

Supporting Information

Quantum Chemical Study of ω -Transaminase Reaction Mechanism

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1. Optimized structures of alternative transition states

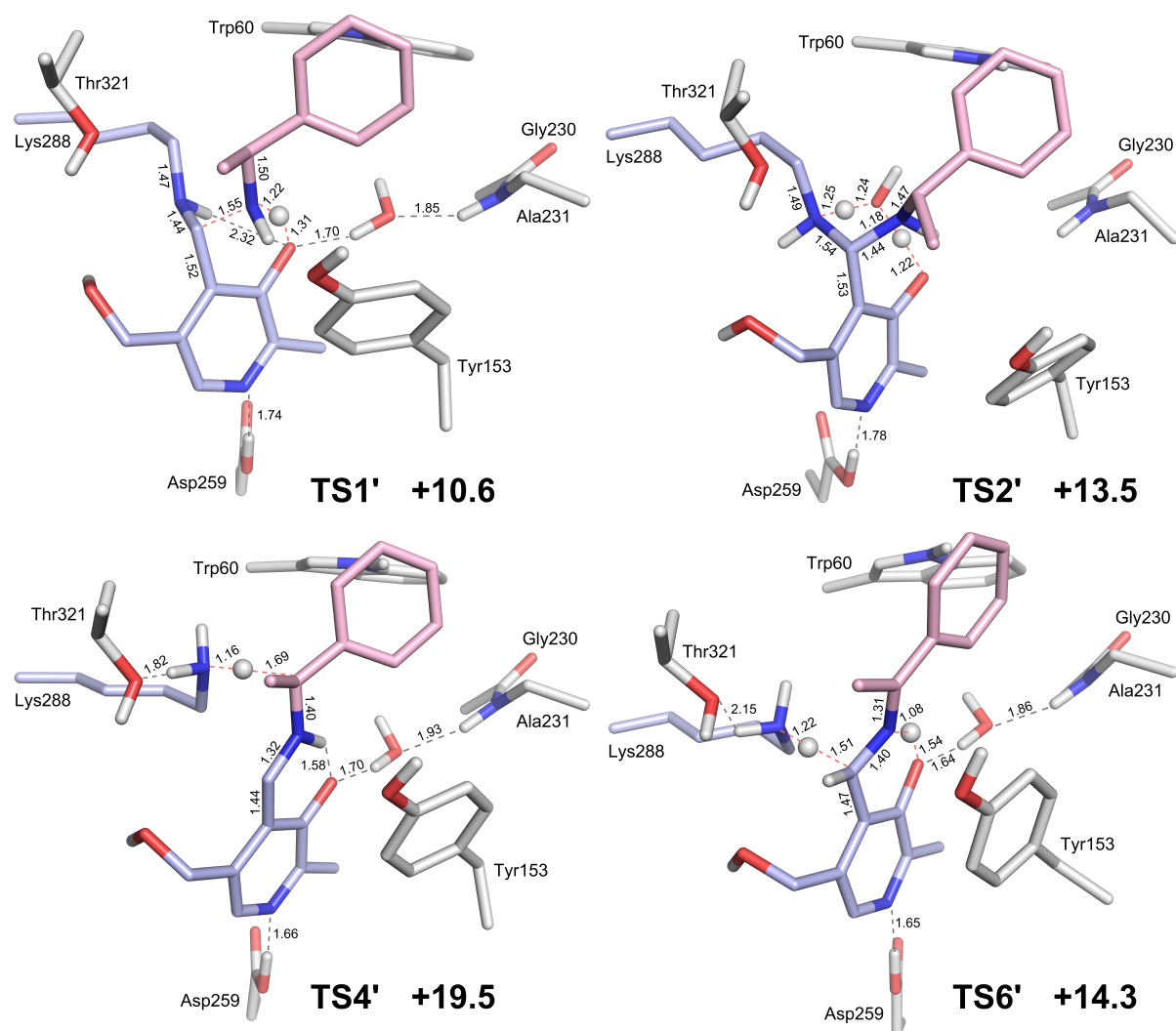


Figure S1. Optimized structures for alternative transition states. Energies are given in kcal/mol relative to **ES**. For clarity, a number of elements and most non-polar hydrogen atoms have been omitted.

2. Absolute energies and energy corrections (a.u.)

	Gas phase B3LYP/ 6-311+G(2d,2p)	ZPE correction	Dispersion correction	Solvation correction ($\epsilon=4.0$)
ES	-3650.463551	1.724039	-0.287023	-0.026080
TS1	-3650.429648	1.720464	-0.302057	-0.026686
Int1	-3650.447919	1.727274	-0.299422	-0.025684
TS2	-3650.428871	1.721865	-0.300488	-0.029947
Int2	-3650.436551	1.726294	-0.301797	-0.029684
TS3	-3650.432552	1.725397	-0.299309	-0.029309
Int3	-3650.461394	1.725568	-0.290875	-0.026329
TS4	-3650.419966	1.719270	-0.294782	-0.026881
Int4	-3650.441555	1.723461	-0.298898	-0.029319
TS5	-3650.421431	1.720546	-0.297801	-0.034684
Int5	-3650.429552	1.724206	-0.297081	-0.032653
TS6'	-3650.417879	1.719943	-0.298818	-0.033147
TS6	-3650.421478	1.719933	-0.297360	-0.029806
Int6	-3650.459851	1.724240	-0.293488	-0.026891
TS7	-3650.422948	1.723395	-0.304560	-0.028561
Int7	-3650.454523	1.729347	-0.302188	-0.026216
Int8	-3650.439543	1.728151	-0.306030	-0.030037
TS8	-3650.438515	1.725399	-0.304116	-0.029230
E:PMP	-3650.452996	1.726227	-0.296915	-0.027548
TS1'	-3650.428680	1.724537	-0.306152	-0.025414
TS2'	-3650.426523	1.720926	-0.297115	-0.028436
TS4'	-3650.410322	1.721548	-0.298255	-0.034534

3. Cartesian coordinates of stationary points

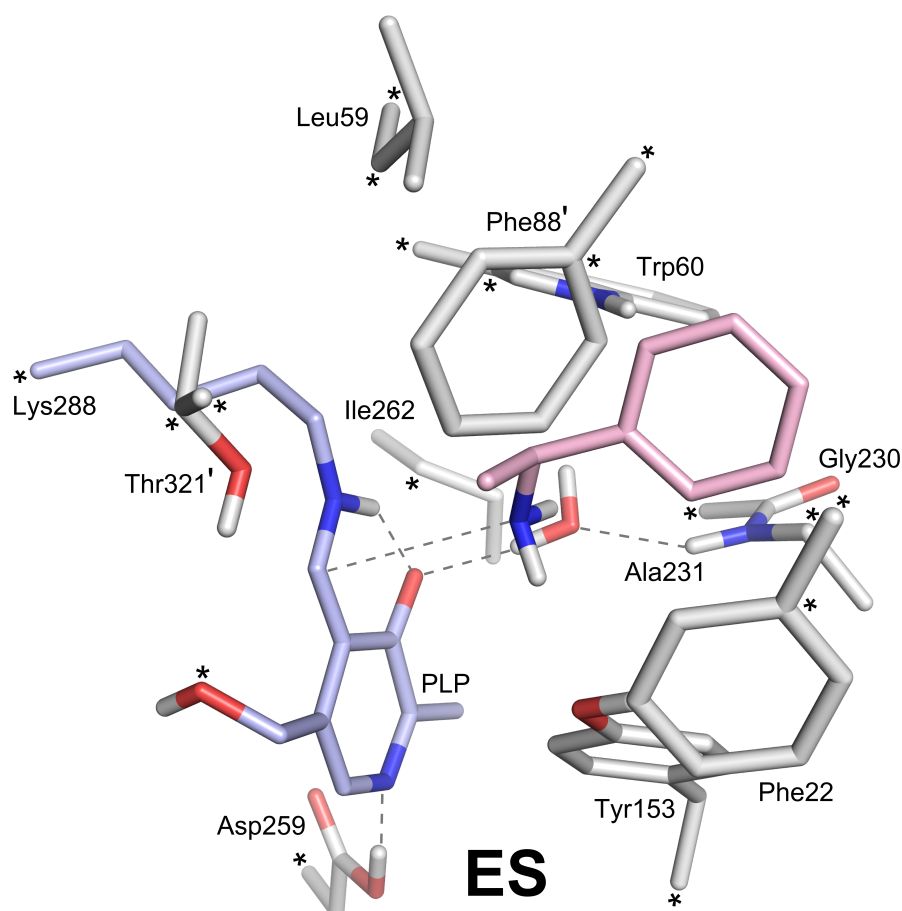


Figure S2. The Cv- ω TA active site model (**ES**) including the substrates (S)-1-PEA and water. Residues from one of the paired subunits are marked with primes. For clarity, non-polar hydrogen atoms have been omitted.

The total size of the active site model is 197 atoms. Atoms kept fixed at their crystallographic positions are indicated with asterisks. The fixed atoms are **1** (Phe22), **2** (Phe22), **8** (Leu59), **12** (Trp60), **13** (Trp60), **30** (Gly230), **34** (Ala231), **37** (Asp259), **42** (Ile262), **46** (Lys288), **70** (Phe88'), **71** (Phe88'), **77** (Thr321'), **78** (Thr321'), **188** (PLP oxygen), **190** (Leu59) and **194** (Tyr153). The imaginary frequencies of transition states are indicated (the small imaginary frequencies resulting from the coordinate fixing are not included).

ES:

C	-31.55570300	-21.11103500	-39.56536800
C	-31.30563900	-19.68982200	-40.00048900
C	-30.01071800	-19.15243400	-40.00965000
C	-32.36955900	-18.85928900	-40.38045200
C	-29.78790900	-17.82393100	-40.37524400
C	-32.15441700	-17.52982500	-40.74561600
C	-30.86015500	-17.00308900	-40.74025500
C	-24.13434200	-23.27918400	-46.91365900
C	-24.71916200	-24.18478200	-45.81156700
C	-23.88241800	-25.45375600	-45.58679400
C	-24.87031400	-23.40668200	-44.49940400
C	-24.78501700	-21.39303100	-51.86126800
C	-26.19604100	-21.48912500	-51.33661400
C	-26.58587300	-21.61704100	-50.02601000
C	-27.41113800	-21.41940100	-52.11169600
C	-28.50082200	-21.50606900	-51.19891400
C	-27.68635700	-21.30522800	-53.48702400
N	-27.96680000	-21.62795500	-49.93376500
C	-29.83468700	-21.46926400	-51.62228800
C	-29.00928600	-21.28013300	-53.91047800
C	-30.07400800	-21.35810200	-52.98678000
C	-31.69281100	-14.17484100	-48.16334400
C	-31.06412300	-14.79764700	-46.93281100
C	-31.82681500	-15.50999800	-46.00058700
C	-29.68775700	-14.67526500	-46.68490700
C	-31.25039300	-16.09105000	-44.86764200
C	-29.09573600	-15.24527500	-45.56074500
C	-29.87643300	-15.96259200	-44.64541900
O	-29.23637200	-16.51750000	-43.57007400
C	-30.93558500	-17.83618600	-53.21863300
C	-31.90373000	-18.40235400	-52.20703400
O	-32.90424100	-19.03931100	-52.53633200
N	-31.58601700	-18.15005100	-50.90881000
C	-32.42873700	-18.65651600	-49.84295900
C	-33.65377800	-17.77679100	-49.57438000
H	-30.69157300	-17.72638000	-50.68642900
C	-25.47400100	-9.01406700	-53.29974600
C	-26.18910300	-8.99241400	-51.94920800
C	-26.05296300	-10.29453400	-51.17626700
O	-25.32192800	-11.21090800	-51.50474500
O	-26.83450000	-10.31081200	-50.08620400
C	-25.65781100	-17.19395600	-53.61267600
C	-27.11925400	-16.93226500	-54.00705600
C	-24.68576100	-17.29420700	-54.79339300
C	-27.35238700	-15.60490500	-54.73665600
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C	-21.51563800	-18.23443100	-49.14783100
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C	-23.95252400	-18.70973200	-48.39211100
N	-24.56719100	-17.41092500	-48.63606100
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H	-27.93053800	-22.09485900	-46.55604700
H	-30.18683300	-18.43906900	-46.58630300
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Int1:

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C	-32.36385900	-18.88723700	-40.45092300
C	-29.82241000	-17.77579300	-40.24562700
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C	-30.06082000	-21.42951300	-53.01881800
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C	-30.93559500	-17.83619300	-53.21863000
C	-31.86867000	-18.45843200	-52.20512400
O	-32.80602400	-19.18887500	-52.52709200
N	-31.60538900	-18.12871700	-50.91212800
C	-32.42873800	-18.65651000	-49.84296300
C	-33.78271200	-17.94912800	-49.71572400
H	-30.75174600	-17.62767700	-50.68703500
C	-25.47400100	-9.01406700	-53.29974600
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C	-25.89020800	-10.12635400	-51.05574500
O	-25.14963900	-11.04891700	-51.34641600
O	-26.66014000	-10.10169500	-49.95901400
C	-25.65780100	-17.19396000	-53.61267100
C	-25.00758000	-15.80157400	-53.60174000
C	-26.13790400	-17.66722300	-54.98879800
C	-23.68100000	-15.71541400	-54.36415300
C	-19.03388700	-18.01802800	-49.78011500
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C	-21.53457300	-18.13302300	-49.23366900
C	-22.88353600	-18.81217900	-49.52253400
C	-23.98926000	-18.48355700	-48.51306100
N	-24.44938600	-17.08586800	-48.64334600
H	-18.74785400	-18.24875500	-48.74759000
N	-26.44149000	-12.56366500	-48.64156100
C	-26.62864300	-13.60410300	-49.46317900
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C	-26.16687600	-14.88792700	-49.10605500
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C	-25.39486100	-13.99493900	-46.99920200
C	-24.78530500	-14.09328600	-45.61412300
C	-25.82983500	-12.75270900	-47.46228200
H	-23.62998000	-16.48881200	-48.75370800

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H	-27.93716500	-12.48356600	-50.72737400	H	-27.25519100	-25.31038100	-42.46367100
H	-26.57578900	-13.23080600	-51.57017200	H	-25.57631600	-23.94019500	-40.76284700
H	-24.83843700	-13.10558000	-45.13472800	H	-24.67089400	-21.66603500	-40.43376800
H	-25.36309700	-14.78181300	-44.99009800	H	-25.95874400	-19.68211500	-41.21192500
C	-27.93588300	-24.66499200	-41.89627700	H	-28.16238200	-20.01079000	-42.32204500
C	-27.38284600	-23.28251300	-41.73911300	H	-29.06243500	-22.28648800	-42.64635000
C	-26.14274500	-23.07994200	-41.11189700	H	-24.97770600	-22.57587400	-46.93198000
C	-28.09591900	-22.15654800	-42.16662700	H	-23.23509100	-22.68681000	-46.70873600
C	-25.63111500	-21.79753500	-40.92451000	H	-22.24324900	-24.68890900	-45.36738600
C	-27.58774700	-20.86696500	-41.98376300	H	-23.34250600	-25.92611300	-44.74487500
C	-26.35349000	-20.68287500	-41.36078700	H	-22.99233300	-25.85056300	-46.47269100
C	-22.71705400	-19.76962500	-43.10278400	H	-25.51136800	-22.88889500	-44.52525200
C	-22.30898400	-19.25678400	-44.49873300	H	-24.83704400	-24.25096100	-43.62705500
C	-22.15453400	-20.38889200	-45.49993700	H	-23.78516900	-22.92958400	-44.13647900
O	-23.27903800	-18.34904600	-45.03447900	H	-25.23843000	-24.87925400	-46.00752800
H	-31.08417400	-21.37903800	-53.37642600	H	-21.95245800	-20.44206500	-42.70019500
H	-30.65703400	-21.56340500	-50.94938800	H	-22.83421500	-18.93563200	-42.40181200
H	-29.20635000	-21.30998200	-54.99896400	H	-23.66742300	-20.30950900	-43.15282300
H	-26.85404900	-21.34471500	-54.21889200	H	-21.45774800	-21.14516900	-45.12599400
H	-25.99288000	-21.61759900	-49.12715400	H	-23.12260800	-20.86560900	-45.66799700
H	-24.05576100	-21.44016600	-51.04739300	H	-21.78065400	-20.01867400	-46.45835800
H	-24.55556700	-22.20812000	-52.55845100	H	-21.34281200	-18.73566000	-44.40491200
H	-24.62018700	-20.45347300	-52.40307000	H	-23.17936000	-17.49127900	-44.60029800
H	-28.49560300	-21.59265100	-49.08405100	H	-30.71806900	-21.76456400	-39.82916100
H	-23.24821900	-14.71227600	-54.29185900	H	-31.68246100	-21.17106000	-38.47738200
H	-22.94712100	-16.42381300	-53.96068800	H	-32.46255800	-21.51737000	-40.02226200
H	-23.80596900	-15.94286300	-55.42795500	H	-29.19209700	-19.72196400	-39.57955100
H	-25.71563800	-15.07280100	-54.01995200	H	-28.82821500	-17.34589200	-40.16158300
H	-24.84801800	-15.50104100	-52.55896600	H	-30.73325500	-15.93196900	-40.90378500
H	-26.84924300	-16.95438000	-55.42210800	H	-33.00226000	-16.94228600	-41.11725300
H	-25.30943200	-17.77855500	-55.69620100	H	-33.35912700	-19.31713800	-40.53195900
H	-26.64396100	-18.63512800	-54.91442100	C	-29.57616200	-21.28324800	-46.68662900
H	-24.94455800	-17.92547700	-53.20458300	C	-28.52279100	-21.49529000	-45.79276500
H	-33.64948900	-16.87959000	-49.52081300	C	-27.51822100	-20.53890400	-45.65966500
H	-34.34851100	-18.06740400	-50.64223700	C	-27.52679300	-19.35998400	-46.42350300
H	-34.36691000	-18.37938300	-48.89458000	C	-28.56820900	-19.17013600	-47.33851700
H	-31.86635900	-18.55221600	-48.90983500	C	-29.59015900	-20.11938300	-47.45655900
H	-32.59998900	-19.72478400	-50.02195400	H	-30.37296300	-22.01571500	-46.78153500
H	-30.57694800	-18.61541500	-53.89477100	H	-28.48463600	-22.39982700	-45.19359500
H	-31.49529200	-17.11105300	-53.81838000	H	-26.71597000	-20.71093200	-44.94767100
H	-30.07948900	-17.33647600	-52.75935500	H	-28.57685000	-18.30458400	-47.99194400
H	-30.36041700	-14.01924500	-48.98057900	H	-30.39519100	-19.94748000	-48.16410000
H	-31.93379800	-14.72759900	-48.66458300	C	-26.42116900	-18.32899400	-46.19904100
H	-28.86508100	-13.41747400	-46.93975300	H	-25.46182500	-18.84747200	-46.26647300
H	-28.06166100	-14.24913900	-44.74116300	C	-26.51226000	-17.74234400	-44.77488800
H	-31.52814400	-16.75779700	-44.42186800	H	-25.68707500	-17.04694400	-44.59454900
H	-32.34009100	-15.91376500	-46.59940500	H	-27.45674000	-17.21509800	-44.61836700
H	-29.81280500	-16.64345500	-42.85675300	H	-26.43581500	-18.53038700	-44.02028800
H	-26.00926500	-9.78425400	-53.86252800	N	-26.43118200	-17.30499900	-47.25528300
H	-25.55274000	-8.07183800	-53.85004900	H	-25.62192400	-16.59413400	-49.71036000
H	-24.42328800	-9.31061000	-53.26043300	H	-27.21977400	-16.67800800	-47.12785800
H	-25.54686800	-8.05400500	-51.34684500	O	-28.75152500	-17.38878500	-50.43085200
H	-27.10858700	-8.59907000	-51.90774400	H	-28.39986600	-18.25240700	-50.68409400
H	-26.54754400	-10.95866000	-49.45357000	H	-27.96610800	-16.83274700	-50.27186300
H	-18.24448100	-18.39729300	-50.43652600	H	-24.55718000	-16.54910800	-46.59107800
H	-19.05359000	-16.92697600	-49.88158700	O	-23.44588100	-14.59889700	-45.58096900
H	-20.32926800	-19.72750800	-50.04679600	H	-22.90401700	-14.02304900	-46.13760100
H	-20.63558600	-18.42344500	-51.17916600	C	-23.99500300	-23.95084800	-48.28391000
H	-21.26651400	-18.30353900	-48.18111600	H	-23.91454300	-23.21026600	-49.08609000
H	-21.61747500	-17.04242000	-49.35090700	H	-23.10423400	-24.58371500	-48.33796100
H	-22.73647800	-19.89948800	-49.50424300	H	-24.86447000	-24.57872300	-48.50886900
H	-23.22318400	-18.56539000	-50.53674600	C	-31.77940500	-12.63992100	-48.11094900
H	-23.61754700	-18.67053500	-47.49707800	H	-31.03700300	-11.93166900	-47.72929900
H	-24.85393100	-19.13202400	-48.68292000	H	-32.13575800	-12.26678800	-49.07684600
H	-26.51051600	-17.18606800	-52.92128700	H	-32.62397000	-12.64189900	-47.41421700

Int2:

C	-31.55570400	-21.11103700	-39.56537000	H	-23.53087900	-16.37719000	-48.51418500
C	-31.30563800	-19.68982000	-40.00048600	H	-25.61492400	-11.75716200	-46.75850100
C	-30.00649500	-19.17188400	-40.08345600	H	-27.75275200	-14.03389300	-51.05938500
C	-32.38185800	-18.82765100	-40.25902700	H	-27.71604900	-12.27386500	-50.74094500
C	-29.79055100	-17.82580500	-40.38637200	H	-26.35329500	-13.07103600	-51.53915100
C	-32.17325400	-17.48319900	-40.56349800	H	-24.78293200	-13.07971800	-45.03826900
C	-30.87369300	-16.97178100	-40.61625400	H	-25.35245700	-14.74659100	-44.93078500
C	-24.13434500	-23.27919200	-46.91365800	C	-27.93588300	-24.66499200	-41.89627700
C	-24.46022200	-24.25176700	-45.76043300	C	-27.38284700	-23.28251300	-41.73911300
C	-23.36894400	-25.31568000	-45.56614500	C	-26.31868500	-23.02368700	-40.86400900
C	-24.69922300	-23.48999800	-44.45046000	C	-27.94273100	-22.20272400	-42.43706400
C	-24.78501800	-21.39301400	-51.86127300	C	-25.83077800	-21.72826500	-40.68696600
C	-26.19064600	-21.48914000	-51.33661100	C	-27.46158900	-20.90470600	-42.26253800
C	-26.58799000	-21.50716200	-50.02237500	C	-26.40224100	-20.66226200	-41.38447400
C	-27.40871600	-21.48532500	-52.11756100	C	-22.71706100	-19.76963100	-43.10278800
C	-28.50054100	-21.49748300	-51.20248000	C	-22.30897400	-19.25677400	-44.49873000
C	-27.68052500	-21.46407500	-53.49752700	C	-22.24159200	-20.38254200	-45.51766000
N	-27.96733700	-21.52739200	-49.93052800	O	-23.22038400	-18.28204000	-45.01933500
C	-29.83211000	-21.47103700	-51.63178700	H	-31.09341500	-21.38938500	-53.35622300
C	-29.00259500	-21.44299900	-53.92566900	H	-30.65630100	-21.46551400	-50.92493300
C	-30.06940200	-21.44232500	-53.00174500	H	-29.22308300	-21.42594100	-54.98912000
C	-31.33280200	-14.10913500	-48.17560200	H	-26.86782700	-21.46113500	-54.21845400
C	-30.79558700	-14.62086200	-46.85641400	H	-25.98456500	-21.49544000	-49.12635000
C	-31.56647600	-15.42911800	-46.01369300	H	-24.05707500	-21.45282200	-51.04662600
C	-29.50966500	-14.26305400	-46.42264800	H	-24.55577300	-22.20015100	-52.56748600
C	-31.07808900	-15.87937300	-44.78455800	H	-24.61876800	-20.44624700	-52.38942200
C	-29.00935000	-14.69895700	-45.20065500	H	-28.48257900	-21.42860600	-49.06837100
C	-29.79058300	-15.51791700	-44.37847000	H	-27.15149300	-14.17282300	-54.64309500
O	-29.23302100	-15.94519000	-43.20272200	H	-25.43165700	-14.57511900	-54.67881900
C	-30.93559500	-17.83619100	-53.21863000	H	-26.56792700	-15.44514200	-55.71800300
C	-31.85628400	-18.48518900	-52.21676400	H	-27.67725600	-16.42676600	-53.66986700
O	-32.69544500	-19.32494200	-52.53089100	H	-26.57834900	-15.52566000	-52.63269500
N	-31.64977800	-18.09975000	-50.92587500	H	-26.77148400	-18.58807000	-54.86652700
C	-32.42873800	-18.65651000	-49.84296300	H	-25.60711300	-17.60250400	-55.76411000
C	-33.67655200	-17.83496100	-49.50232900	H	-25.04363000	-18.94317300	-54.76541900
H	-30.97833000	-17.37471600	-50.72633100	H	-24.63711800	-16.78866300	-53.56230600
C	-25.47400100	-9.01406700	-53.29974600	H	-33.41271100	-16.81501000	-49.20199100
C	-25.94027400	-8.78121700	-51.86156900	H	-34.33844500	-17.77730200	-50.37066400
C	-25.71037700	-9.99334100	-50.97050800	H	-34.23032800	-18.29865600	-48.67858400
O	-24.87430700	-10.84929500	-51.20149000	H	-31.78048400	-18.75339600	-48.96542400
O	-26.52533000	-10.00361900	-49.90992800	H	-32.72685200	-19.66083800	-50.15423200
C	-25.65779800	-17.19395600	-53.61267300	H	-30.17507500	-18.56522300	-53.51641500
C	-26.65511300	-16.02508500	-53.60428800	H	-31.50645500	-17.57312900	-54.11188000
C	-25.77666200	-18.13053000	-54.81986500	H	-30.43386700	-16.94167900	-52.83826900
C	-26.44051600	-15.00170800	-54.72466700	H	-30.56213200	-14.21263300	-48.95018000
C	-19.03388800	-18.01802800	-49.78011500	H	-32.17933700	-14.73051200	-48.49280500
C	-20.41163900	-18.57617700	-50.15061900	H	-28.88206200	-13.64143900	-47.05633800
C	-21.53489800	-18.08281900	-49.22805500	H	-28.01091900	-14.42628900	-44.87722900
C	-22.90335300	-18.69822400	-49.56071100	H	-31.69082200	-16.51256500	-44.14694200
C	-24.01028400	-18.39917300	-48.54576300	H	-32.56973000	-15.71700200	-46.31954400
N	-24.37413300	-16.95328600	-48.53387000	H	-29.82436200	-16.57901700	-42.76941600
H	-18.75174600	-18.30240100	-48.76005800	H	-26.06304800	-9.80079400	-53.78081900
N	-26.31922600	-12.42529500	-48.58914900	H	-25.57475800	-8.10143400	-53.89483600
C	-26.49231200	-13.44744000	-49.43045100	H	-24.42913900	-9.33210400	-53.31499800
C	-27.12295600	-13.18964800	-50.76862400	H	-25.39357600	-7.94149200	-51.41098000
C	-26.07658400	-14.77856200	-49.10344300	H	-26.99948100	-8.50980800	-51.81382600
O	-26.11287100	-15.73713400	-49.99508200	H	-26.39022200	-10.85106300	-49.37988800
C	-25.58704500	-14.99373500	-47.78735000	H	-18.25928000	-18.39295300	-50.45606000
C	-25.28508400	-16.42530100	-47.36628900	H	-19.01973200	-16.92366200	-49.83467500
C	-25.39507000	-13.90026000	-46.92364500	H	-20.38198600	-19.67356300	-50.11831200
C	-24.77831700	-14.05114300	-45.55089100	H	-20.65170600	-18.30954600	-51.18812300
C	-25.76115300	-12.63657200	-47.38179000	H	-21.27631100	-18.31812800	-48.18582100
				H	-21.57812300	-16.98483900	-49.28975900
				H	-22.79929900	-19.78962000	-49.59783700
				H	-23.22767900	-18.39246400	-50.56357200
				H	-23.68921000	-18.66259400	-47.53495400
				H	-24.92389500	-18.93703700	-48.80344600

H	-25.79892000	-17.77348200	-52.68997300
H	-28.78578200	-24.83358400	-41.22249300
H	-28.29584300	-24.84330100	-42.91438300
H	-27.18790900	-25.42959800	-41.66549800
H	-25.86809500	-23.84752800	-40.31568300
H	-25.00395900	-21.55230400	-40.00454700
H	-26.02539700	-19.65284300	-41.24738300
H	-27.91432600	-20.08552400	-42.81232700
H	-28.76224100	-22.37950100	-43.12924600
H	-24.92343300	-22.51642400	-46.96273500
H	-23.20435400	-22.74867300	-46.67640000
H	-22.40315200	-24.84646700	-45.33943900
H	-23.61706700	-25.97851400	-44.73029800
H	-23.23610100	-25.94157700	-46.45316800
H	-25.50001200	-22.74916100	-44.54609400
H	-24.97893800	-24.16893600	-43.63890300
H	-23.79233500	-22.96080800	-44.13443100
H	-25.39317200	-24.77336400	-46.02450700
H	-21.98138400	-20.49047800	-42.73205700
H	-22.76914100	-18.94388700	-42.38436700
H	-23.69724100	-20.25493400	-43.13634300
H	-21.58387500	-21.18382300	-45.16807600
H	-23.23908900	-20.80020400	-45.67304500
H	-21.86238200	-20.02198300	-46.47816400
H	-21.30894300	-18.80132300	-44.41470500
H	-23.08833500	-17.44603800	-44.55202400
H	-30.75527300	-21.77966200	-39.89700800
H	-31.60467500	-21.18092900	-38.47166700
H	-32.50308700	-21.49201900	-39.95811000
H	-29.15667400	-19.82421600	-39.90314200
H	-28.77639800	-17.43857300	-40.43208000
H	-30.70536400	-15.91811900	-40.82036800
H	-33.02300800	-16.83129900	-40.74557900
H	-33.39652600	-19.21488200	-40.20666800
C	-30.01583500	-20.74595000	-46.56138600
C	-28.76067300	-21.34803100	-46.44273700
C	-27.61281200	-20.55543800	-46.34128500
C	-27.69708700	-19.15822700	-46.35605200
C	-28.96194900	-18.56433000	-46.47336100
C	-30.10931900	-19.35155400	-46.57184600
H	-30.91155300	-21.35630600	-46.63306300
H	-28.67267700	-22.43105700	-46.42073500
H	-26.64046100	-21.02962600	-46.23583200
H	-29.04608700	-17.48257800	-46.47995600
H	-31.08030900	-18.87002900	-46.64049300
C	-26.44623200	-18.31148400	-46.17192700
H	-25.57789200	-18.97125700	-46.30187500
C	-26.39214800	-17.76971700	-44.73207900
H	-25.50830000	-17.14612000	-44.57777000
H	-27.28392100	-17.18526900	-44.49523200
H	-26.31912400	-18.60413900	-44.02826300
N	-26.45187900	-17.20951100	-47.15239200
H	-24.96383800	-16.64553700	-49.38999800
H	-26.95246400	-17.44036000	-48.00747900
O	-26.98626500	-18.24541800	-49.93864400
H	-27.48993300	-18.69257700	-50.62863700
H	-26.89745000	-17.29958500	-50.18621600
H	-24.64879400	-16.45641500	-46.48449900
O	-23.44588000	-14.59889700	-45.58096900
H	-22.91439400	-14.00728000	-46.13142800
C	-23.99500300	-23.95084700	-48.28390900
H	-23.83593700	-23.21113400	-49.07520200
H	-23.14848200	-24.64311600	-48.31268800
H	-24.89707600	-24.51552000	-48.54485700
C	-31.77940500	-12.63992100	-48.11094900
H	-30.94620000	-11.98933200	-47.82755500
H	-32.15759200	-12.29937900	-49.08070200

H	-32.57326700	-12.50493500	-47.36911800
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Int3:

C	-31.55571200	-21.11103000	-39.56534800
C	-31.30562700	-19.68982900	-40.00051200
C	-30.12264300	-19.02522800	-39.64485400
C	-32.31599300	-18.95113500	-40.63298400
C	-29.97086500	-17.65701500	-39.87430000
C	-32.17325900	-17.58233000	-40.86087800
C	-31.00597400	-16.92419200	-40.46376500
C	-24.13437400	-23.27916400	-46.91365000
C	-25.47454300	-23.53970100	-46.20485700
C	-25.70704700	-25.02361100	-45.88448800
C	-25.56708800	-22.68645900	-44.93482500
C	-24.78504200	-21.39299800	-51.86127800
C	-26.19601200	-21.48912900	-51.33660800
C	-26.57519900	-21.40865500	-50.01719000
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C	-28.49792200	-21.51911500	-51.18314800
C	-27.69929600	-21.61836000	-53.48190800
N	-27.95484400	-21.44766600	-49.91742100
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C	-29.02539800	-21.62274200	-53.89892200
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C	-31.61395800	-14.14170300	-47.83732600
C	-31.04764500	-14.47114100	-46.47084900
C	-31.75077800	-15.26323800	-45.55713400
C	-29.77356200	-14.02116000	-46.09054600
C	-31.19711300	-15.63485900	-44.32877200
C	-29.20900000	-14.37466400	-44.86992200
C	-29.90933000	-15.20874000	-43.99210500
O	-29.27275300	-15.58546200	-42.83941800
C	-30.93554200	-17.83618000	-53.21864500
C	-31.87165000	-18.46274900	-52.21624600
O	-32.75453000	-19.25450400	-52.53548800
N	-31.63684700	-18.10852700	-50.92159300
C	-32.42874500	-18.65650800	-49.84295200
C	-33.67286900	-17.82195700	-49.51918400
H	-30.90096900	-17.45255800	-50.71001600
C	-25.47400100	-9.01406700	-53.29974500
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C	-25.83911700	-10.39351500	-51.21516100
O	-26.13542400	-11.35101400	-51.91203100
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C	-25.65785300	-17.19398400	-53.61265800
C	-26.52376200	-16.27185200	-54.48723200
C	-24.23002700	-17.39748700	-54.13220100
C	-26.03802100	-14.81972100	-54.56305900
C	-19.03389100	-18.01802900	-49.78011400
C	-20.40638900	-18.68146800	-49.89359800
C	-21.56775500	-17.68505200	-49.80570200
C	-22.93785200	-18.36612400	-49.83610600
C	-24.11322600	-17.39434800	-49.71269000
N	-25.36975300	-18.12924600	-49.48695400
H	-18.92469900	-17.49313000	-48.82393000
N	-26.27879100	-12.81082900	-48.72618300
C	-26.96519200	-13.86790700	-49.10650900
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C	-27.01115000	-15.08210100	-48.29579100
O	-27.69000400	-16.08505600	-48.69164100
C	-26.25967700	-15.06614200	-47.06121300
C	-26.32701100	-16.19922600	-46.20303000
C	-25.51345700	-13.89513000	-46.70879600
C	-24.63519100	-13.80398800	-45.48116600

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H	-25.57100700	-18.74539200	-50.27344100	H	-26.15329200	-18.17053200	-53.53474500
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H	-27.63300100	-14.78945500	-50.91287200	H	-28.83247400	-24.67560700	-42.52330300
H	-28.81361000	-13.72286700	-50.17953300	H	-27.20596300	-25.34707600	-42.34437400
H	-27.40452500	-13.01402000	-51.02024000	H	-25.42435700	-23.95673100	-41.14694600
H	-24.38248700	-12.74984400	-45.30420800	H	-24.55203800	-21.69209700	-40.67902000
H	-25.14786500	-14.16309400	-44.58333900	H	-26.01753500	-19.70309000	-40.98130800
C	-27.93588700	-24.66499200	-41.89626400	H	-28.35699400	-20.01355000	-41.77338200
C	-27.38283400	-23.28251100	-41.73914000	H	-29.21512300	-22.27670500	-42.26028700
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C	-28.19161200	-22.15303800	-41.91509000	H	-23.31537800	-23.60904000	-46.25642500
C	-25.57404700	-21.81501500	-41.02611500	H	-24.91400000	-25.40831600	-45.23040200
C	-27.70590700	-20.87205800	-41.64377200	H	-26.66192200	-25.16959800	-45.36645700
C	-26.39562300	-20.69843400	-41.19523800	H	-25.72391300	-25.64350000	-46.78601900
C	-22.71708000	-19.76963800	-43.10279600	H	-25.40035200	-21.62946500	-45.16590700
C	-22.30895000	-19.25677200	-44.49872500	H	-26.54140100	-22.78055300	-44.44621600
C	-21.83546700	-20.37486600	-45.41819500	H	-24.80919800	-22.99345000	-44.20372500
O	-23.42894600	-18.57577200	-45.12043600	H	-26.27256000	-23.21656700	-46.89207200
H	-31.11096400	-21.54320800	-53.31536600	H	-21.87631700	-20.28203200	-42.62426800
H	-30.64952700	-21.47873100	-50.88527900	H	-23.02557900	-18.93793000	-42.46205700
H	-29.25543800	-21.66389800	-54.95974100	H	-23.55302800	-20.47063000	-43.18501800
H	-26.89305100	-21.65517100	-54.20966200	H	-20.96848500	-20.88348800	-44.98425800
H	-25.96303400	-21.29975000	-49.13204100	H	-22.62566500	-21.11422800	-45.56977400
H	-24.06822100	-21.31621300	-51.03926900	H	-21.54790500	-19.97756700	-46.39594100
H	-24.50850900	-22.27014600	-52.45941200	H	-21.49299700	-18.53097000	-44.37660200
H	-24.65517900	-20.51648500	-52.50895000	H	-23.23424700	-17.63032600	-45.16093200
H	-28.47245000	-21.32180600	-49.06124800	H	-30.65054300	-21.72247200	-39.63759800
H	-26.71351200	-14.21200600	-55.17379000	H	-31.88422500	-21.13720500	-38.51952500
H	-25.99074600	-14.35712600	-53.57077800	H	-32.33686200	-21.58641000	-40.16562600
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H	-26.57909800	-16.69259900	-55.50100600	H	-29.05661100	-17.15621100	-39.56867100
H	-27.55087200	-16.28564700	-54.09980800	H	-30.91318600	-15.84830300	-40.58584500
H	-24.23686000	-17.80140300	-55.15139300	H	-32.98398900	-17.02382100	-41.32058300
H	-23.66492000	-16.46013200	-54.15242600	H	-33.23902800	-19.44929600	-40.91838800
H	-23.67427700	-18.10126900	-53.50271000	C	-30.92703400	-20.49648800	-46.43260700
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H	-33.40125600	-16.80307500	-49.22219500	C	-28.51497000	-20.55497800	-46.24320900
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H	-34.24011600	-18.27672400	-48.69931000	C	-29.68907200	-18.46316300	-45.98172900
H	-31.79053200	-18.75120900	-48.95833800	C	-30.90203100	-19.12101800	-46.19648100
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H	-30.21430600	-18.59318900	-53.54342200	H	-29.73607900	-22.28564700	-46.63251000
H	-31.50708700	-17.52616700	-54.09627500	H	-27.58270900	-21.11110200	-46.26396500
H	-30.38617900	-16.97605000	-52.82535100	H	-29.68744400	-17.39309500	-45.80428800
H	-30.95704900	-14.57400300	-48.60486100	H	-31.82703700	-18.55247100	-46.17416700
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H	-28.21830300	-14.03156100	-44.59128100	C	-26.88266800	-18.29254700	-44.22628800
H	-31.75302000	-16.27363700	-43.64749500	H	-25.84185100	-18.00754300	-44.04675000
H	-32.74770200	-15.61452500	-45.81248400	H	-27.55412500	-17.53938900	-43.79968000
H	-29.81334000	-16.23578100	-42.36494200	H	-27.04262900	-19.23837700	-43.70682800
H	-26.48250200	-9.22622100	-53.66410000	N	-27.05162500	-17.25121900	-46.48800500
H	-25.16936200	-8.03338400	-53.67810900	H	-26.15801600	-17.48626700	-49.40824200
H	-24.81114200	-9.77098100	-53.72655600	H	-27.53305000	-17.15590400	-47.40816900
H	-24.42272400	-8.82094100	-51.39855900	O	-24.81103600	-19.90945300	-47.35781400
H	-26.08316600	-8.28677800	-51.33453000	H	-24.26442200	-19.43062000	-46.71107900
H	-26.08900300	-11.33090100	-49.55680700	H	-25.04598700	-19.25166300	-48.06381600
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H	-18.88080500	-17.28206800	-50.57769300	O	-23.44588700	-14.59890200	-45.58097200
H	-20.51737400	-19.43250400	-49.09939700	H	-23.00161300	-14.33676100	-46.39905500
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H	-21.48918600	-16.95798300	-50.62630700	H	-24.00782000	-25.04386900	-48.21562900
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Int4:

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C	-30.63540900	-15.14645700	-46.20435700
C	-29.19835400	-13.25755000	-45.87712000
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C	-29.38134700	-14.93704900	-44.15303900
O	-28.97038700	-15.38567100	-42.92088600
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C	-32.42874700	-18.65650800	-49.84295400
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O	-27.29405300	-16.57518700	-48.74476400
C	-26.11009100	-15.23039000	-47.12530700
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C	-24.61761100	-13.76494800	-45.64486900
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C	-22.71708300	-19.76964300	-43.10280200
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H	-24.01526000	-16.84148400	-48.76322300
H	-26.18833100	-18.11550100	-53.33728300
H	-28.10247400	-25.12980000	-40.91656900
H	-28.89649500	-24.66382400	-42.42047400
H	-27.25330200	-25.31925400	-42.44877100
H	-25.35638700	-23.94449400	-41.42994100
H	-24.48121300	-21.70135500	-40.87500800
H	-26.01280300	-19.73980300	-40.82451200
H	-28.42495000	-20.05375400	-41.35449600
H	-29.28668900	-22.29371400	-41.93475700
H	-24.11221800	-22.19145400	-47.04612400
H	-23.26938300	-23.54082200	-46.28597300
H	-24.69186900	-25.46633900	-45.22081100
H	-26.45667400	-25.35375700	-45.28986700
H	-25.54275800	-25.75271700	-46.74589900
H	-25.46668700	-21.73419500	-45.10202200
H	-26.47717100	-22.97781400	-44.35815500
H	-24.72373300	-23.05225500	-44.18334900
H	-26.27381200	-23.37030800	-46.80794400
H	-21.85194500	-20.20328300	-42.59093400
H	-23.10440500	-18.95184900	-42.48708800
H	-23.49488500	-20.53404900	-43.18921900
H	-20.88419500	-20.82867000	-44.92068100
H	-22.51215200	-21.14091500	-45.54661900
H	-21.45935500	-19.96697100	-46.36103400
H	-21.54155500	-18.47968500	-44.38087600
H	-23.47450400	-17.71387500	-45.02256200
H	-30.62445700	-21.68588600	-39.51754400
H	-32.00540300	-21.14357900	-38.56584000
H	-32.23623400	-21.62607300	-40.24905800
H	-29.70828600	-19.36000300	-38.59040700
H	-29.36010000	-16.99326500	-39.21591400
H	-30.77548700	-15.94103200	-40.96704700
H	-32.50883900	-17.30516800	-42.12861600
H	-32.84395500	-19.67498500	-41.50656800
C	-30.04042400	-21.36944900	-46.78795300
C	-29.40138000	-21.45823100	-45.54796800
C	-28.56100800	-20.44521100	-45.10196100
C	-28.31080200	-19.28330800	-45.88039100
C	-28.97162700	-19.21069700	-47.13793900
C	-29.81429800	-20.23026100	-47.56834900
H	-30.70509600	-22.15630400	-47.13086200
H	-29.55539600	-22.32921800	-44.91685000
H	-28.07471700	-20.56792600	-44.14208900
H	-28.85019200	-18.34218900	-47.77891000
H	-30.30828800	-20.12679100	-48.52951900
C	-27.41133100	-18.24322300	-45.41371800
H	-25.95890800	-19.82035600	-46.63012500
C	-26.87265000	-18.14105200	-44.01951600
H	-25.77794500	-18.24858500	-43.99460600
H	-27.11064000	-17.15632800	-43.59092500
H	-27.28842700	-18.89987600	-43.35977900
N	-27.04845800	-17.27108400	-46.26855600
H	-26.25535700	-17.52454500	-49.20107100
H	-27.40870400	-17.25293100	-47.25505100
O	-25.10425700	-19.80614900	-47.08953900
H	-24.48696300	-19.40847000	-46.43612800
H	-25.33829500	-18.84240800	-48.53804800
H	-25.75690300	-16.08601700	-45.13287600
O	-23.44588700	-14.59890100	-45.58097200
H	-22.97182000	-14.45542100	-46.41133100
C	-23.99499000	-23.95085400	-48.28390600
H	-23.09817600	-23.59885100	-48.80588000
H	-23.91344900	-25.03938600	-48.20264100
H	-24.85635700	-23.73179000	-48.92415700
C	-31.77940000	-12.63992500	-48.11094700

H	-31.71875500	-11.75914000	-47.46334200
H	-32.00442400	-12.29904100	-49.12704200
H	-32.62135500	-13.24788700	-47.76287600

Int5:

C	-31.55571400	-21.11103700	-39.56535000
C	-31.30562700	-19.68982000	-40.00050900
C	-30.26847100	-18.93702100	-39.42774300
C	-32.14146000	-19.06227500	-40.93330100
C	-30.08704000	-17.59496300	-39.76038200
C	-31.96626400	-17.71809100	-41.26856200
C	-30.94428100	-16.97473900	-40.67464600
C	-24.13433200	-23.27915200	-46.91363200
C	-25.40988300	-23.66675600	-46.14538500
C	-25.47002700	-25.16388500	-45.80828300
C	-25.53383100	-22.82085300	-44.87595800
C	-24.78501800	-21.39301800	-51.86127000
C	-26.19603400	-21.48913800	-51.33661600
C	-26.59475900	-21.47478500	-50.02330200
C	-27.39903000	-21.55377100	-52.12690300
C	-28.49605700	-21.57826200	-51.22071300
C	-27.65828000	-21.56878600	-53.50896600
N	-27.97351700	-21.54761500	-49.94547400
C	-29.82359900	-21.59825500	-51.66181000
C	-28.97676300	-21.58750800	-53.94919500
C	-30.05032900	-21.59633600	-53.03382700
C	-30.40798200	-13.32622300	-48.00639700
C	-30.08972900	-13.85668000	-46.62397900
C	-30.56927300	-15.10111300	-46.19734600
C	-29.30371100	-13.12118500	-45.72634500
C	-30.26697500	-15.60722000	-44.93373300
C	-28.98887300	-13.61040800	-44.46090000
C	-29.46200700	-14.86412700	-44.06643400
O	-29.08748600	-15.32351100	-42.82679200
C	-30.93557400	-17.83618200	-53.21865100
C	-31.81885700	-18.51578800	-52.20290700
O	-32.61558000	-19.40291100	-52.49816300
N	-31.64095700	-18.09551400	-50.91938900
C	-32.42874200	-18.65651500	-49.84294700
C	-33.83810800	-18.06108200	-49.74368800
H	-31.01018300	-17.33292400	-50.72768000
C	-25.47400100	-9.01406700	-53.29974600
C	-25.48695300	-9.06545900	-51.77793300
C	-25.70848100	-10.47156100	-51.24654800
O	-25.72499300	-11.46067800	-51.96516400
O	-25.87665300	-10.49102300	-49.93110600
C	-25.65782500	-17.19396100	-53.61265900
C	-27.05542100	-17.36455900	-54.22875800
C	-24.51780400	-17.77526400	-54.45743300
C	-27.25764500	-16.62509500	-55.55592900
C	-19.03388700	-18.01802900	-49.78011500
C	-20.46540100	-18.18147400	-50.30088200
C	-21.50848200	-17.45609500	-49.43991800
C	-22.94369700	-17.62040500	-49.96216800
C	-23.99791900	-16.83970000	-49.17908100
N	-24.14798900	-17.34059200	-47.77507900
H	-18.93049800	-18.41958500	-48.76551300
N	-26.11949100	-12.86025600	-48.80826900
C	-26.80384800	-13.97010800	-49.16063500
C	-27.45931300	-13.99398700	-50.51477200
C	-26.90105100	-15.06298400	-48.29500700
O	-27.57978600	-16.16437200	-48.71709400
C	-26.26663700	-15.04894500	-47.01480800
C	-26.36372800	-16.15726700	-46.10405900

C	-25.49985500	-13.88241100	-46.71308900	H	-22.99411200	-17.26903400	-50.99960700
C	-24.64181000	-13.78752600	-45.48233000	H	-24.98740600	-16.92522800	-49.63286600
C	-25.48822000	-12.83839000	-47.62753000	H	-23.74968100	-15.77720100	-49.11695400
H	-24.51320100	-18.32481200	-47.72436900	H	-25.65373000	-17.67747000	-52.62645400
H	-24.93924800	-11.92412600	-47.40286300	H	-28.12604200	-25.12121200	-40.91687100
H	-27.42033300	-14.99776100	-50.94638500	H	-28.88418000	-24.66617300	-42.44223700
H	-28.51975700	-13.72274300	-50.43900800	H	-27.24224700	-25.32541500	-42.42726400
H	-26.96638900	-13.28172400	-51.17979000	H	-25.36980100	-23.94962400	-41.35965500
H	-24.36847900	-12.73983800	-45.29841700	H	-24.49562500	-21.70035500	-40.82942500
H	-25.15954200	-14.14947400	-44.58996300	H	-26.01481100	-19.72713700	-40.87160600
C	-27.93589200	-24.66499900	-41.89626200	H	-28.41283400	-20.03981400	-41.45911900
C	-27.38283200	-23.28250400	-41.73914100	H	-29.27333800	-22.28616900	-42.01249300
C	-26.03496800	-23.09041500	-41.39932800	H	-24.13691400	-22.19183900	-47.05201300
C	-28.22191600	-22.16104800	-41.76599800	H	-23.25802000	-23.52108000	-46.29318300
C	-25.54138500	-21.82189400	-41.09796000	H	-24.61561300	-25.45814300	-45.18520200
C	-27.73552200	-20.88813500	-41.45687500	H	-26.38329100	-25.40284800	-45.25195800
C	-26.39227900	-20.71444300	-41.12106700	H	-25.45999100	-25.79097700	-46.70452000
C	-22.71706300	-19.76962400	-43.10279400	H	-25.53220500	-21.75322000	-45.11594800
C	-22.30898300	-19.25680300	-44.49872800	H	-26.45676700	-23.03389000	-44.33183800
C	-21.77145200	-20.35675200	-45.40070600	H	-24.69960500	-23.01724800	-44.19091600
O	-23.42839400	-18.65266400	-45.18985800	H	-26.26888600	-23.43123100	-46.79146300
H	-31.07222300	-21.57302700	-53.39718900	H	-21.85004100	-20.20012200	-42.59247200
H	-30.65552400	-21.60137400	-50.96396800	H	-23.09835300	-18.95145000	-42.48189700
H	-29.18851500	-21.59395300	-55.01458200	H	-23.49461100	-20.53514600	-43.18240800
H	-26.83902000	-21.56151300	-54.22316200	H	-20.87277000	-20.79802600	-44.96041600
H	-25.99900400	-21.39402600	-49.12436700	H	-22.51075700	-21.15111900	-45.53642100
H	-24.06177700	-21.36068300	-51.04019200	H	-21.50703900	-19.95874800	-46.38512600
H	-24.52573000	-22.25159100	-52.49274500	H	-21.53502400	-18.48507200	-44.37599100
H	-24.64205900	-20.49294000	-52.47241600	H	-23.77009000	-17.92228200	-44.65317700
H	-28.50734800	-21.47693500	-49.09197600	H	-30.62392400	-21.68303500	-39.50316200
H	-28.28541400	-16.73913000	-55.91588000	H	-32.01955500	-21.14082200	-38.57197300
H	-27.06172300	-15.55225600	-55.44483100	H	-32.22677100	-21.63030900	-40.25541300
H	-26.59444300	-17.00359700	-56.34054300	H	-29.60619400	-19.40701700	-38.70481400
H	-27.26089300	-18.43495300	-54.36476100	H	-29.28575600	-17.02630600	-39.29700100
H	-27.79760400	-17.00538500	-53.50493800	H	-30.81870200	-15.92251300	-40.91153700
H	-24.67533100	-18.84274900	-54.65221300	H	-32.63689600	-17.24830000	-41.98259900
H	-24.43120000	-17.27261700	-55.42591500	H	-32.94772000	-19.62949000	-41.39144500
H	-23.55206800	-17.66956300	-53.95028200	C	-30.00403900	-21.42503100	-46.77397400
H	-25.47125400	-16.12604200	-53.43378900	C	-29.25679600	-21.51614200	-45.59875400
H	-33.79874300	-16.98052500	-49.57042600	C	-28.45364000	-20.45716000	-45.18338500
H	-34.38619100	-18.24661800	-50.67031300	C	-28.35953700	-19.25664100	-45.92827100
H	-34.39097000	-18.51951200	-48.91670000	C	-29.12554100	-19.18407300	-47.11722400
H	-31.88695700	-18.49699300	-48.90598200	C	-29.92882200	-20.24515500	-47.52490600
H	-32.50327700	-19.73494300	-50.01260200	H	-30.63871400	-22.24550400	-47.09493600
H	-30.15072100	-18.53602200	-53.52268600	H	-29.29283400	-22.42013800	-44.99706700
H	-31.52838000	-17.60047600	-54.10543700	H	-27.87786100	-20.57786000	-44.27398600
H	-30.46482600	-16.92155100	-52.84789100	H	-29.10760600	-18.27265200	-47.70372400
H	-29.62765600	-12.61815600	-48.30681100	H	-30.51197700	-20.14723600	-48.43493000
H	-30.36157700	-14.15355200	-48.72524800	C	-27.49626300	-18.14741300	-45.49500600
H	-28.91186100	-12.15414000	-46.03114400	H	-24.84384500	-16.77435700	-47.22075600
H	-28.36933600	-13.04151200	-43.77495000	C	-26.99476100	-18.06784500	-44.07299000
H	-30.63142800	-16.58727000	-44.63449100	H	-25.91148500	-18.25265600	-43.99567900
H	-31.17958200	-15.69880400	-46.87037800	H	-27.17490600	-17.06490700	-43.66496400
H	-29.49368600	-16.18770800	-42.66930600	H	-27.48498400	-18.78561300	-43.41700900
H	-26.43030700	-9.34944100	-53.71055700	N	-27.18747400	-17.20591800	-46.36677400
H	-25.28524600	-7.99639600	-53.65633900	H	-23.27847600	-17.32502400	-47.23865100
H	-24.70187700	-9.67324000	-53.70410500	H	-27.59627000	-16.78731100	-47.93036000
H	-24.54189400	-8.69802100	-51.35696000	O	-25.15305800	-19.80531900	-47.09099100
H	-26.26546600	-8.42003400	-51.35472400	H	-26.09042200	-19.65183400	-46.88300400
H	-26.01018700	-11.45746200	-49.60539900	H	-24.68541300	-19.67923700	-46.24260100
H	-18.31816600	-18.54423900	-50.41878800	H	-25.93161100	-16.03716200	-45.11312400
H	-18.73993100	-16.96294900	-49.75068800	O	-23.44588200	-14.59889800	-45.58097000
H	-20.71964500	-19.24827300	-50.35241300	H	-22.93251000	-14.21557400	-46.30518800
H	-20.52768700	-17.80406500	-51.32977300	C	-23.99501500	-23.95086000	-48.28392200
H	-21.42924300	-17.83470400	-48.40903000	H	-23.09973700	-23.59702400	-48.80708300
H	-21.25992900	-16.38627200	-49.39324100	H	-23.91151300	-25.03911700	-48.20209400
H	-23.21941500	-18.68286400	-49.98800500	H	-24.85729500	-23.72901200	-48.92201800

C	-31.77940400	-12.63992000	-48.11094800
H	-31.84249900	-11.78352600	-47.43149800
H	-31.96144000	-12.27858700	-49.12868300
H	-32.58842400	-13.32947100	-47.84695500

Int6:

C	-31.55573300	-21.11103900	-39.56532900
C	-31.30561900	-19.68981600	-40.00052500
C	-30.19762600	-18.97484200	-39.51986800
C	-32.22101000	-19.01794600	-40.82234000
C	-30.02468300	-17.62543300	-39.82837700
C	-32.05606300	-17.66649000	-41.13214100
C	-30.96225700	-16.96016700	-40.62537300
C	-24.13433200	-23.27913000	-46.91362400
C	-25.46110300	-23.61013000	-46.19934000
C	-25.49258000	-25.04896500	-45.66325400
C	-25.74812100	-22.59435500	-45.08728100
C	-24.78502000	-21.39304800	-51.86127100
C	-26.19603400	-21.48909700	-51.33661000
C	-26.57062200	-21.48940300	-50.01405700
C	-27.41228700	-21.56281100	-52.10713000
C	-28.49363800	-21.61362400	-51.18267000
C	-27.69606700	-21.56862300	-53.48430800
N	-27.94808600	-21.57210000	-49.91584100
C	-29.82787200	-21.65696000	-51.60068200
C	-29.02158900	-21.60712800	-53.90172200
C	-30.07878600	-21.64629900	-52.96867800
C	-31.38362200	-14.11797200	-47.97288300
C	-30.82851700	-14.50688700	-46.61601000
C	-31.38236600	-15.56207000	-45.88389800
C	-29.71444100	-13.85281900	-46.06695400
C	-30.83871600	-15.97704400	-44.66680500
C	-29.16368600	-14.24617400	-44.85118600
C	-29.71527100	-15.32541600	-44.15375600
O	-29.09876000	-15.70871400	-42.98814200
C	-30.93556700	-17.83618500	-53.21864400
C	-31.82874200	-18.50777700	-52.20606300
O	-32.64252600	-19.37687600	-52.50743500
N	-31.63591500	-18.10360700	-50.91925500
C	-32.42874300	-18.65652000	-49.84295200
C	-33.80252200	-17.99234200	-49.69554500
H	-30.99543700	-17.34997800	-50.72384500
C	-25.47400100	-9.01406700	-53.29974600
C	-25.48561800	-9.04143400	-51.77638000
C	-25.92217500	-10.38532000	-51.22410700
O	-26.28956500	-11.31334200	-51.92691300
O	-25.86289300	-10.42952500	-49.89426900
C	-25.65783100	-17.19396200	-53.61265800
C	-27.02833100	-17.38635100	-54.28128200
C	-24.48993000	-17.84652300	-54.36104600
C	-27.15716800	-16.73419000	-55.66248500
C	-19.03389000	-18.01802900	-49.78011600
C	-20.39757500	-18.70730200	-49.68824000
C	-21.57735200	-17.72979000	-49.75327900
C	-22.94156100	-18.41885900	-49.64843900
C	-24.12140600	-17.44974500	-49.74515200
N	-25.39455800	-18.14693700	-49.49767200
H	-18.89366700	-17.30354400	-48.96074500
N	-26.28563800	-12.82660700	-48.74015700
C	-26.97674100	-13.91828400	-49.08222900
C	-27.74922900	-13.91088700	-50.37057000
C	-26.98642800	-15.05939000	-48.24625700
O	-27.73372000	-16.11300900	-48.65462000
C	-26.23065500	-15.07398600	-47.05940800

C	-26.16202300	-16.30038300	-46.16306800
C	-25.50709100	-13.90569500	-46.73361200
C	-24.62467100	-13.78753900	-45.51201300
C	-25.57916000	-12.82129900	-47.60187900
H	-25.56828200	-18.84675400	-50.21794500
H	-25.04434800	-11.90003600	-47.37919300
H	-27.63260700	-14.86353900	-50.89498800
H	-28.82235000	-13.79041700	-50.17556800
H	-27.40828700	-13.09334300	-51.00814300
H	-24.35743100	-12.73147900	-45.36600300
H	-25.14453700	-14.11361100	-44.60576500
C	-27.93592500	-24.66502200	-41.89620200
C	-27.38279400	-23.28249700	-41.73922600
C	-26.03002100	-23.09689500	-41.41564600
C	-28.21110900	-22.15458100	-41.78205500
C	-25.52197000	-21.82966200	-41.13618800
C	-27.70907800	-20.88247200	-41.49705800
C	-26.36292500	-20.71525700	-41.17040600
C	-22.71706100	-19.76961800	-43.10284800
C	-22.30897200	-19.25680700	-44.49867500
C	-21.96453500	-20.38971300	-45.45380800
O	-23.37134800	-18.48457700	-45.10073700
H	-31.10660700	-21.64080000	-53.31567200
H	-30.64766600	-21.68638100	-50.88862800
H	-29.25168300	-21.60692100	-54.96321200
H	-26.88972400	-21.54031300	-54.21228600
H	-25.96430400	-21.40169000	-49.12223500
H	-24.06427800	-21.36877200	-51.03928700
H	-24.53123700	-22.25098000	-52.49590100
H	-24.63459500	-20.49336000	-52.47110700
H	-28.45736200	-21.60493800	-49.04778900
H	-28.16848200	-16.85918500	-56.06316400
H	-26.95033500	-15.65877700	-55.61242500
H	-26.46320100	-17.17160600	-56.38764600
H	-27.24475200	-18.46058700	-54.35758100
H	-27.79868600	-16.97014500	-53.61955600
H	-24.66005800	-18.92084000	-54.49998900
H	-24.34437300	-17.40607600	-55.35259500
H	-23.55045000	-17.72691500	-53.81083400
H	-25.46082300	-16.11905700	-53.49800800
H	-33.70385200	-16.92049800	-49.49179200
H	-34.37930700	-18.11948200	-50.61488300
H	-34.36301400	-18.44586600	-48.87076600
H	-31.85806500	-18.56093700	-48.91470200
H	-32.56262800	-19.72245900	-50.04970700
H	-30.15800700	-18.54410100	-53.52319200
H	-31.52339800	-17.59082500	-54.10600100
H	-30.45449200	-16.92821100	-52.84441900
H	-30.63779700	-14.36181300	-48.74217200
H	-32.25629900	-14.74549200	-48.19071000
H	-29.25642900	-13.02737900	-46.60487000
H	-28.30044800	-13.73658300	-44.43533900
H	-31.27359100	-16.81734100	-44.13172700
H	-32.24903100	-16.08740300	-46.27750900
H	-29.61000500	-16.41827400	-42.57112700
H	-26.46363600	-9.24673300	-53.70066300
H	-25.17217600	-8.02929600	-53.66968100
H	-24.78087500	-9.75927400	-53.69906100
H	-24.49861900	-8.81117200	-51.35757300
H	-26.16158700	-8.28098900	-51.36504600
H	-26.12066400	-11.35454300	-49.57571900
H	-18.21441700	-18.74243100	-49.73213000
H	-18.93229500	-17.46395000	-50.72017900
H	-20.45604700	-19.28198200	-48.75367500
H	-20.49274300	-19.44151600	-50.49940700
H	-21.47848700	-16.99033400	-48.94498800
H	-21.52268100	-17.16023400	-50.69209900

H	-23.02229000	-18.96924600	-48.70306500
H	-23.03030100	-19.16890000	-50.44670300
H	-24.09686400	-16.93378900	-50.71865200
H	-24.01870100	-16.67046800	-48.97896700
H	-25.70622400	-17.60451500	-52.59534500
H	-28.08560800	-25.14007700	-40.91865300
H	-28.90356500	-24.66104300	-42.40693800
H	-27.25970400	-25.31044800	-42.46632000
H	-25.37158400	-23.96109100	-41.37292100
H	-24.47222900	-21.71252000	-40.88282700
H	-25.97294900	-19.72770000	-40.94217300
H	-28.37560100	-20.02557300	-41.50914200
H	-29.26297700	-22.27472100	-42.02938400
H	-24.08811800	-22.19340900	-47.05557500
H	-23.29069000	-23.55779400	-46.26573000
H	-24.72285200	-25.19239400	-44.89398000
H	-26.46272200	-25.28013900	-45.20848800
H	-25.31494700	-25.78825100	-46.45110700
H	-25.78953100	-21.58077300	-45.49725400
H	-26.69864800	-22.80328200	-44.58584100
H	-24.96616200	-22.62599900	-44.31805900
H	-26.26314200	-23.51429300	-46.94760600
H	-21.89947600	-20.34234200	-42.65290400
H	-22.95574000	-18.93481200	-42.43529000
H	-23.59766500	-20.41409800	-43.17879400
H	-21.14392000	-20.99195700	-45.05158400
H	-22.82770900	-21.04183100	-45.60375100
H	-21.65963200	-19.99457400	-46.42695300
H	-21.42931800	-18.60569600	-44.39059300
H	-23.27613700	-17.55678000	-44.84706500
H	-30.63947200	-21.70967100	-39.59776300
H	-31.92570700	-21.14158500	-38.53355500
H	-32.30394100	-21.59932500	-40.19603600
H	-29.47331900	-19.47886100	-38.88534700
H	-29.16912100	-17.08591700	-39.43224500
H	-30.84926600	-15.89946700	-40.83075200
H	-32.79112000	-17.16002900	-41.75130000
H	-33.08618400	-19.55432500	-41.20392500
C	-30.89859200	-20.68576900	-46.41597300
C	-30.60031200	-20.35259100	-45.09550600
C	-29.49801500	-19.54701400	-44.81004800
C	-28.68584900	-19.04685000	-45.83870700
C	-28.98955600	-19.39356200	-47.16410700
C	-30.08602900	-20.20585200	-47.44750900
H	-31.75350800	-21.31572800	-46.64301400
H	-31.22439400	-20.71565400	-44.28435600
H	-29.28239800	-19.29257400	-43.77817700
H	-28.34535900	-19.04367000	-47.96275500
H	-30.31853300	-20.45272800	-48.47901300
C	-27.54848200	-18.13515800	-45.53441200
H	-25.21737600	-16.83044800	-46.35435500
C	-26.79965200	-18.30677200	-44.23426400
H	-25.72305900	-18.33593300	-44.42395500
H	-27.01506400	-17.46623900	-43.56208100
H	-27.06764400	-19.23456500	-43.73173500
N	-27.27301600	-17.22032200	-46.39093100
H	-25.29680800	-19.15846000	-47.90263000
H	-27.78058300	-16.73259700	-47.85365900
O	-25.19981800	-19.75268800	-47.12081100
H	-26.17586700	-17.49308700	-49.52224700
H	-24.54786400	-19.32590600	-46.54413800
H	-26.12152500	-15.97765800	-45.11615800
O	-23.44588300	-14.59889900	-45.58097000
H	-22.99526200	-14.37391600	-46.40638600
C	-23.99501600	-23.95087200	-48.28391800
H	-23.05364200	-23.67127000	-48.77014200
H	-24.00855600	-25.04413800	-48.21265600

H	-24.81177800	-23.65354800	-48.95012700
C	-31.77940200	-12.63992300	-48.11094600
H	-30.92441200	-11.97627000	-47.94873700
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Int7:

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C	-30.04776300	-17.61392600	-39.80197700
C	-32.02458300	-17.68612500	-41.18563200
C	-30.95678700	-16.96556900	-40.64490000
C	-24.13430600	-23.27911600	-46.91359500
C	-25.46161500	-23.60197300	-46.19817000
C	-25.50972900	-25.05067600	-45.69067700
C	-25.72232300	-22.60675700	-45.06262000
C	-24.78500800	-21.39308000	-51.86129200
C	-26.19605900	-21.48903000	-51.33657700
C	-26.59415400	-21.65136000	-50.03158400
C	-27.40162000	-21.47060200	-52.12811900
C	-28.49740400	-21.62919300	-51.23543100
C	-27.65814800	-21.33418700	-53.50364600
N	-27.97345800	-21.74427100	-49.96427800
C	-29.82419300	-21.63648600	-51.67977400
C	-28.97467400	-21.34393800	-53.94793000
C	-30.04841500	-21.48945000	-53.04402500
C	-31.38059200	-14.12413800	-48.09947500
C	-30.85136000	-14.62449300	-46.76961400
C	-31.46088500	-15.69018400	-46.09831300
C	-29.71168000	-14.05536700	-46.18052200
C	-30.95618100	-16.18828000	-44.89538000
C	-29.19944300	-14.52979700	-44.97576500
C	-29.81825500	-15.60686400	-44.32906400
O	-29.24690600	-16.05406700	-43.16695500
C	-30.93555500	-17.83618700	-53.21865000
C	-31.82450600	-18.51176100	-52.20554900
O	-32.63058600	-19.38891700	-52.50509700
N	-31.63637600	-18.10312000	-50.91939700
C	-32.42873300	-18.65653100	-49.84294700
C	-33.80561700	-17.99804200	-49.69934000
H	-31.00609300	-17.34026300	-50.72674400
C	-25.47400100	-9.01406800	-53.29974500
C	-25.69490800	-9.00457500	-51.79265500
C	-26.07145000	-10.37289600	-51.25632400
O	-26.35720400	-11.32020400	-51.97183600
O	-26.06317700	-10.41472500	-49.92594500
C	-25.65783900	-17.19397000	-53.61265600
C	-26.77567900	-17.09253000	-54.66342900
C	-24.30522600	-17.65226300	-54.17030300
C	-26.53714400	-16.02946100	-55.74123700
C	-19.03389200	-18.01802900	-49.78011600
C	-20.30121700	-18.64394700	-49.18325000
C	-21.58334000	-17.88132800	-49.54346800
C	-22.87175600	-18.52927000	-49.01362100
C	-24.12084100	-17.75818300	-49.44451500
N	-25.37728100	-18.44861800	-49.07410200
H	-18.89648100	-16.98887400	-49.42941300
N	-26.27744900	-12.83888800	-48.81231200
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O	-27.46364200	-16.22931500	-48.67845000

C	-26.06626700	-15.04276700	-47.09116200	H	-21.64906800	-17.79281200	-50.63770900
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C	-25.41814900	-13.82539300	-46.79416000	H	-22.93671400	-19.56034200	-49.39143600
C	-24.52355600	-13.66722200	-45.58718700	H	-24.07614800	-17.56830700	-50.52854100
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H	-26.15440900	-17.84287400	-49.33969900	H	-25.97775600	-17.89453500	-52.82991200
H	-25.08381500	-11.80839400	-47.48347100	H	-28.10701000	-25.13106200	-40.91771400
H	-27.40995600	-14.98714800	-50.96418400	H	-28.89360300	-24.66367700	-42.42578200
H	-28.72231200	-14.06142300	-50.25426100	H	-27.25026000	-25.31793000	-42.44616700
H	-27.38457400	-13.20341100	-51.06640000	H	-25.36357400	-23.95550200	-41.40833400
H	-24.16113100	-12.62962500	-45.53897600	H	-24.46931500	-21.70693900	-40.90329300
H	-25.07096100	-13.85688600	-44.65695800	H	-25.98078700	-19.73141100	-40.91456200
C	-27.93593700	-24.66504600	-41.89616900	H	-28.38944700	-20.03339800	-41.45325700
C	-27.38276200	-23.28246200	-41.73929900	H	-29.27295900	-22.28198400	-41.98724500
C	-26.02693700	-23.09426200	-41.43167400	H	-24.06637700	-22.19142200	-47.04609200
C	-28.21793100	-22.15835900	-41.75487300	H	-23.29225700	-23.56180800	-46.26666600
C	-25.52193600	-21.82776200	-41.14184900	H	-24.72969700	-25.22287800	-44.93829600
C	-27.71920600	-20.88756700	-41.45920600	H	-26.47585000	-25.27132700	-45.22338600
C	-26.36935200	-20.71792700	-41.14845600	H	-25.36065900	-25.77695700	-46.49603400
C	-22.71704000	-19.76961000	-43.10283100	H	-25.75292300	-21.58077400	-45.44259600
C	-22.30902700	-19.25684000	-44.49869200	H	-26.67268300	-22.80833000	-44.55911600
C	-21.77786300	-20.39194900	-45.37691500	H	-24.93505300	-22.66687700	-44.30154300
O	-23.33629700	-18.51759000	-45.14812700	H	-26.26886600	-23.48118800	-46.93799100
H	-31.06957800	-21.45698300	-53.40831400	H	-21.86145200	-20.23052400	-42.59752800
H	-30.65575900	-21.74990200	-50.99044900	H	-23.07992000	-18.94246800	-42.48534800
H	-29.18567000	-21.23880800	-55.00812100	H	-23.51432500	-20.51816800	-43.17646800
H	-26.83854900	-21.22226700	-54.20817900	H	-20.92299500	-20.88819600	-44.90439200
H	-26.00055700	-21.71818700	-49.13112700	H	-22.55165500	-21.14949600	-45.54312200
H	-24.05480200	-21.44199900	-51.04793200	H	-21.45741400	-20.01187700	-46.35096200
H	-24.56142200	-22.21387200	-52.55314100	H	-21.50257900	-18.52512300	-44.35786500
H	-24.61693600	-20.45848600	-52.40964400	H	-24.05875700	-19.09453000	-45.45506000
H	-28.50201500	-21.82158600	-49.11027500	H	-30.63539100	-21.70412600	-39.57875100
H	-27.38738800	-15.96846900	-56.42842500	H	-31.94469000	-21.14134100	-38.54050900
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H	-25.64791300	-16.24799100	-56.34143000	H	-29.52188600	-19.45049800	-38.81407200
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H	-24.39144200	-18.62789300	-54.66362100	H	-32.73977500	-17.19254400	-41.83801200
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H	-34.38049300	-18.13003800	-50.61918700	C	-28.22540700	-19.26183500	-45.95893300
H	-34.36567100	-18.45195800	-48.87448900	C	-28.63228600	-19.50838300	-47.27793900
H	-31.85939400	-18.55638600	-48.91382200	C	-29.84373800	-20.14255500	-47.55052100
H	-32.55760900	-19.72343300	-50.04741900	H	-31.61610600	-21.05348500	-46.71646500
H	-30.14355100	-18.53286700	-53.51174900	H	-30.90383100	-20.64975000	-44.36402900
H	-31.52150200	-17.60899700	-54.11197900	H	-28.77627100	-19.52167700	-43.89049800
H	-30.47268900	-16.91635100	-52.84989200	H	-27.99678200	-19.20383700	-48.10277600
H	-30.61878200	-14.29259200	-48.87288400	H	-30.14948500	-20.29309300	-48.58182300
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H	-29.80683500	-16.73259000	-42.76005400	H	-26.46548200	-19.45778500	-43.79573300
H	-26.36404000	-9.37636400	-53.81960200	N	-27.08657500	-17.15556800	-46.28580500
H	-25.23976000	-8.01002400	-53.66690800	H	-25.47839700	-19.29546000	-49.63435900
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H	-24.80704100	-8.66000200	-51.25055100	O	-25.82323400	-19.16189800	-46.37384200
H	-26.49834400	-8.31098600	-51.51151300	H	-27.45497300	-16.83133700	-47.86374100
H	-26.25413600	-11.36208300	-49.62047200	H	-25.73984100	-18.89281300	-47.33514300
H	-18.14001500	-18.58572400	-49.50260000	H	-25.81475400	-15.87906200	-45.12671600
H	-19.08445500	-17.98952700	-50.87444600	O	-23.44588400	-14.59890000	-45.58097000
H	-20.20438100	-18.69491600	-48.09068700	H	-22.95862400	-14.48475600	-46.40807500
H	-20.39104200	-19.68272900	-49.52930900	C	-23.99502800	-23.95087800	-48.28392600
H	-21.50903300	-16.85230700	-49.16311200	H	-23.06483900	-23.65318300	-48.78020300

H	-23.98127400	-25.04297700	-48.20363600
H	-24.82484000	-23.68324700	-48.94571900
C	-31.77939900	-12.63992800	-48.11094300
H	-30.92926000	-11.99397300	-47.87120900
H	-32.15044300	-12.34566300	-49.09781700
H	-32.56657800	-12.43933900	-47.37716300

Int8:

C	-31.55577100	-21.11102400	-39.56528800
C	-31.30558600	-19.68983400	-40.00056600
C	-30.25658900	-18.94086200	-39.44380600
C	-32.14848200	-19.06093600	-40.92614100
C	-30.06770700	-17.60340400	-39.78808600
C	-31.96788000	-17.71884300	-41.27178000
C	-30.93093700	-16.98113600	-40.69629000
C	-24.13430600	-23.27911600	-46.91359500
C	-25.46519800	-23.59141900	-46.20071900
C	-25.53137700	-25.04379000	-45.70582000
C	-25.71282200	-22.60106700	-45.05809300
C	-24.78500800	-21.39308100	-51.86129200
C	-26.19605900	-21.48902800	-51.33657700
C	-26.59048400	-21.64671800	-50.02784200
C	-27.40414100	-21.46193400	-52.12304300
C	-28.49741900	-21.61163600	-51.22639400
C	-27.66394100	-21.32845700	-53.49860600
N	-27.97128800	-21.72257900	-49.95578500
C	-29.82598900	-21.61298500	-51.66604600
C	-28.98153500	-21.33537700	-53.93821600
C	-30.05322500	-21.47189900	-53.02977600
C	-30.75360500	-13.78262700	-48.20921600
C	-30.35187200	-14.36006000	-46.86753600
C	-30.97925600	-15.49601200	-46.34280200
C	-29.33735400	-13.76677100	-46.10140200
C	-30.61313000	-16.03345100	-45.10732700
C	-28.96231600	-14.28183900	-44.86248700
C	-29.59950800	-15.42318000	-44.36047700
O	-29.16001000	-15.91057800	-43.15552400
C	-30.93555500	-17.83618700	-53.21865000
C	-31.83737700	-18.50391700	-52.21172800
O	-32.66200100	-19.36031600	-52.52086100
N	-31.63559800	-18.11203100	-50.92219800
C	-32.42873300	-18.65653100	-49.84294700
C	-33.70456400	-17.85496500	-49.56130000
H	-30.96756700	-17.38308000	-50.72411900
C	-25.47400100	-9.01406800	-53.29974500
C	-25.99974200	-9.13160700	-51.87346300
C	-26.20361000	-10.57454200	-51.44025700
O	-26.30521600	-11.50660800	-52.22246000
O	-26.27804000	-10.69218300	-50.11747200
C	-25.65783900	-17.19397000	-53.61265600
C	-26.92283400	-17.20029700	-54.48582900
C	-24.41822600	-17.79173100	-54.28875700
C	-26.82818500	-16.32981600	-55.74371800
C	-19.03389200	-18.01802900	-49.78011600
C	-20.26448800	-18.73172400	-49.20548000
C	-21.57463200	-17.98339200	-49.48320000
C	-22.83192300	-18.68679200	-48.94531000
C	-24.08237700	-17.87493300	-49.27155500
N	-25.36982100	-18.52372500	-48.87892000
H	-18.92278200	-17.01443200	-49.35458500
N	-26.22019400	-13.12356300	-49.04605000
C	-26.73776100	-14.32253700	-49.32243800
C	-27.45125900	-14.51009900	-50.63170900
C	-26.61581800	-15.42332200	-48.41719800

O	-27.14491000	-16.59426000	-48.72515400
C	-25.93100900	-15.18802200	-47.19380100
C	-25.81310500	-16.28927400	-46.16267300
C	-25.35311900	-13.92622400	-46.95628400
C	-24.50867400	-13.65666800	-45.73263400
C	-25.52955100	-12.93168300	-47.91003800
H	-26.14627300	-17.77717300	-48.96175400
H	-25.10704500	-11.93894200	-47.77066400
H	-27.09943700	-15.42023500	-51.12803500
H	-28.52806400	-14.64829600	-50.47312200
H	-27.28504100	-13.64862300	-51.28162000
H	-24.12984600	-12.62473800	-45.76914900
H	-25.09816500	-13.74521000	-44.81208900
C	-27.93593700	-24.66504500	-41.89616800
C	-27.38276200	-23.28246300	-41.73930100
C	-26.02484700	-23.09782900	-41.43820700
C	-28.22004500	-22.16007100	-41.72746100
C	-25.52036300	-21.83729700	-41.12305400
C	-27.72202800	-20.89575900	-41.40503700
C	-26.37120500	-20.73046900	-41.09627400
C	-22.71704000	-19.76961000	-43.10283100
C	-22.30902700	-19.25684000	-44.49869200
C	-21.72888100	-20.39452000	-45.34567300
O	-23.33456000	-18.55388200	-45.18726800
H	-31.07529900	-21.43583500	-53.39127000
H	-30.65567600	-21.71634100	-50.97315400
H	-29.19580200	-21.23416300	-54.99797100
H	-26.84622700	-21.22324500	-54.20618200
H	-25.99478000	-21.74780200	-49.13129300
H	-24.05358600	-21.46834600	-51.05075800
H	-24.56993800	-22.20081700	-52.57067300
H	-24.60960300	-20.44952300	-52.39167600
H	-28.49507500	-21.84693500	-49.10429500
H	-27.77284000	-16.33531000	-56.29719100
H	-26.60064300	-15.28925500	-55.48582000
H	-26.04807500	-16.68104800	-56.42690900
H	-27.15988100	-18.23562800	-54.76722900
H	-27.76699500	-16.85345600	-53.87657500
H	-24.60215000	-18.82359500	-54.61159800
H	-24.12034200	-17.21926800	-55.17264100
H	-23.56010600	-17.80375100	-53.60753900
H	-25.44177600	-16.16348900	-53.29985200
H	-33.47218000	-16.81952400	-49.28845600
H	-34.34445700	-17.84081300	-50.44767400
H	-34.26876400	-18.30474200	-48.73706600
H	-31.80468400	-18.70557000	-48.94422400
H	-32.69503000	-19.67772300	-50.12791400
H	-30.14435000	-18.53657000	-53.50408100
H	-31.51319000	-17.60669000	-54.11665500
H	-30.47074200	-16.91868100	-52.84688500
H	-29.85899800	-13.41582000	-48.72492100
H	-31.16696900	-14.58187200	-48.83683400
H	-28.81912500	-12.89254700	-46.48647200
H	-28.18000400	-13.81539600	-44.27215800
H	-31.09560400	-16.93452100	-44.73767900
H	-31.76279200	-15.98635200	-46.91539400
H	-29.73662600	-16.62848300	-42.85419700
H	-26.12977100	-9.54254400	-53.99555200
H	-25.40650300	-7.96598600	-53.60740900
H	-24.47860200	-9.45950300	-53.38945600
H	-25.33583500	-8.64583200	-51.15089300
H	-26.97010000	-8.62651400	-51.77290200
H	-26.35079000	-11.67429000	-49.85815400
H	-18.11606300	-18.57388900	-49.56483600
H	-19.11057500	-17.90943600	-50.86779100
H	-20.14171300	-18.85802500	-48.12203300
H	-20.32958900	-19.74444200	-49.62558100

H	-21.51145400	-16.97654600	-49.04684500
H	-21.67937800	-17.83633800	-50.56780800
H	-22.76577900	-18.81088200	-47.85807000
H	-22.91036700	-19.68962500	-49.38768000
H	-24.14521800	-17.66153400	-50.34354500
H	-24.05303500	-16.91204500	-48.75487500
H	-25.86966400	-17.75615700	-52.69278200
H	-28.11266400	-25.12677200	-40.91672200
H	-28.89103300	-24.66518700	-42.43065000
H	-27.24786000	-25.32047800	-42.44009100
H	-25.36026200	-23.95847100	-41.43649700
H	-24.46641900	-21.71942200	-40.88860700
H	-25.98439400	-19.74896300	-40.83928900
H	-28.39378400	-20.04344300	-41.37598200
H	-29.27595000	-22.27983900	-41.95726400
H	-24.05807000	-22.19132500	-47.04217000
H	-23.29588400	-23.56907400	-46.26513300
H	-24.75122500	-25.23272200	-44.95756800
H	-26.49862500	-25.25441800	-45.23638400
H	-25.39552300	-25.76605300	-46.51728300
H	-25.72974600	-21.57085900	-45.42861200
H	-26.66563200	-22.79658700	-44.55662500
H	-24.92704500	-22.68038500	-44.29691000
H	-26.27100600	-23.45458900	-46.93979000
H	-21.85097100	-20.19842800	-42.58761000
H	-23.11111400	-18.95077900	-42.49317900
H	-23.48934200	-20.54367700	-43.17692600
H	-20.87831400	-20.86777300	-44.84243800
H	-22.48362700	-21.16825900	-45.52401000
H	-21.38534000	-20.02279300	-46.31524200
H	-21.52262000	-18.50407800	-44.35334000
H	-24.09334800	-19.11815500	-45.45232700
H	-30.63564300	-21.70464400	-39.58558600
H	-31.93826400	-21.14462900	-38.53826700
H	-32.29170100	-21.60366100	-40.20663900
H	-29.58843100	-19.41149100	-38.72713600
H	-29.25509800	-17.03928400	-39.33967700
H	-30.79804800	-15.93170700	-40.94140900
H	-32.64976500	-17.24590100	-41.97344600
H	-32.96942700	-19.62257200	-41.36502600
C	-30.71029500	-20.46473400	-46.26866900
C	-30.31248700	-20.13292300	-44.97545900
C	-29.05871400	-19.55596900	-44.75102000
C	-28.17199500	-19.31373000	-45.80737800
C	-28.57867400	-19.66902700	-47.10093000
C	-29.83613400	-20.22524100	-47.33285500
H	-31.68706300	-20.90370400	-46.44963000
H	-30.97476700	-20.31524800	-44.13351800
H	-28.77147200	-19.31234700	-43.73557300
H	-27.90620700	-19.50313600	-47.93496800
H	-30.14435300	-20.45650100	-48.34897400
C	-26.78119900	-18.66464700	-45.60259500
H	-24.97065600	-16.96105900	-46.34947400
C	-26.41531900	-18.47460700	-44.12105900
H	-25.41811800	-18.03784500	-44.05694200
H	-27.12335900	-17.83717200	-43.58041500
H	-26.38290700	-19.45120300	-43.63376300
N	-27.04015600	-17.14220900	-46.14734000
H	-25.59015200	-19.32549800	-49.47700500
H	-27.78568400	-16.68486400	-45.61695800
O	-25.80580100	-19.21171600	-46.32789700
H	-27.34994600	-17.17417600	-47.15527300
H	-25.44054400	-18.84079300	-47.84740600
H	-25.65573400	-15.88757800	-45.16277800
O	-23.44588400	-14.59890000	-45.58097000
H	-22.92909300	-14.58062900	-46.39776800
C	-23.99502800	-23.95087800	-48.28392600

H	-23.06532000	-23.65314300	-48.78146700
H	-23.98020800	-25.04284500	-48.20335200
H	-24.82605600	-23.68601900	-48.94557400
C	-31.77939900	-12.63992800	-48.11094300
H	-31.38464200	-11.80874800	-47.51787900
H	-32.03143800	-12.25589200	-49.10460100
H	-32.70361700	-12.97955000	-47.63189300

E:PMP:

C	-31.55577100	-21.11102400	-39.56528800
C	-31.30558600	-19.68983400	-40.00056600
C	-30.29614700	-18.92229100	-39.39818100
C	-32.13774200	-19.06799700	-40.94111900
C	-30.13987300	-17.57178100	-39.70720700
C	-31.98973400	-17.71357500	-41.25104000
C	-30.99774100	-16.95601200	-40.62405300
C	-24.13430600	-23.27911600	-46.91359500
C	-25.35309900	-23.76485200	-46.10880000
C	-25.30318800	-25.26911900	-45.80198700
C	-25.49760800	-22.95514000	-44.81949400
C	-24.78500800	-21.39308100	-51.86129200
C	-26.19605900	-21.48902800	-51.33657700
C	-26.59406700	-21.67302700	-50.03452000
C	-27.40247300	-21.45446500	-52.12725600
C	-28.49893600	-21.62447400	-51.23844900
C	-27.65792500	-21.30162100	-53.50131500
N	-27.97650900	-21.74895500	-49.96689300
C	-29.82515800	-21.62936800	-51.68366800
C	-28.97392000	-21.31099400	-53.94735200
C	-30.04843700	-21.46956200	-53.04645600
C	-30.54684900	-13.55860700	-48.07158000
C	-30.22446200	-14.08572700	-46.68881400
C	-30.80720200	-15.26315100	-46.20420300
C	-29.33590700	-13.40640700	-45.84278100
C	-30.51331000	-15.75802700	-44.93300200
C	-29.03000200	-13.88273200	-44.56963400
C	-29.61354400	-15.06957300	-44.11194200
O	-29.24294400	-15.51698000	-42.87246100
C	-30.93555500	-17.83618700	-53.21865000
C	-31.84014600	-18.50197800	-52.21284600
O	-32.66625800	-19.35696800	-52.52142800
N	-31.63956200	-18.10861100	-50.92314800
C	-32.42873300	-18.65653100	-49.84294700
C	-33.70299700	-17.85552200	-49.55254400
H	-30.97023100	-17.38071400	-50.72595000
C	-25.47400100	-9.01406800	-53.29974500
C	-25.88340000	-9.01341500	-51.83350100
C	-26.12840700	-10.41744000	-51.31514200
O	-26.17283800	-11.39733500	-52.04330100
O	-26.29457800	-10.45428500	-49.99672800
C	-25.65783900	-17.19397000	-53.61265600
C	-26.92470500	-17.19977300	-54.48338500
C	-24.42166800	-17.79875900	-54.28838100
C	-26.82875600	-16.33936400	-55.74822900
C	-19.03389200	-18.01802900	-49.78011600
C	-20.29491300	-18.75321800	-49.31825600
C	-21.57806400	-17.96230500	-49.59392500
C	-22.86004800	-18.66516900	-49.13032900
C	-24.10440800	-17.81605000	-49.40131000
N	-25.39444000	-18.41999000	-49.00828700
H	-18.92944000	-17.05331700	-49.27084100
N	-26.24867700	-12.89792000	-48.96119800
C	-26.73972700	-14.08103900	-49.35595900
C	-27.47035400	-14.15421500	-50.66738000

C	-26.57543400	-15.23021800	-48.55390500	H	-20.35502200	-19.73044800	-49.81618000
O	-27.14043200	-16.38507000	-48.99635500	H	-21.50715300	-16.98245000	-49.10022100
C	-25.91482900	-15.13168900	-47.31416200	H	-21.64680700	-17.75224600	-50.67114900
C	-25.92138400	-16.31195000	-46.35927100	H	-22.80536600	-18.86652600	-48.05209300
C	-25.35202200	-13.88848100	-46.96124600	H	-22.95598400	-19.63617200	-49.63618700
C	-24.54449600	-13.69583700	-45.69590200	H	-24.17365000	-17.56432600	-50.46595400
C	-25.55370000	-12.81267700	-47.81957400	H	-24.00465500	-16.86367800	-48.86712700
H	-26.49864600	-17.17904200	-48.95348300	H	-25.86947800	-17.74845500	-52.68866400
H	-25.14825800	-11.83015500	-47.58441400	H	-28.15435400	-25.10172400	-40.91406600
H	-27.22646600	-15.08643900	-51.18310800	H	-28.86932800	-24.67344900	-42.46822800
H	-28.55590200	-14.15950600	-50.50681200	H	-27.23020300	-25.33621300	-42.39656100
H	-27.20533600	-13.29925300	-51.29162400	H	-25.35885400	-23.95915500	-41.45249800
H	-24.20932700	-12.64907000	-45.64035100	H	-24.48906200	-21.75253000	-40.75642900
H	-25.15865400	-13.88016800	-44.80727100	H	-26.03211900	-19.80864600	-40.57147300
C	-27.93593700	-24.66504500	-41.89616800	H	-28.43029000	-20.08587600	-41.16514200
C	-27.38276200	-23.28246300	-41.73930100	H	-29.28461000	-22.28484900	-41.90562100
C	-26.02943500	-23.10436200	-41.41294300	H	-24.21709800	-22.19228600	-47.04561100
C	-28.23038800	-22.16958700	-41.66608200	H	-23.22154400	-23.44843200	-46.32487800
C	-25.53916900	-21.86325500	-41.01057200	H	-24.40546400	-25.51783600	-45.22189300
C	-27.74913900	-20.92724700	-41.24816200	H	-26.17363900	-25.57435500	-45.21056400
C	-26.40362600	-20.77169700	-40.90890000	H	-25.29380000	-25.88030400	-46.70918000
C	-22.71704000	-19.76961000	-43.10283100	H	-25.52440000	-21.88276300	-45.02958900
C	-22.30902700	-19.25684000	-44.49869200	H	-26.41345400	-23.21397700	-44.28282800
C	-21.65415100	-20.36363000	-45.32935700	H	-24.65664800	-23.14638600	-44.14184900
O	-23.38264900	-18.63801000	-45.20195000	H	-26.24653300	-23.57848700	-46.72557900
H	-31.06922800	-21.43629500	-53.41194200	H	-21.84389900	-20.15014700	-42.56203400
H	-30.65709300	-21.74991100	-50.99599700	H	-23.16346700	-18.96277200	-42.51424700
H	-29.18390200	-21.19521600	-55.00657400	H	-23.44802600	-20.58292500	-43.18217800
H	-26.83790900	-21.18015600	-54.20367400	H	-20.77358400	-20.77211500	-44.82129900
H	-25.99893500	-21.76740600	-49.13737000	H	-22.35599600	-21.18869200	-45.49702300
H	-24.05463100	-21.47500800	-51.05109700	H	-21.34013700	-19.98041200	-46.30428700
H	-24.57405500	-22.19589800	-52.57762200	H	-21.58001000	-18.44855500	-44.36017900
H	-24.60665800	-20.44505100	-52.38238600	H	-24.08562300	-19.27931000	-45.41016400
H	-28.50115600	-21.93853000	-49.12865900	H	-30.62210700	-21.67527900	-39.47177600
H	-27.77474200	-16.34372400	-56.29963500	H	-32.04808100	-21.13543200	-38.58580300
H	-26.59423400	-15.29800700	-55.49943000	H	-32.20306200	-21.64035600	-40.27025000
H	-26.05206300	-16.70020600	-56.43032700	H	-29.63967600	-19.38674600	-38.66673000
H	-27.16775600	-18.23560700	-54.75735700	H	-29.36091500	-16.99204200	-39.22066500
H	-27.76602800	-16.84445300	-53.87475800	H	-30.89661000	-15.89603700	-40.83579100
H	-24.60997500	-18.83112500	-54.60732100	H	-32.66478700	-17.24555200	-41.96240900
H	-24.12219800	-17.23059600	-55.17474100	H	-32.93076200	-19.64369900	-41.41231300
H	-23.56387900	-17.81248300	-53.60704100	C	-30.93430600	-20.37027200	-46.18371100
H	-25.43681100	-16.16228800	-53.30662400	C	-30.57755500	-20.05041500	-44.87351600
H	-33.46900300	-16.82174500	-49.27544600	C	-29.26313100	-19.68697800	-44.57573200
H	-34.34578900	-17.83737100	-50.43669100	C	-28.28650400	-19.65378800	-45.58017200
H	-34.26469100	-18.30881600	-48.72844100	C	-28.65217100	-19.98899600	-46.89212800
H	-31.80084300	-18.70849900	-48.94646600	C	-29.96713800	-20.33272200	-47.19387300
H	-32.69599400	-19.67668300	-50.13089900	H	-31.95814500	-20.64505900	-46.42021100
H	-30.13910600	-18.53474600	-53.49407200	H	-31.31830900	-20.07976400	-44.07966700
H	-31.50859700	-17.61518200	-54.12166800	H	-28.99721000	-19.44701300	-43.55291500
H	-30.47746500	-16.91424000	-52.84948800	H	-27.89515200	-19.95637200	-47.66766900
H	-29.67978300	-13.01268700	-48.45988500	H	-30.24789600	-20.55847400	-48.21883400
H	-30.70824400	-14.40440000	-48.75170300	C	-26.85606000	-19.31207000	-45.28290200
H	-28.85947400	-12.49438100	-46.19300800	H	-25.30719000	-17.13174400	-46.74001900
H	-28.33526300	-13.35675100	-43.92274000	C	-26.49224100	-18.75608800	-43.92922900
H	-30.95563100	-16.69174900	-44.59425200	H	-25.50601800	-18.29629200	-43.99201300
H	-31.49569500	-15.81845400	-46.83695600	H	-27.22018100	-18.02563000	-43.57555600
H	-29.72722600	-16.32664600	-42.65532600	H	-26.44370200	-19.58114700	-43.21017700
H	-26.23424000	-9.50230300	-53.91387000	N	-27.27089800	-16.82303100	-46.08815200
H	-25.33062400	-7.99317900	-53.66785000	H	-25.65277700	-19.16560300	-49.65421700
H	-24.54037000	-9.56463100	-53.44465300	H	-27.81009300	-16.11408500	-45.59682800
H	-25.12763200	-8.54089700	-51.19580700	O	-25.97212900	-19.62885600	-46.08974400
H	-26.80464200	-8.43756200	-51.67472200	H	-27.75194500	-16.98030500	-46.97164700
H	-26.37230500	-11.42674100	-49.70160400	H	-25.33553700	-18.84967300	-48.08348600
H	-18.13069500	-18.60145400	-49.57408600	H	-25.45212300	-16.03649200	-45.41529700
H	-19.06281100	-17.82000500	-50.85762500	O	-23.44588400	-14.59890000	-45.58097000
H	-20.22272600	-18.96333500	-48.24288700	H	-22.93500500	-14.53767100	-46.39926500

C	-23.99502800	-23.95087800	-48.28392600
H	-23.17476400	-23.50961500	-48.86071400
H	-23.78506700	-25.02101600	-48.19394800
H	-24.90966700	-23.84413100	-48.87715600
C	-31.77939900	-12.63992800	-48.11094300
H	-31.63659900	-11.76563000	-47.46776400
H	-31.97013700	-12.28393600	-49.12861800
H	-32.67456100	-13.16482800	-47.76096000

TS1:

Imaginary frequency -1215 cm⁻¹

C	-31.55570300	-21.11103500	-39.56536900
C	-31.30564000	-19.68982200	-40.00048800
C	-30.00761900	-19.16607300	-40.06657700
C	-32.38074900	-18.83688000	-40.29206300
C	-29.79224800	-17.82442800	-40.38894900
C	-32.17289500	-17.49657600	-40.61536200
C	-30.87489900	-16.98001200	-40.65488800
C	-24.13434300	-23.27918900	-46.91366000
C	-24.37782800	-24.26444100	-45.75032500
C	-23.22433400	-25.26516600	-45.57999600
C	-24.63046500	-23.51664100	-44.43467500
C	-24.78501600	-21.39302300	-51.86126700
C	-26.19604300	-21.48913300	-51.33661600
C	-26.58028800	-21.43563000	-50.01920800
C	-27.41474200	-21.52953000	-52.10864200
C	-28.50088000	-21.49879500	-51.18839200
C	-27.69670100	-21.56864400	-53.48627900
N	-27.96200200	-21.43929300	-49.91999600
C	-29.83575700	-21.50224000	-51.60718800
C	-29.02158500	-21.57272900	-53.90567900
C	-30.08195600	-21.53787500	-52.97502000
C	-31.06519000	-13.99409900	-48.26162900
C	-30.58263100	-14.55475800	-46.94104000
C	-31.36424300	-15.44469600	-46.19470000
C	-29.35022500	-14.15880900	-46.39942100
C	-30.93994200	-15.93449400	-44.95718200
C	-28.91144500	-14.63458200	-45.16497500
C	-29.70688500	-15.52907700	-44.43842400
O	-29.21319400	-15.98171400	-43.24478300
C	-30.93558900	-17.83619000	-53.21863400
C	-31.91869900	-18.36886400	-52.20744500
O	-32.93894300	-18.97324000	-52.52831900
N	-31.58202900	-18.15197000	-50.90384000
C	-32.42873800	-18.65651200	-49.84295800
C	-33.59350700	-17.72208200	-49.50047700
H	-30.70165300	-17.71582100	-50.67026400
C	-25.47400100	-9.01406700	-53.29974600
C	-25.79596000	-8.72504800	-51.83304400
C	-25.63924300	-9.95838300	-50.95789300
O	-24.91100200	-10.89394300	-51.23776800
O	-26.38847500	-9.89615700	-49.85010600
C	-25.65780600	-17.19395400	-53.61267600
C	-26.90248900	-16.29825000	-53.51371600
C	-25.63285700	-18.11832800	-54.83531900
C	-27.00461600	-15.23712400	-54.61532300
C	-19.03097600	-18.02626600	-49.77497900
C	-20.44810600	-18.50295200	-50.12241200
C	-21.53939600	-18.02706900	-49.14836500
C	-22.89963600	-18.68482700	-49.42554500
C	-24.01256700	-18.37807000	-48.41042100
N	-24.54302700	-17.02621800	-48.55168700
H	-18.72564000	-18.38180300	-48.78411400
N	-26.29611000	-12.35772100	-48.58491000
C	-26.59840900	-13.36119600	-49.41261000

C	-27.28422500	-13.04370000	-50.71027900
C	-26.28062500	-14.71801500	-49.10602400
O	-26.55413300	-15.64114600	-50.02019000
C	-25.65832400	-14.99188300	-47.86185400
C	-25.29248400	-16.42727500	-47.49803000
C	-25.38047300	-13.91592000	-46.98752800
C	-24.76966200	-14.06823300	-45.60720100
C	-25.70273200	-12.62841200	-47.41170100
H	-24.97472000	-16.84672800	-49.45434900
H	-25.48333500	-11.77211900	-46.77766500
H	-28.00031100	-13.82773600	-50.96473800
H	-27.78809500	-12.07800200	-50.64526500
H	-26.55134000	-12.98858500	-51.52223900
H	-24.79200500	-13.08730500	-45.11148900
H	-25.36556500	-14.74721800	-44.98714100
C	-27.93588100	-24.66498800	-41.89627700
C	-27.38284900	-23.28251800	-41.73911300
C	-26.27703500	-23.04147600	-40.90989700
C	-27.97606600	-22.18897900	-42.38358000
C	-25.78176800	-21.75079700	-40.72724900
C	-27.48703100	-20.89362100	-42.20208500
C	-26.38739200	-20.66926900	-41.37163100
C	-22.71705400	-19.76962500	-43.10278300
C	-22.30898300	-19.25678400	-44.49873400
C	-22.17047900	-20.38512500	-45.50722200
O	-23.28271600	-18.33375600	-45.01424400
H	-31.10852800	-21.52076100	-53.32759300
H	-30.65320600	-21.46756200	-50.89316700
H	-29.24924600	-21.60272400	-54.96709700
H	-26.88915200	-21.59418400	-54.21255900
H	-25.97007100	-21.39323900	-49.12819500
H	-24.06201900	-21.35752800	-51.04143500
H	-24.52585200	-22.24869600	-52.49644300
H	-24.64561900	-20.49004600	-52.46769400
H	-28.47829600	-21.43103000	-49.05335100
H	-27.88669100	-14.60400500	-54.47176200
H	-26.12526500	-14.58238600	-54.61262100
H	-27.08257300	-15.68270400	-55.61280300
H	-27.79943300	-16.93372100	-53.53581600
H	-26.89333100	-15.80616200	-52.53493500
H	-26.49928000	-18.78997400	-54.83578400
H	-25.64866000	-17.55415800	-55.77366300
H	-24.73061900	-18.74019000	-54.84547000
H	-24.76009400	-16.56026200	-53.61175900
H	-33.23185300	-16.74181900	-49.17188600
H	-34.22639900	-17.58092500	-50.37993400
H	-34.20798300	-18.14836400	-48.69953900
H	-31.79994400	-18.82459400	-48.96199800
H	-32.82627100	-19.62407500	-50.16437600
H	-30.31046300	-18.66133800	-53.57560200
H	-31.48631400	-17.44042100	-54.07426000
H	-30.28217500	-17.05671900	-52.81715600
H	-30.21275500	-13.87789200	-48.94105400
H	-31.74506000	-14.71042700	-48.73815400
H	-28.72198800	-13.46377200	-46.95065300
H	-27.96709900	-14.30794800	-44.74129500
H	-31.56314100	-16.62788300	-44.39707400
H	-32.32622900	-15.76694400	-46.58603300
H	-29.83399200	-16.60628700	-42.83889300
H	-26.18679500	-9.72720400	-53.72489800
H	-25.51369000	-8.09755600	-53.89610400
H	-24.47780900	-9.45224200	-53.39175500
H	-25.11869400	-7.95729400	-51.43455100
H	-26.80872500	-8.33058800	-51.70509000
H	-26.29816800	-10.75806100	-49.33897000
H	-18.30000700	-18.39514700	-50.50149200
H	-18.96833900	-16.93218600	-49.76656800

H	-20.45494500	-19.60168600	-50.15077200
H	-20.70489200	-18.17602500	-51.13890300
H	-21.23184000	-18.26543600	-48.11947000
H	-21.63984900	-16.93572600	-49.19160700
H	-22.76328600	-19.77515700	-49.43699400
H	-23.24477600	-18.41798900	-50.43440500
H	-23.61883700	-18.47988200	-47.39366500
H	-24.79933200	-19.14571100	-48.53194900
H	-25.59592400	-17.80661000	-52.70307300
H	-28.60647800	-24.92317600	-41.06668800
H	-28.51282400	-24.76697700	-42.82016000
H	-27.14311800	-25.41977600	-41.91048700
H	-25.80029000	-23.87674100	-40.40236800
H	-24.92318200	-21.58872500	-40.08174000
H	-26.00453000	-19.66298300	-41.22832300
H	-27.96842600	-20.06238300	-42.70785400
H	-28.82804400	-22.35172600	-43.03875100
H	-24.96599100	-22.56298800	-46.94662700
H	-23.22976800	-22.69708000	-46.70365000
H	-22.28131700	-24.74230700	-45.37641600
H	-23.41548800	-25.93922300	-44.73813200
H	-23.07738600	-25.88420800	-46.46952400
H	-25.47622800	-22.82490700	-44.50993200
H	-24.85030100	-24.21103700	-43.61755100
H	-23.74975900	-22.93447200	-44.13922100
H	-25.28539500	-24.83908100	-45.99272300
H	-21.96177600	-20.45630000	-42.70654000
H	-22.81950000	-18.93596400	-42.40005600
H	-23.67551200	-20.29561100	-43.15079900
H	-21.48225200	-21.15317200	-45.14079300
H	-23.14509000	-20.84952600	-45.67363300
H	-21.79751400	-20.01336200	-46.46526300
H	-21.34055200	-18.74206700	-44.41003300
H	-23.04883600	-17.43689900	-44.73986100
H	-30.75402500	-21.77883500	-39.89568400
H	-31.60650500	-21.18177400	-38.47181500
H	-32.50201900	-21.49221200	-39.96011500
H	-29.15829000	-19.81115400	-39.86002800
H	-28.77929600	-17.43265700	-40.42090800
H	-30.70758100	-15.92874400	-40.87234300
H	-33.02245700	-16.85218300	-40.82323000
H	-33.39437000	-19.22824400	-40.25300200
C	-29.71582800	-21.19741600	-46.50998600
C	-28.38984300	-21.60542800	-46.34513700
C	-27.37433300	-20.65051800	-46.24558700
C	-27.66047200	-19.28112900	-46.30658400
C	-28.99509200	-18.88281800	-46.46834000
C	-30.01183200	-19.83286000	-46.56877400
H	-30.51083600	-21.93365900	-46.58464400
H	-28.14351500	-22.66193500	-46.29113700
H	-26.34671300	-20.97368100	-46.10578100
H	-29.25396100	-17.83051900	-46.52496400
H	-31.04018900	-19.50453800	-46.68652200
C	-26.52854000	-18.27687400	-46.13098500
H	-25.58560400	-18.78169900	-46.34160600
C	-26.46557400	-17.75764600	-44.68778500
H	-25.62081300	-17.07808700	-44.55117400
H	-27.38894300	-17.24832800	-44.39687600
H	-26.31163300	-18.59944500	-44.00792700
N	-26.63965700	-17.15191700	-47.12167100
H	-27.22147000	-17.47669100	-48.17511100
H	-27.25169400	-16.43550900	-46.72068500
O	-27.82803700	-17.54281100	-49.28422900
H	-27.55772200	-18.33475100	-49.77058800
H	-27.22610500	-16.58925500	-49.71381500
H	-24.69111100	-16.45070800	-46.58831300
O	-23.44297000	-14.60713500	-45.57583300

H	-22.94051600	-14.17853000	-46.28233800
C	-23.99500400	-23.95084800	-48.28390800
H	-23.91212100	-23.20857000	-49.08408300
H	-23.10556400	-24.58544000	-48.33685100
H	-24.86537600	-24.57711700	-48.51062300
C	-31.77940500	-12.63991800	-48.11094800
H	-31.11322500	-11.89239400	-47.66869600
H	-32.11276500	-12.26269100	-49.08315300
H	-32.65638500	-12.72905600	-47.46150600

TS2:

Imaginary frequency -891 cm⁻¹

C	-31.55570400	-21.11103600	-39.56537000
C	-31.30563900	-19.68982100	-40.00048500
C	-30.00882200	-19.16380800	-40.06633100
C	-32.38425000	-18.83324400	-40.26889400
C	-29.79833300	-17.81404300	-40.35764400
C	-32.18111700	-17.48572500	-40.56208300
C	-30.88438900	-16.96522100	-40.59292000
C	-24.13434300	-23.27918900	-46.91365700
C	-24.41243500	-24.25827600	-45.75302700
C	-23.29032700	-25.29305300	-45.57780700
C	-24.64788800	-23.50209600	-44.43896300
C	-24.78501800	-21.39302800	-51.86127300
C	-26.19604300	-21.48911800	-51.33661200
C	-26.58821900	-21.47557000	-50.02337100
C	-27.40691700	-21.50892100	-52.11982400
C	-28.50137500	-21.49504300	-51.21079900
C	-27.67355300	-21.52170500	-53.50031000
N	-27.97288100	-21.46331500	-49.93555600
C	-29.83116100	-21.49122600	-51.64365300
C	-28.99405100	-21.51870300	-53.93402500
C	-30.06397200	-21.50147100	-53.01461200
C	-31.03399600	-13.98204300	-48.20115300
C	-30.56792800	-14.48342500	-46.85128100
C	-31.31274600	-15.41354000	-46.11680000
C	-29.39104000	-13.98519700	-46.27074800
C	-30.90433700	-15.84304800	-44.85137800
C	-28.97180600	-14.39842100	-45.00986000
C	-29.72698500	-15.33464000	-44.29442300
O	-29.25162800	-15.72561300	-43.07281500
C	-30.93559500	-17.83619200	-53.21863000
C	-31.86088500	-18.48402800	-52.22070000
O	-32.70614700	-19.31717700	-52.53467600
N	-31.65193300	-18.10164600	-50.92716500
C	-32.42873800	-18.65651000	-49.84296300
C	-33.62098700	-17.78349500	-49.43631600
H	-30.96394300	-17.39176500	-50.73008400
C	-25.47400100	-9.01406700	-53.29974600
C	-26.04402900	-8.79059400	-51.89857300
C	-25.81875400	-9.97793900	-50.97548900
O	-24.99679900	-10.85208400	-51.18304600
O	-26.62861400	-9.94714800	-49.90790900
C	-25.65780000	-17.19395900	-53.61267200
C	-26.87446600	-16.27383800	-53.43308700
C	-25.71724700	-18.08751800	-54.85750600
C	-27.04544000	-15.21655600	-54.52969700
C	-19.03388700	-18.01802800	-49.78011500
C	-20.42713800	-18.47415700	-50.23037000
C	-21.55365200	-17.98918300	-49.30671800
C	-22.93755300	-18.55176900	-49.67368200
C	-24.03130500	-18.26604200	-48.63995900
N	-24.42645700	-16.83407800	-48.63712200
H	-18.80127800	-18.39074800	-48.77611000
N	-26.41135500	-12.36529400	-48.52194000

C	-26.58617000	-13.39203800	-49.35892600	H	-18.96178600	-16.92480300	-49.75232300
C	-27.25973800	-13.15687400	-50.67999000	H	-20.45272300	-19.57133900	-50.27468200
C	-26.11936800	-14.69881400	-49.03634500	H	-20.61868700	-18.12530700	-51.25329600
O	-26.16760300	-15.67813200	-49.92081900	H	-21.31568900	-18.27763400	-48.27246100
C	-25.56383700	-14.90951700	-47.74976700	H	-21.56519700	-16.88858500	-49.31710800
C	-25.19511100	-16.34682500	-47.41087800	H	-22.85869100	-19.64237600	-49.76044100
C	-25.37817300	-13.81236100	-46.89103900	H	-23.25895900	-18.19309800	-50.65905600
C	-24.72424300	-13.94771800	-45.53466100	H	-23.66475300	-18.52280800	-47.63890400
C	-25.80297500	-12.56236600	-47.33767800	H	-24.93382800	-18.83137100	-48.87032300
H	-23.59132400	-16.25073400	-48.70484700	H	-25.58578700	-17.82541500	-52.72186100
H	-25.65628800	-11.67829500	-46.72115700	H	-28.80293500	-24.82470000	-41.24249800
H	-27.87376600	-14.01770400	-50.95590700	H	-28.27069500	-24.85287200	-42.92124300
H	-27.87470600	-12.25608600	-50.63933800	H	-27.19595200	-25.42888500	-41.63926700
H	-26.51071500	-13.02142600	-51.46769800	H	-25.88941700	-23.84397300	-40.29228500
H	-24.64058000	-12.95686400	-45.06729500	H	-25.02175200	-21.55015300	-39.98240800
H	-25.33101300	-14.56720600	-44.86659400	H	-26.01776500	-19.65491700	-41.25091400
C	-27.93588300	-24.66499000	-41.89627600	H	-27.88612000	-20.09068800	-42.84122000
C	-27.38284600	-23.28251500	-41.73911400	H	-28.73968300	-22.38312200	-43.15340500
C	-26.32990900	-23.02191500	-40.85123100	H	-24.94749300	-22.54235500	-46.95343300
C	-27.92930000	-22.20490500	-42.45097400	H	-23.21753200	-22.72000900	-46.69288800
C	-25.83988300	-21.72725900	-40.67488100	H	-22.33282800	-24.79844700	-45.37089400
C	-27.44511800	-20.90768100	-42.27829300	H	-23.50491800	-25.96017700	-44.73609500
C	-26.39739400	-20.66353500	-41.38697600	H	-23.15858900	-25.91700000	-46.46631800
C	-22.71705500	-19.76962600	-43.10278400	H	-25.46680100	-22.77977800	-44.52136400
C	-22.30898300	-19.25678200	-44.49873300	H	-24.89845100	-24.18719300	-43.62284200
C	-22.11530100	-20.38496500	-45.49702800	H	-23.74813900	-22.95244000	-44.13778400
O	-23.30051700	-18.37965100	-45.05193300	H	-25.33580100	-24.80511000	-45.99972400
H	-31.08704200	-21.46753700	-53.37432000	H	-21.94207200	-20.42391600	-42.69057500
H	-30.65794600	-21.46974400	-50.93989100	H	-22.85520000	-18.93400800	-42.40756200
H	-29.21022200	-21.52722100	-54.99842300	H	-23.65626700	-20.32857400	-43.15583900
H	-26.85774300	-21.52951900	-54.21777300	H	-21.38568100	-21.11141000	-45.12673000
H	-25.98668500	-21.44618300	-49.12628400	H	-23.06389200	-20.90125000	-45.65842600
H	-24.05636700	-21.46733600	-51.04829500	H	-21.76356500	-19.99984300	-46.45833200
H	-24.56276700	-22.19118400	-52.57956700	H	-21.35965700	-18.70656000	-44.40060600
H	-24.62226300	-20.43653000	-52.37110900	H	-23.25048800	-17.52930600	-44.59486600
H	-28.49559600	-21.48044100	-49.07316000	H	-30.74307700	-21.77577700	-39.87413500
H	-27.89946200	-14.56216700	-54.32172200	H	-31.63058800	-21.17532300	-38.47280400
H	-26.15514700	-14.58066200	-54.60551400	H	-32.49085400	-21.50056400	-39.97853400
H	-27.21301700	-15.66665400	-55.51409800	H	-29.15710700	-19.81163000	-39.87868400
H	-27.77833800	-16.89604100	-53.37558400	H	-28.78623400	-17.41956400	-40.38625400
H	-26.78180000	-15.77801000	-52.46073600	H	-30.72143900	-15.90762100	-40.78075300
H	-26.60336900	-18.73261300	-54.83100200	H	-33.03281100	-16.83813100	-40.75038900
H	-25.75509100	-17.50596800	-55.78524200	H	-33.39688800	-19.22731000	-40.23042800
H	-24.83783900	-18.73903600	-54.91941500	C	-29.64220800	-20.96881000	-46.54861400
H	-24.74660800	-16.57855600	-53.64902500	C	-28.32298900	-21.40624300	-46.41018600
H	-33.29568600	-16.78900600	-49.11021000	C	-27.28845800	-20.47536000	-46.27568000
H	-34.30356000	-17.65874400	-50.28138000	C	-27.54670000	-19.09989100	-46.26883500
H	-34.17572900	-18.24571700	-48.61223100	C	-28.87750600	-18.67336900	-46.39689400
H	-31.76737000	-18.82150400	-48.98386300	C	-29.91306500	-19.59715100	-46.53997600
H	-32.78721700	-19.63064200	-50.18408700	H	-30.45185700	-21.68632500	-46.64712300
H	-30.14388400	-18.54814300	-53.47381800	H	-28.09659900	-22.46891100	-46.40005700
H	-31.49153500	-17.61640400	-54.13239400	H	-26.26607300	-20.82352900	-46.16035700
H	-30.46956100	-16.91809500	-52.85041200	H	-29.12114600	-17.61449500	-46.37088100
H	-30.17053000	-13.86774400	-48.86817600	H	-30.93697500	-19.24498900	-46.62759200
H	-31.69028600	-14.72902100	-48.66492300	C	-26.40700400	-18.10604100	-46.07805300
H	-28.79046700	-13.26134700	-46.81568900	H	-25.46905100	-18.66476900	-46.09747600
H	-28.06327800	-14.00707200	-44.56441500	C	-26.49641300	-17.43533200	-44.69379300
H	-31.49684300	-16.56894600	-44.29898300	H	-25.65405000	-16.75410400	-44.53776100
H	-32.23327100	-15.81302100	-46.53661000	H	-27.42307900	-16.86985700	-44.57155200
H	-29.81652300	-16.42155800	-42.70375800	H	-26.45230900	-18.19288500	-43.90462100
H	-25.97755400	-9.84652400	-53.79982300	N	-26.37051900	-17.16952500	-47.21572100
H	-25.59872300	-8.11907300	-53.91653000	H	-25.23922500	-16.44378800	-49.47998600
H	-24.41097400	-9.26014900	-53.24786400	H	-27.21693000	-16.61757100	-47.28708000
H	-25.57815100	-7.91710200	-51.42245200	O	-26.64812000	-18.31505100	-50.64236500
H	-27.11745100	-8.57550200	-51.92467300	H	-27.24181900	-18.89461400	-50.15076200
H	-26.49349300	-10.77566000	-49.35777300	H	-26.86020900	-17.40732200	-50.36887300
H	-18.25750100	-18.38361200	-50.45931800	H	-24.51126400	-16.40676900	-46.56315200

O	-23.44588100	-14.59889700	-45.58096900
H	-22.87745500	-14.06952800	-46.15706500
C	-23.99500300	-23.95084800	-48.28391000
H	-23.88538200	-23.20883600	-49.08109300
H	-23.12060200	-24.60670300	-48.32801600
H	-24.87757800	-24.55488900	-48.52293400
C	-31.77940500	-12.63992100	-48.11094900
H	-31.13811400	-11.86486500	-47.67975200
H	-32.09996800	-12.30048800	-49.10138400
H	-32.66734400	-12.72739400	-47.47655800

TS3:

Imaginary frequency -151 cm⁻¹

C	-31.55571000	-21.11103300	-39.56535500
C	-31.30563100	-19.68982500	-40.00050500
C	-30.03424200	-19.10902000	-39.89719200
C	-32.37170800	-18.88208300	-40.42305900
C	-29.84084100	-17.75489800	-40.17665600
C	-32.18601300	-17.52841500	-40.70214000
C	-30.91953800	-16.95382400	-40.56514600
C	-24.13434400	-23.27918600	-46.91365900
C	-24.42432100	-24.26073700	-45.75876500
C	-23.28903100	-25.27609700	-45.55641800
C	-24.70602200	-23.50964400	-44.45166900
C	-24.78502100	-21.39303900	-51.86126900
C	-26.19604000	-21.48909900	-51.33661900
C	-26.59459400	-21.43634900	-50.02176100
C	-27.40588500	-21.55222300	-52.12015000
C	-28.50075300	-21.53497200	-51.21173500
C	-27.66944700	-21.59417500	-53.50118100
N	-27.97634100	-21.47898300	-49.93747000
C	-29.83044900	-21.53770600	-51.64692700
C	-28.98906800	-21.60156700	-53.93575400
C	-30.06029900	-21.56745700	-53.01738100
C	-31.55535700	-14.15870500	-48.02587900
C	-30.99619600	-14.62643500	-46.69773000
C	-31.71934200	-15.46923200	-45.84769300
C	-29.71190300	-14.23576200	-46.28686400
C	-31.18351700	-15.92892500	-44.64050600
C	-29.16358100	-14.68007000	-45.08958600
C	-29.89481000	-15.54089600	-44.26443700
O	-29.28526900	-15.97891700	-43.11767800
C	-30.93559400	-17.83619300	-53.21863100
C	-31.83904700	-18.50189100	-52.21192800
O	-32.65880100	-19.36333300	-52.52106200
N	-31.64751500	-18.09937900	-50.92397300
C	-32.42873800	-18.65651000	-49.84296200
C	-33.68849700	-17.84533500	-49.52105000
H	-30.98012800	-17.36974300	-50.72472700
C	-25.47400100	-9.01406700	-53.29974600
C	-25.74589700	-8.93063700	-51.79947600
C	-25.96627900	-10.29217000	-51.15902100
O	-25.84609700	-11.34501600	-51.76428600
O	-26.30199600	-10.19411700	-49.87273700
C	-25.65780300	-17.19396200	-53.61266400
C	-26.91251200	-16.31828300	-53.47521900
C	-25.67866300	-18.13960600	-54.81955600
C	-27.08634900	-15.27243200	-54.58193200
C	-19.03388600	-18.01802800	-49.78011500
C	-20.44662500	-18.56266100	-50.01512700
C	-21.49176200	-18.02689200	-49.02488900
C	-22.86559200	-18.69214000	-49.19762000
C	-23.90355700	-18.34301300	-48.12084900
N	-24.45473800	-16.97521500	-48.22285400
H	-18.67063400	-18.27696400	-48.77898900

N	-26.51186200	-12.59996500	-48.60715600
C	-27.11478300	-13.67122300	-49.11689400
C	-27.97822200	-13.49225600	-50.33345900
C	-26.96495800	-14.98800600	-48.53670700
O	-27.62159500	-16.00262300	-48.99732100
C	-26.04729400	-15.08875100	-47.44310400
C	-25.71573700	-16.43782100	-46.91454700
C	-25.48068400	-13.92125800	-46.87820000
C	-24.70918100	-13.91130700	-45.57252700
C	-25.74567100	-12.70864100	-47.50157900
H	-23.72804000	-16.26251200	-48.20069200
H	-25.34040200	-11.77906100	-47.10811100
H	-28.28345100	-14.46596800	-50.71692300
H	-28.88158700	-12.91971500	-50.08746100
H	-27.43132000	-12.93523800	-51.09988100
H	-24.56876800	-12.86966500	-45.25407700
H	-25.28711800	-14.41041300	-44.78756500
C	-27.93588500	-24.66499100	-41.89627300
C	-27.38284300	-23.28251300	-41.73911800
C	-26.19181200	-23.06029000	-41.03297700
C	-28.08201500	-22.16925900	-42.22460200
C	-25.71509900	-21.76777300	-40.81307900
C	-27.61472300	-20.87352300	-42.00071400
C	-26.42857000	-20.66744100	-41.29247700
C	-22.71704900	-19.76962400	-43.10278500
C	-22.30899300	-19.25678500	-44.49873200
C	-22.30414400	-20.37353500	-45.52882900
O	-23.20613900	-18.23645500	-44.96135800
H	-31.08270700	-21.53279700	-53.37863200
H	-30.65822300	-21.50049700	-50.94552300
H	-29.20443700	-21.62805300	-54.99993900
H	-26.85265400	-21.61239600	-54.21723500
H	-25.99343300	-21.39190100	-49.12411900
H	-24.06319700	-21.32056800	-51.04209800
H	-24.51482600	-22.26769200	-52.46521800
H	-24.65750200	-20.51001700	-52.49809900
H	-28.50360200	-21.40943600	-49.08011600
H	-27.97707400	-14.65866100	-54.41044200
H	-26.22520100	-14.59554800	-54.62038600
H	-27.19187000	-15.73340400	-55.57004600
H	-27.79756200	-16.96962500	-53.44292200
H	-26.87384800	-15.81229600	-52.50385200
H	-26.53183600	-18.82641200	-54.76495100
H	-25.75048400	-17.59712000	-55.76852900
H	-24.76761600	-18.74788400	-54.86329000
H	-24.77489700	-16.54127300	-53.67713500
H	-33.43711000	-16.81985200	-49.22970000
H	-34.34347500	-17.80381400	-50.39558400
H	-34.24486400	-18.30643100	-48.69734900
H	-31.78834600	-18.73640200	-48.95767400
H	-32.71266200	-19.66708500	-50.14733600
H	-30.17529400	-18.55708300	-53.53621700
H	-31.52074800	-17.56674900	-54.10090700
H	-30.43199400	-16.94473800	-52.83552500
H	-30.86812700	-14.46253900	-48.82672100
H	-32.50416400	-14.67373300	-48.21934500
H	-29.11940800	-13.58510200	-46.92318400
H	-28.16556800	-14.38164700	-44.78723400
H	-31.76097000	-16.59010800	-43.99851300
H	-32.72086300	-15.78334300	-46.13212100
H	-29.86314500	-16.60421200	-42.65448500
H	-26.31882200	-9.46692600	-53.82559900
H	-25.30030000	-8.01804700	-53.71869800
H	-24.59769200	-9.63485000	-53.50237600
H	-24.91504800	-8.44769000	-51.26914100
H	-26.62625300	-8.31408600	-51.58176400
H	-26.42439200	-11.11532800	-49.46669600

H	-18.32536800	-18.42701400	-50.50706500
H	-19.00662500	-16.92608200	-49.86951600
H	-20.42590200	-19.65889600	-49.94708300
H	-20.76728200	-18.33024700	-51.03891800
H	-21.13510300	-18.19473000	-47.99828400
H	-21.57452400	-16.93668100	-49.14379000
H	-22.72830700	-19.78184600	-49.16406700
H	-23.28016300	-18.46799800	-50.18798000
H	-23.49048300	-18.45836300	-47.11912200
H	-24.76390100	-19.00903600	-48.22544000
H	-25.54715100	-17.77027000	-52.69008300
H	-28.59254200	-24.92559600	-41.05643600
H	-28.53026900	-24.76296400	-42.80992700
H	-27.14347600	-25.41924000	-41.92846500
H	-25.63595800	-23.91123300	-40.64648400
H	-24.79011200	-21.62029500	-40.26272900
H	-26.06437800	-19.65930500	-41.11772000
H	-28.18116800	-20.02659300	-42.37370700
H	-29.00455200	-22.31721600	-42.78046500
H	-24.94426400	-22.53745000	-46.95534900
H	-23.21664100	-22.72379100	-46.68692400
H	-22.34680900	-24.76577900	-45.31963600
H	-23.51542500	-25.95185400	-44.72475500
H	-23.12061700	-25.89273000	-46.44385200
H	-25.54315400	-22.81043000	-44.55189500
H	-24.95536000	-24.20148300	-43.64131900
H	-23.82918300	-22.93496500	-44.13059600
H	-25.33205600	-24.82292900	-46.02727000
H	-22.00783200	-20.52362100	-42.74598800
H	-22.73003900	-18.94939100	-42.37668800
H	-23.71608300	-20.21505900	-43.13244700
H	-21.69080500	-21.20952400	-45.17991400
H	-23.32187300	-20.73908400	-45.68538700
H	-21.90374900	-20.03454200	-46.48762800
H	-21.29369400	-18.83597300	-44.43107500
H	-22.98044000	-17.39704600	-44.53823700
H	-30.71019800	-21.76216100	-39.80918300
H	-31.70292500	-21.16312600	-38.47971000
H	-32.45196600	-21.52493200	-40.03643500
H	-29.19108100	-19.71881600	-39.58470800
H	-28.85104200	-17.31848900	-40.07618000
H	-30.77460500	-15.89261500	-40.74563400
H	-33.03093800	-16.91782900	-41.00792400
H	-33.36377900	-19.31732600	-40.51404400
C	-30.27827300	-20.91390000	-46.55803200
C	-29.02206000	-21.52177300	-46.49044500
C	-27.87614600	-20.73937100	-46.31846200
C	-27.96532900	-19.34618700	-46.20727300
C	-29.23123700	-18.74700700	-46.26901300
C	-30.37633000	-19.52539800	-46.44340000
H	-31.17141000	-21.51730000	-46.69054600
H	-28.93190300	-22.60209300	-46.56491700
H	-26.90232600	-21.21903700	-46.25710300
H	-29.32720000	-17.66977100	-46.17688200
H	-31.34753500	-19.04126400	-46.47785500
C	-26.71275000	-18.52005400	-45.95905500
H	-25.84583900	-19.14855300	-46.19650200
C	-26.59847200	-18.12519400	-44.47527100
H	-25.66187600	-17.59441100	-44.28827100
H	-27.43875700	-17.49740000	-44.16590200
H	-26.58274000	-19.02824400	-43.85973000
N	-26.72263400	-17.33715900	-46.82930400
H	-24.97838900	-16.93354500	-49.10978000
H	-27.42685600	-17.21810600	-47.56281200
O	-26.11982400	-17.70403300	-50.38304000
H	-26.47165900	-18.60410100	-50.39826400
H	-26.83332300	-17.11927200	-50.02050500

H	-25.01074500	-16.46197700	-46.08979600
O	-23.44588200	-14.59889700	-45.58097000
H	-22.88645100	-14.14940200	-46.22929200
C	-23.99500000	-23.95085000	-48.28390800
H	-23.87113700	-23.21006600	-49.08035800
H	-23.12844800	-24.61734200	-48.32337200
H	-24.88340400	-24.54407100	-48.52797000
C	-31.77940400	-12.63992100	-48.11094800
H	-30.84475500	-12.09021700	-47.96186700
H	-32.17844500	-12.35872300	-49.09105800
H	-32.48705800	-12.30359600	-47.34616800

TS4:

Imaginary frequency -1302 cm⁻¹

C	-31.55571000	-21.11103200	-39.56535300
C	-31.30563000	-19.68982600	-40.00050600
C	-30.10896400	-19.03545100	-39.67344800
C	-32.31290800	-18.94989200	-40.63576200
C	-29.93637000	-17.67718800	-39.94309300
C	-32.14912000	-17.59048700	-40.90398500
C	-30.96380100	-16.94326500	-40.54456600
C	-24.13436500	-23.27918200	-46.91365700
C	-25.40229300	-23.65985800	-46.13171500
C	-25.48190100	-25.15883000	-45.80826900
C	-25.49113900	-22.81886200	-44.85392400
C	-24.78503900	-21.39299200	-51.86127600
C	-26.19602000	-21.48914700	-51.33661600
C	-26.57480500	-21.46808900	-50.01142300
C	-27.41570700	-21.51920900	-52.10588100
C	-28.49722000	-21.51785600	-51.17990100
C	-27.70104400	-21.52831000	-53.48312400
N	-27.95341200	-21.49692800	-49.91265100
C	-29.83318300	-21.51045100	-51.59477600
C	-29.02726800	-21.52341100	-53.89729200
C	-30.08429900	-21.50990100	-52.96218400
C	-31.59208400	-14.15396400	-47.93397200
C	-31.00897200	-14.55774300	-46.59464000
C	-31.70656700	-15.38892400	-45.71181600
C	-29.72993700	-14.12846400	-46.20625600
C	-31.14636200	-15.81105500	-44.50285900
C	-29.16136800	-14.52934900	-45.00256300
C	-29.85910400	-15.39465800	-44.15313500
O	-29.22297300	-15.80529800	-43.01237300
C	-30.93554300	-17.83617700	-53.21864400
C	-31.86776200	-18.47343300	-52.21927400
O	-32.72174000	-19.29684300	-52.53853100
N	-31.65738400	-18.09284000	-50.92869800
C	-32.42874800	-18.65650900	-49.84295600
C	-33.65853100	-17.81973500	-49.47449500
H	-30.93686100	-17.41841000	-50.72119700
C	-25.47400100	-9.01406700	-53.29974600
C	-25.37799300	-9.17880100	-51.78857800
C	-25.70810700	-10.58803600	-51.32966400
O	-25.94943900	-11.50736000	-52.09693300
O	-25.70180800	-10.69509800	-50.00416800
C	-25.65785200	-17.19398100	-53.61265500
C	-26.57280100	-16.35234000	-54.51818400
C	-24.30241600	-17.54503000	-54.23801100
C	-26.04825100	-14.94506200	-54.82592900
C	-19.03388900	-18.01802900	-49.78011400
C	-20.37363500	-18.75875600	-49.74698600
C	-21.58487800	-17.81800900	-49.71235600
C	-22.92226700	-18.56551100	-49.64148800
C	-24.12159400	-17.61951500	-49.59766900
N	-25.39678900	-18.35706100	-49.36701800

H	-18.90971100	-17.38202100	-48.89636800	H	-25.90791100	-11.65156000	-49.72755200
N	-26.08410600	-13.10550100	-48.91652100	H	-18.19291600	-18.71791900	-49.80633700
C	-26.71929600	-14.20820700	-49.30243200	H	-18.95800200	-17.37416900	-50.66343100
C	-27.36977500	-14.24125700	-50.65448400	H	-20.40570400	-19.41883200	-48.86945300
C	-26.82625100	-15.36099100	-48.44906100	H	-20.45160200	-19.41636900	-50.62293500
O	-27.44244300	-16.42625200	-48.87114200	H	-21.49805300	-17.14839700	-48.84491300
C	-26.22397700	-15.27656400	-47.14508800	H	-21.56931000	-17.17086000	-50.60027300
C	-26.37800200	-16.37420600	-46.22341700	H	-22.94334800	-19.20556500	-48.75078700
C	-25.51737600	-14.09196100	-46.79123200	H	-23.01620100	-19.23320600	-50.50787500
C	-24.71989500	-13.93616000	-45.51706800	H	-24.20390700	-17.03756700	-50.52097000
C	-25.48860100	-13.05362000	-47.70575700	H	-24.02309600	-16.91097000	-48.76951300
H	-25.60093600	-19.01923700	-50.12076600	H	-26.18201700	-18.12209900	-53.34895600
H	-24.97927400	-12.12133500	-47.47095800	H	-28.24799600	-25.07524800	-40.92766600
H	-27.14397100	-15.18414600	-51.16243900	H	-28.81219000	-24.68077100	-42.55137000
H	-28.46240200	-14.20945100	-50.55370000	H	-27.19447500	-25.35563000	-42.31163500
H	-27.03810000	-13.39740700	-51.26166500	H	-25.44649900	-23.95960800	-41.08068700
H	-24.58373900	-12.86584700	-45.30960400	H	-24.57745600	-21.69407800	-40.60982800
H	-25.22858100	-14.36709100	-44.65026500	H	-26.02409200	-19.70133000	-40.97927600
C	-27.93588800	-24.66499400	-41.89627000	H	-28.33694700	-20.00898800	-41.84024700
C	-27.38283700	-23.28251000	-41.73912500	H	-29.19369200	-22.27322000	-42.32627600
C	-26.07943200	-23.09275700	-41.25545500	H	-24.14219800	-22.19133800	-47.05265900
C	-28.18114500	-22.15140100	-41.94970200	H	-23.25348500	-23.51616100	-46.29833100
C	-25.58932900	-21.81588800	-40.98621600	H	-24.61849800	-25.47359100	-45.20827300
C	-27.69736600	-20.87000700	-41.67702600	H	-26.38536000	-25.38780500	-45.23188400
C	-26.40029900	-20.69774700	-41.19138600	H	-25.50326100	-25.77700700	-46.71091000
C	-22.71708500	-19.76964000	-43.10280000	H	-25.41746000	-21.75140800	-45.08546500
C	-22.30893700	-19.25676000	-44.49871700	H	-26.42857000	-22.98599400	-44.31713700
C	-21.78631000	-20.37740300	-45.38943300	H	-24.67499900	-23.07005700	-44.16518800
O	-23.40985400	-18.63153700	-45.18839600	H	-26.26565900	-23.40679400	-46.76690900
H	-31.11193900	-21.46834500	-53.30787300	H	-21.85589600	-20.22200100	-42.60076100
H	-30.64869600	-21.49166500	-50.87832700	H	-23.08406500	-18.94837300	-42.47875100
H	-29.25935000	-21.52700600	-54.95831000	H	-23.51020300	-20.51871800	-43.18490600
H	-26.89561100	-21.53585100	-54.21256500	H	-20.93115800	-20.87474100	-44.92135500
H	-25.96756700	-21.41659700	-49.11676400	H	-22.56439100	-21.12642300	-45.56137500
H	-24.05877700	-21.43754100	-51.04436800	H	-21.46743600	-19.98275200	-46.35884500
H	-24.54997200	-22.21329900	-52.55006400	H	-21.51209700	-18.50937500	-44.37367100
H	-24.62012100	-20.46045600	-52.41684800	H	-23.38692300	-17.67861800	-45.02901300
H	-28.46872400	-21.43971900	-49.04643800	H	-30.65832200	-21.72915900	-39.67104500
H	-26.75472600	-14.39509200	-55.45591000	H	-31.85132500	-21.14451400	-38.50980100
H	-25.90315000	-14.35989700	-53.91100800	H	-32.35893300	-21.57493400	-40.14497700
H	-25.09220900	-14.97324900	-55.35924100	H	-29.31267600	-19.59267500	-39.18751200
H	-26.73896100	-16.89719000	-55.45793800	H	-29.00851200	-17.18487800	-39.66603300
H	-27.55711100	-16.26966300	-54.03976300	H	-30.84671400	-15.87640200	-40.71295700
H	-24.43485300	-18.08903200	-55.18031900	H	-32.95411500	-17.03129100	-41.37278500
H	-23.70842900	-16.65123200	-54.45307700	H	-33.24624500	-19.44038900	-40.90031900
H	-23.70734600	-18.18100900	-53.57249300	C	-30.96088900	-20.76073600	-46.50837200
H	-25.49619600	-16.64991700	-52.67039000	C	-29.76019000	-21.46055400	-46.35263200
H	-33.37332000	-16.80839000	-49.16505000	C	-28.56320400	-20.76857700	-46.16629600
H	-34.33189200	-17.73955200	-50.33229700	C	-28.53365000	-19.36112200	-46.12902600
H	-34.20915500	-18.28570100	-48.64954700	C	-29.74556500	-18.67271600	-46.29579200
H	-31.77147000	-18.77614000	-48.97708100	C	-30.94481000	-19.36598700	-46.47540700
H	-32.74768600	-19.65135900	-50.16470200	H	-31.89515700	-21.29703800	-46.64637200
H	-30.16014600	-18.56141200	-53.48627600	H	-29.75652500	-22.54734400	-46.37140700
H	-31.49349900	-17.59800200	-54.12663700	H	-27.63508300	-21.31783000	-46.04170000
H	-30.45121500	-16.92907100	-52.84571300	H	-29.75966500	-17.58851300	-46.25603500
H	-30.93969100	-14.52596000	-48.73618300	H	-31.87196600	-18.80759500	-46.56960700
H	-32.55806800	-14.65481400	-48.06986800	C	-27.22869300	-18.66512600	-45.87482800
H	-29.15625500	-13.48273700	-46.86558700	H	-26.22167000	-19.33965200	-46.57852100
H	-28.16802500	-14.20104700	-44.71693400	C	-26.77969500	-18.64744100	-44.42018900
H	-31.69866700	-16.47793500	-43.84569300	H	-25.70914600	-18.43742600	-44.32628300
H	-32.70501200	-15.72951200	-45.97586100	H	-27.33988200	-17.90331100	-43.83202200
H	-29.77154900	-16.45557100	-42.54783500	H	-26.95022900	-19.62752800	-43.97378200
H	-26.48528000	-9.23228500	-53.65339400	N	-27.13652500	-17.40642900	-46.51658200
H	-25.21778800	-7.99268900	-53.59814600	H	-26.19624100	-17.68945200	-49.29379300
H	-24.79821600	-9.70435000	-53.81102800	H	-27.55898900	-17.28722900	-47.46998400
H	-24.37195300	-8.93939700	-51.42112000	O	-25.25951000	-19.74883700	-47.22003200
H	-26.05113400	-8.49174300	-51.26186300	H	-24.51687000	-19.48073400	-46.64843500

H	-25.32257300	-18.96547700	-48.39324700
H	-25.86458000	-16.37496600	-45.26920300
O	-23.44588700	-14.59890100	-45.58097200
H	-23.01070700	-14.27885400	-46.38298800
C	-23.99499100	-23.95085600	-48.28390500
H	-23.10492900	-23.58812900	-48.80997100
H	-23.90075300	-25.03861700	-48.20293400
H	-24.86210600	-23.73968800	-48.91956100
C	-31.77940200	-12.63992200	-48.11094800
H	-30.82793800	-12.10600500	-48.02522300
H	-32.20008000	-12.41141200	-49.09561900
H	-32.45539000	-12.23653400	-47.35011500

TS5:

Imaginary frequency -443 cm⁻¹

C	-31.55571400	-21.11103700	-39.56535000
C	-31.30562700	-19.68982000	-40.00050900
C	-30.28148600	-18.93102000	-39.41225000
C	-32.13531700	-19.06563600	-40.94098300
C	-30.10836600	-17.58568900	-39.73546500
C	-31.96881700	-17.71790600	-41.26661900
C	-30.96158000	-16.96815100	-40.65528600
C	-24.13433200	-23.27915200	-46.91363200
C	-25.42493400	-23.65432100	-46.16222200
C	-25.47439500	-25.14012500	-45.77676000
C	-25.59829600	-22.76732100	-44.92683800
C	-24.78501800	-21.39301800	-51.86127000
C	-26.19603400	-21.48913800	-51.33661600
C	-26.59389700	-21.51467900	-50.02368100
C	-27.39832600	-21.55130000	-52.12827300
C	-28.49394000	-21.61603400	-51.22268700
C	-27.65826700	-21.53620300	-53.51015500
N	-27.97062300	-21.61418800	-49.94740800
C	-29.82162700	-21.64385200	-51.66337500
C	-28.97678700	-21.56205000	-53.95003800
C	-30.04943200	-21.60902500	-53.03473500
C	-30.55005700	-13.56256500	-48.07207600
C	-30.20407400	-14.05621000	-46.68317700
C	-30.68125500	-15.28201200	-46.20557200
C	-29.39731700	-13.29380600	-45.82596500
C	-30.35769700	-15.74583200	-44.92997700
C	-29.06426300	-13.73891700	-44.54969000
C	-29.53702400	-14.97559600	-44.10294000
O	-29.14193200	-15.39332300	-42.85422600
C	-30.93557400	-17.83618200	-53.21865100
C	-31.81779800	-18.51602100	-52.20224100
O	-32.62371100	-19.39424400	-52.49976400
N	-31.63133900	-18.10451400	-50.91714400
C	-32.42874200	-18.65651500	-49.84294700
C	-33.83497000	-18.05165900	-49.75589400
H	-30.98787000	-17.35321900	-50.72215600
C	-25.47400100	-9.01406700	-53.29974600
C	-25.51137900	-9.15505300	-51.78391600
C	-25.82288000	-10.57225600	-51.33068300
O	-26.07913300	-11.48352500	-52.10321900
O	-25.78809400	-10.68909700	-50.00919200
C	-25.65782500	-17.19396100	-53.61265900
C	-27.05590000	-17.35261500	-54.23072100
C	-24.51962600	-17.77047200	-54.46329000
C	-27.25553600	-16.59720400	-55.54926800
C	-19.03388700	-18.01802900	-49.78011500
C	-20.46185300	-18.25287400	-50.28500800
C	-21.52249100	-17.48800000	-49.48095400
C	-22.95455000	-17.72015100	-49.98816000
C	-24.02296000	-16.90036600	-49.26715700

N	-24.16830900	-17.30545700	-47.82933800
H	-18.92187200	-18.33796900	-48.73777500
N	-26.09880000	-13.05579400	-48.90001300
C	-26.77454200	-14.18248700	-49.17859100
C	-27.42750100	-14.31336500	-50.52604700
C	-26.87677400	-15.24710900	-48.24219400
O	-27.49571800	-16.36557400	-48.54389500
C	-26.24178400	-15.08411600	-46.95882000
C	-26.37389700	-16.12394200	-45.97477300
C	-25.48097500	-13.90496100	-46.73359500
C	-24.61722700	-13.74916600	-45.51451000
C	-25.46216500	-12.93272800	-47.72234500
H	-24.58021800	-18.26861200	-47.71521500
H	-24.91671100	-12.00194100	-47.57371800
H	-27.15836000	-15.26847500	-50.99114800
H	-28.52018500	-14.32340400	-50.42921100
H	-27.12938100	-13.48948800	-51.17749300
H	-24.31625500	-12.70031600	-45.39344900
H	-25.13406500	-14.04733300	-44.59787100
C	-27.93589200	-24.66499900	-41.89626200
C	-27.38283200	-23.28250400	-41.73914100
C	-26.03036600	-23.08894200	-41.42015600
C	-28.22609500	-22.16358700	-41.74137800
C	-25.53666100	-21.82191500	-41.11175100
C	-27.73967100	-20.89257100	-41.42517200
C	-26.39187200	-20.71785000	-41.10761100
C	-22.71706300	-19.76962400	-43.10279400
C	-22.30898300	-19.25680300	-44.49872800
C	-21.78598200	-20.35970600	-45.40548400
O	-23.42318700	-18.63743100	-45.18678100
H	-31.07165900	-21.59003700	-53.39749300
H	-30.65273300	-21.67884000	-50.96537600
H	-29.18932600	-21.54454300	-55.01513900
H	-26.83982400	-21.49949400	-54.22440700
H	-25.99884400	-21.44646100	-49.12336600
H	-24.06113600	-21.36524600	-51.04053200
H	-24.52875600	-22.25049600	-52.49547900
H	-24.63957300	-20.49154900	-52.46979300
H	-28.50498500	-21.55627100	-49.09346200
H	-28.28348200	-16.70460300	-55.91074900
H	-27.05755300	-15.52621600	-55.42525400
H	-26.59301200	-16.96802300	-56.33821300
H	-27.26506600	-18.42072200	-54.37869600
H	-27.79636600	-16.99896500	-53.50268200
H	-24.68072100	-18.83537400	-54.66908200
H	-24.43137500	-17.25817800	-55.42654900
H	-23.55313000	-17.67333200	-53.95553900
H	-25.46765700	-16.12868400	-53.42235100
H	-33.78957500	-16.97062900	-49.58675400
H	-34.37857200	-18.23736000	-50.68510800
H	-34.39600700	-18.50304700	-48.93046500
H	-31.89199100	-18.49589800	-48.90385200
H	-32.50881400	-19.73549400	-50.00658200
H	-30.15892500	-18.53977400	-53.53495000
H	-31.53324000	-17.58767600	-54.09869600
H	-30.45400800	-16.92894100	-52.84378700
H	-29.68786800	-13.03040500	-48.48988700
H	-30.72362700	-14.42535300	-48.72636700
H	-29.00443100	-12.34106500	-46.17188700
H	-28.42978600	-13.14986600	-43.89518400
H	-30.72046400	-16.71338300	-44.59052200
H	-31.30558500	-15.89970700	-46.84670200
H	-29.56846600	-16.23785100	-42.64962000
H	-26.42812900	-9.31214400	-53.74179500
H	-25.26393000	-7.98024800	-53.59203900
H	-24.70409300	-9.65780400	-53.73398900
H	-24.56008900	-8.85859700	-51.32554100

H	-26.26676800	-8.49533300	-51.33840400
H	-25.98023200	-11.65723700	-49.72756800
H	-18.30702800	-18.57616900	-50.37770400
H	-18.76316100	-16.95767400	-49.83250600
H	-20.69169700	-19.32603600	-50.25540700
H	-20.53206300	-17.95610100	-51.33945400
H	-21.43481900	-17.78673300	-48.42449200
H	-21.29690000	-16.41269400	-49.51419800
H	-23.21091200	-18.78625000	-49.93373400
H	-23.01128000	-17.44935300	-51.04906300
H	-25.01381700	-17.03083800	-49.70696200
H	-23.78859600	-15.83278300	-49.27794000
H	-25.65618500	-17.68825100	-52.63167900
H	-28.12591100	-25.12074800	-40.91663800
H	-28.88425100	-24.66608000	-42.44213500
H	-27.24242900	-25.32527600	-42.42746500
H	-25.36173400	-23.94613100	-41.40012100
H	-24.48732200	-21.69960700	-40.85797000
H	-26.01433700	-19.73240300	-40.85094100
H	-28.42022300	-20.04694200	-41.40539300
H	-29.28128300	-22.29073000	-41.97043600
H	-24.12250700	-22.19145100	-47.05188100
H	-23.26701600	-23.53096100	-46.28494700
H	-24.64071600	-25.39732000	-45.11068200
H	-26.40519200	-25.37705400	-45.24951900
H	-25.41714600	-25.79660600	-46.64998600
H	-25.60695800	-21.70908900	-45.20494700
H	-26.53335400	-22.97733800	-44.40196500
H	-24.78166800	-22.92421300	-44.21122500
H	-26.26914600	-23.45331900	-46.83896200
H	-21.85258000	-20.21187700	-42.59830900
H	-23.08622100	-18.94948800	-42.47722400
H	-23.50376500	-20.52581900	-43.18173500
H	-20.89070800	-20.81173100	-44.96920100
H	-22.53396000	-21.14584500	-45.54114600
H	-21.52065400	-19.96147700	-46.38951100
H	-21.52646600	-18.49374200	-44.37655600
H	-23.74424600	-17.89289700	-44.65683100
H	-30.62167200	-21.67521300	-39.47357100
H	-32.04723200	-21.13866600	-38.58533000
H	-32.20332500	-21.63960700	-40.27065900
H	-29.62453000	-19.39862800	-38.68296200
H	-29.31802600	-17.01219400	-39.25949200
H	-30.84465200	-15.91298900	-40.88326300
H	-32.63566000	-17.24999000	-41.98543800
H	-32.93145800	-19.63738600	-41.41098400
C	-30.08422300	-21.32213800	-46.93072800
C	-29.45707100	-21.43586800	-45.68735000
C	-28.63440000	-20.42253100	-45.20823700
C	-28.39811800	-19.23653000	-45.95252300
C	-29.04232500	-19.14076400	-47.21582400
C	-29.86374000	-20.16215400	-47.68272900
H	-30.73503400	-22.10852200	-47.30057400
H	-29.60604600	-22.32517200	-45.08086900
H	-28.15711900	-20.56440100	-44.24632000
H	-28.92294500	-18.25154600	-47.82544800
H	-30.34071500	-20.04564900	-48.65024600
C	-27.53312100	-18.18078700	-45.44382900
H	-24.80310300	-16.66374700	-47.31157700
C	-27.03214200	-18.13048300	-44.03041000
H	-25.93514100	-18.23173900	-43.97577300
H	-27.28071400	-17.16449500	-43.56843100
H	-27.45376300	-18.91614700	-43.40761700
N	-27.17543700	-17.17693200	-46.25260600
H	-23.28536200	-17.30693000	-47.31435500
H	-27.48455300	-17.02524700	-47.34845600
O	-25.16241900	-19.74820100	-47.07949900

H	-26.10625800	-19.67351700	-46.85976900
H	-24.69227300	-19.62600400	-46.23122000
H	-25.96092400	-16.01395100	-44.98005600
O	-23.44588200	-14.59889800	-45.58097000
H	-22.91894800	-14.25391300	-46.31469100
C	-23.99501500	-23.95086000	-48.28392200
H	-23.08858600	-23.61408200	-48.79908900
H	-23.93320100	-25.04069200	-48.20289500
H	-24.84766700	-23.71227100	-48.92847500
C	-31.77940400	-12.63992000	-48.11094800
H	-31.62351800	-11.75326900	-47.48763300
H	-31.98594600	-12.30264000	-49.13219500
H	-32.67065000	-13.15404000	-47.73562600

TS6:

Imaginary frequency -1133 cm⁻¹

C	-31.55571400	-21.11103900	-39.56534900
C	-31.30562700	-19.68981800	-40.00051000
C	-30.25811700	-18.94215200	-39.43988200
C	-32.14393900	-19.06011200	-40.92971900
C	-30.06748900	-17.60382200	-39.78249100
C	-31.95950600	-17.71969800	-41.27523300
C	-30.92542600	-16.98208600	-40.69527700
C	-24.13432700	-23.27915000	-46.91362900
C	-25.42607400	-23.64825100	-46.16253200
C	-25.50716800	-25.14184400	-45.81426000
C	-25.56615600	-22.78920600	-44.90341000
C	-24.78501700	-21.39301700	-51.86127000
C	-26.19603400	-21.48914000	-51.33661600
C	-26.59174600	-21.46781400	-50.02274800
C	-27.40083100	-21.55585600	-52.12436600
C	-28.49683600	-21.57484400	-51.21670200
C	-27.66244600	-21.57641500	-53.50578900
N	-27.97173700	-21.53760300	-49.94233500
C	-29.82483800	-21.59652400	-51.65563500
C	-28.98162800	-21.59634300	-53.94418100
C	-30.05383300	-21.60100200	-53.02745200
C	-30.39524400	-13.29790700	-47.99625600
C	-30.07112700	-13.83143400	-46.61609100
C	-30.53055200	-15.08624000	-46.19757400
C	-29.29120300	-13.09276300	-45.71547600
C	-30.21351400	-15.59918300	-44.94004700
C	-28.96329700	-13.58764500	-44.45556500
C	-29.41528500	-14.85193900	-44.06939100
O	-29.02694400	-15.31620700	-42.83626600
C	-30.93557400	-17.83618200	-53.21865100
C	-31.81747100	-18.51671100	-52.20248200
O	-32.60971000	-19.40860200	-52.49475100
N	-31.64392700	-18.09154300	-50.91944200
C	-32.42874200	-18.65651400	-49.84294800
C	-33.84849500	-18.08420600	-49.75562600
H	-31.01888000	-17.32385000	-50.72939100
C	-25.47400100	-9.01406700	-53.29974600
C	-25.57628200	-9.00502500	-51.77972300
C	-25.78435100	-10.39577600	-51.20599000
O	-25.73198600	-11.41085600	-51.88465300
O	-26.02522600	-10.37347000	-49.90001500
C	-25.65782500	-17.19396100	-53.61265900
C	-27.06156300	-17.35233200	-54.21793900
C	-24.53051400	-17.79279300	-54.46206700
C	-27.26595600	-16.61665700	-55.54692300
C	-19.03388600	-18.01802900	-49.78011500
C	-20.43835500	-18.02299300	-50.38823400
C	-21.48294400	-17.37822200	-49.47045800
C	-22.90869700	-17.42432300	-50.03331500

C	-23.95187400	-16.73700000	-49.14752200	H	-24.67029100	-8.58932500	-51.31972400
N	-24.08998200	-17.35471300	-47.80510200	H	-26.39890600	-8.37035300	-51.42990600
H	-19.00901700	-18.57238200	-48.83483800	H	-26.14235500	-11.32858900	-49.55096800
N	-26.23066900	-12.75699100	-48.74477600	H	-18.30511000	-18.47982900	-50.45347000
C	-26.88259100	-13.86676600	-49.14097000	H	-18.69367600	-16.99696100	-49.57362400
C	-27.55727000	-13.85225200	-50.48539500	H	-20.74031500	-19.05511600	-50.60992300
C	-26.91015200	-15.01026800	-48.33061900	H	-20.42745000	-17.49546800	-51.35090900
O	-27.57166700	-16.10629800	-48.79140700	H	-21.44834200	-17.88986600	-48.49713900
C	-26.21141200	-15.04317500	-47.09776600	H	-21.20015300	-16.33301700	-49.27722100
C	-26.11197700	-16.27433300	-46.30425900	H	-23.20817600	-18.46706800	-50.20452800
C	-25.49963200	-13.87081900	-46.73647600	H	-22.93197300	-16.93343100	-51.01445100
C	-24.64363500	-13.79684900	-45.49803100	H	-24.94091500	-16.77386600	-49.61122100
C	-25.56735700	-12.76879300	-47.58282900	H	-23.70129000	-15.68218900	-48.99911700
H	-24.37639400	-18.34550100	-47.85506300	H	-25.65114200	-17.67069300	-52.62360500
H	-25.05639300	-11.84369300	-47.31906100	H	-28.08986600	-25.13681300	-40.91797400
H	-27.55426700	-14.85183800	-50.92642400	H	-28.90228600	-24.66188100	-42.40931700
H	-28.60574000	-13.54334300	-50.39500500	H	-27.25856000	-25.31429000	-42.46106400
H	-27.04617000	-13.15052300	-51.14793200	H	-25.36798300	-23.94782800	-41.36570500
H	-24.38224300	-12.74910800	-45.29490200	H	-24.48974000	-21.69525300	-40.85866900
H	-25.17719000	-14.17411700	-44.62033000	H	-26.00564300	-19.72091300	-40.91043400
C	-27.93589000	-24.66499400	-41.89626700	H	-28.40873900	-20.03600000	-41.48005400
C	-27.38283300	-23.28250900	-41.73913400	H	-29.27426900	-22.28716100	-42.00794200
C	-26.03311800	-23.08877600	-41.40791700	H	-24.11823300	-22.19298400	-47.04976800
C	-28.22086900	-22.16031500	-41.77038600	H	-23.26962000	-23.53964400	-46.28434600
C	-25.53703900	-21.81826600	-41.11994600	H	-24.66940900	-25.43749700	-45.16958900
C	-27.73155900	-20.88465900	-41.47597200	H	-26.43476600	-25.36920400	-45.27669700
C	-26.38638000	-20.70959500	-41.14933900	H	-25.48153400	-25.77686700	-46.70465200
C	-22.71705900	-19.76962100	-43.10278900	H	-25.54909300	-21.72534000	-45.15734300
C	-22.30899100	-19.25681000	-44.49873500	H	-26.50017200	-22.99123400	-44.37309100
C	-21.75287300	-20.35545700	-45.39166400	H	-24.74605000	-22.98510300	-44.20148400
O	-23.43652700	-18.67760600	-45.19308200	H	-26.27096800	-23.41042600	-46.82655100
H	-31.07625100	-21.57944900	-53.38938100	H	-21.84872000	-20.18679300	-42.58322000
H	-30.65601200	-21.59662900	-50.95668300	H	-23.11547000	-18.95457100	-42.48859200
H	-29.19480900	-21.60712700	-55.00924600	H	-23.48324500	-20.54597200	-43.18703600
H	-26.84414600	-21.57233000	-54.22102000	H	-20.85498300	-20.78856600	-44.94146600
H	-25.99257000	-21.38341200	-49.12637400	H	-22.48523100	-21.15572700	-45.53104800
H	-24.06323800	-21.35156600	-51.03976700	H	-21.48499000	-19.95806900	-46.37503800
H	-24.52313300	-22.25527000	-52.48664600	H	-21.54633400	-18.47368100	-44.37856000
H	-24.64523400	-20.49648700	-52.47809200	H	-23.72060900	-17.87960200	-44.72510900
H	-28.50431900	-21.46940300	-49.08884300	H	-30.62758300	-21.69163000	-39.53587400
H	-28.19471300	-16.72204300	-55.90003500	H	-31.98786700	-21.14303800	-38.55791900
H	-27.05869200	-15.54530300	-55.44171900	H	-32.25284800	-21.61983500	-40.23702200
H	-26.61138100	-17.00472800	-56.33407100	H	-29.59376800	-19.41341000	-38.71974200
H	-27.27884300	-18.42119400	-54.34825200	H	-29.25811400	-17.03928700	-39.32820800
H	-27.79500900	-16.98246100	-53.49034700	H	-30.79256600	-15.93232400	-40.93957700
H	-24.70275600	-18.85906000	-54.65138000	H	-32.63190400	-17.24845100	-41.98666800
H	-24.44321200	-17.29558800	-55.43342700	H	-32.95871200	-19.62305100	-41.37801600
H	-23.56147900	-17.69737400	-53.95987000	C	-30.06535600	-21.35492100	-46.68889500
H	-25.45781900	-16.12717400	-53.44148900	C	-29.30753600	-21.42720100	-45.52130100
H	-33.82782700	-17.00174300	-49.59144500	C	-28.47804900	-20.36940000	-45.15150100
H	-34.38829100	-18.28690300	-50.68338800	C	-28.37458800	-19.20513200	-45.94002100
H	-34.39784600	-18.54489400	-48.92751300	C	-29.14873200	-19.14765700	-47.11797000
H	-31.89518900	-18.47830900	-48.90456400	C	-29.97915100	-20.20481200	-47.48217000
H	-32.48462600	-19.73772100	-50.00307600	H	-30.71731400	-22.17400200	-46.97747100
H	-30.14673000	-18.53324300	-53.51869000	H	-29.35263800	-22.31088200	-44.89167900
H	-31.52759100	-17.60632400	-54.10748000	H	-27.88947400	-20.47139300	-44.24806200
H	-30.46970400	-16.91825600	-52.84995800	H	-29.10625200	-18.25883700	-47.73714600
H	-29.62836900	-12.57137600	-48.28645500	H	-30.56857700	-20.12974300	-48.38960800
H	-30.32541400	-14.11985200	-48.71920000	C	-27.45080100	-18.10389700	-45.56468600
H	-28.91546300	-12.11732500	-46.01347400	H	-24.98380400	-16.83598800	-47.08164700
H	-28.35021700	-13.01468800	-43.76726600	C	-26.93014900	-18.02057200	-44.14530400
H	-30.56533600	-16.58571300	-44.64644900	H	-25.89643100	-18.38144000	-44.05965600
H	-31.13596100	-15.68683100	-46.87253300	H	-26.94891800	-16.98123700	-43.80012000
H	-29.43715100	-16.17743400	-42.67314400	H	-27.53316100	-18.60942400	-43.45452400
H	-26.39256400	-9.39868300	-53.75137400	N	-27.10154600	-17.24896300	-46.47977500
H	-25.29749400	-8.00524400	-53.68622900	H	-23.22928100	-17.32379000	-47.26123300
H	-24.65777700	-9.66112900	-53.63008500	H	-27.54903600	-16.77318900	-48.04858400

O	-25.10096300	-19.92981500	-47.13397000
H	-26.03222600	-19.71297400	-46.97855500
H	-24.64680700	-19.69753500	-46.30190700
H	-25.73524300	-16.12421800	-45.29034700
O	-23.44588200	-14.59889800	-45.58097000
H	-22.94515100	-14.25278700	-46.33229000
C	-23.99501700	-23.95085800	-48.28392400
H	-23.08956000	-23.61131300	-48.79890300
H	-23.93148500	-25.04088600	-48.20522900
H	-24.84790200	-23.71205200	-48.92856400
C	-31.77940400	-12.63992000	-48.11094800
H	-31.86693500	-11.78713300	-47.42973100
H	-31.95831700	-12.27921600	-49.12934500
H	-32.57703100	-13.34656400	-47.85745400

TS7:

Imaginary frequency -902 cm⁻¹

C	-31.55573400	-21.11103800	-39.56532800
C	-31.30561900	-19.68981700	-40.00052500
C	-30.19779100	-18.97577000	-39.51719400
C	-32.20644500	-19.02404600	-40.84124900
C	-30.00703400	-17.63520300	-39.84916500
C	-32.02385500	-17.67938000	-41.17401300
C	-30.92683900	-16.97582200	-40.67130100
C	-24.13432600	-23.27913300	-46.91361800
C	-25.39930500	-23.69783200	-46.14098900
C	-25.33943500	-25.15553900	-45.66217900
C	-25.65090700	-22.73915200	-44.97367100
C	-24.78502000	-21.39305400	-51.86127100
C	-26.19603600	-21.48908500	-51.33660900
C	-26.60350000	-21.62310700	-50.03056900
C	-27.39359500	-21.50226700	-52.13945900
C	-28.49429100	-21.65020200	-51.25206900
C	-27.63893800	-21.39715200	-53.51979600
N	-27.98028400	-21.74223300	-49.97564800
C	-29.81781200	-21.66777600	-51.70645100
C	-28.95214100	-21.41831200	-53.97373600
C	-30.03211300	-21.54555700	-53.07460200
C	-31.34554900	-14.11376800	-48.16068900
C	-30.83281700	-14.65729300	-46.84182900
C	-31.48170900	-15.70343400	-46.17874000
C	-29.66958100	-14.13711800	-46.25229600
C	-30.98691100	-16.23421300	-44.98444700
C	-29.17000000	-14.64458100	-45.05837400
C	-29.82081400	-15.70817000	-44.42573000
O	-29.25752400	-16.19772500	-43.27324400
C	-30.93556800	-17.83618600	-53.21864400
C	-31.79816500	-18.53345900	-52.19749600
O	-32.58099400	-19.43438800	-52.48939400
N	-31.61984100	-18.11324000	-50.91319400
C	-32.42874100	-18.65652100	-49.84295200
C	-33.84035800	-18.06067400	-49.78310500
H	-31.02394700	-17.32112600	-50.72707200
C	-25.47400100	-9.01406700	-53.29974600
C	-25.68428700	-9.08836900	-51.79289800
C	-25.98750400	-10.49890400	-51.31618400
O	-26.18126000	-11.43433300	-52.07759500
O	-26.02471300	-10.58338800	-49.99141800
C	-25.65783100	-17.19396200	-53.61265900
C	-26.92899900	-17.24031100	-54.47548100
C	-24.40728500	-17.75965700	-54.29587800
C	-26.86575600	-16.38164100	-55.74350400
C	-19.03389000	-18.01802900	-49.78011600
C	-20.32612500	-18.78225300	-49.46492300
C	-21.58140600	-17.89968500	-49.50924800

C	-22.88087500	-18.64945000	-49.17679600
C	-24.10727500	-17.74219600	-49.27346500
N	-25.38371000	-18.43259200	-48.95136000
H	-18.87112500	-17.20325200	-49.06566800
N	-26.20449400	-12.99235700	-48.90542400
C	-26.77684600	-14.14619900	-49.25041200
C	-27.47104700	-14.23959900	-50.57877800
C	-26.74163500	-15.30591000	-48.40264300
O	-27.29432300	-16.41928200	-48.81529600
C	-26.08936000	-15.15934100	-47.14285400
C	-26.03040200	-16.29835100	-46.14305000
C	-25.45372500	-13.93951300	-46.83177900
C	-24.61294600	-13.75570900	-45.59094300
C	-25.54224700	-12.89174600	-47.74028800
H	-25.58272300	-19.16461700	-49.63701400
H	-25.07415800	-11.93095300	-47.53716900
H	-27.18003500	-15.16375700	-51.08808700
H	-28.55915500	-14.30108700	-50.44412800
H	-27.22980200	-13.37646300	-51.20143900
H	-24.32222400	-12.70001600	-45.49954600
H	-25.15799000	-14.01852000	-44.67820100
C	-27.93592500	-24.66502400	-41.89619800
C	-27.38279100	-23.28249400	-41.73923600
C	-26.04074100	-23.09012800	-41.37971600
C	-28.21236000	-22.15582500	-41.81698200
C	-25.54313500	-21.81673200	-41.10593300
C	-27.72096000	-20.87726200	-41.54143600
C	-26.38311300	-20.70378800	-41.18280600
C	-22.71705900	-19.76961700	-43.10284100
C	-22.30897900	-19.25681200	-44.49868200
C	-21.92873800	-20.39924300	-45.43027700
O	-23.36166600	-18.50634600	-45.13305700
H	-31.05076600	-21.51821400	-53.44605000
H	-30.65472400	-21.76648000	-51.02176200
H	-29.15542300	-21.33447100	-55.03732200
H	-26.81430000	-21.29728900	-54.22037200
H	-26.01971900	-21.65487000	-49.12115800
H	-24.05436800	-21.44158000	-51.04794900
H	-24.56057700	-22.21579500	-52.55061800
H	-24.61689100	-20.46070900	-52.41330700
H	-28.52037500	-21.73638800	-49.12453500
H	-27.81617400	-16.41189200	-56.28636500
H	-26.65579000	-15.33399900	-55.49940100
H	-26.08619800	-16.72466100	-56.43162500
H	-27.14398400	-18.28385200	-54.74411700
H	-27.77537100	-16.90689500	-53.86226700
H	-24.56311700	-18.79901200	-54.60967800
H	-24.13398800	-17.18514200	-55.18660200
H	-23.54389000	-17.74187900	-53.62155600
H	-25.46804900	-16.15575800	-53.30805800
H	-33.80409000	-16.97730600	-49.62554300
H	-34.37082200	-18.25967200	-50.71720700
H	-34.41041600	-18.50578700	-48.96034200
H	-31.90667100	-18.47882400	-48.89884300
H	-32.49897600	-19.73762900	-49.99578900
H	-30.13979800	-18.51870900	-53.53364600
H	-31.54087100	-17.60873200	-54.09910400
H	-30.47791000	-16.91432800	-52.84933300
H	-30.56262000	-14.22551600	-48.92280500
H	-32.19032300	-14.72773500	-48.49665400
H	-29.13207700	-13.33070700	-46.74365200
H	-28.26808000	-14.23952700	-44.61170900
H	-31.49771200	-17.06303000	-44.49947300
H	-32.38827300	-16.12583000	-46.60618400
H	-29.85021500	-16.85040500	-42.87218700
H	-26.34973100	-9.39258800	-53.83252200
H	-25.28981100	-7.98341500	-53.61941700

H	-24.62131300	-9.62613000	-53.60682500
H	-24.80967300	-8.72545300	-51.24050700
H	-26.51764500	-8.44885800	-51.47389400
H	-26.17854500	-11.55337700	-49.70363800
H	-18.16137100	-18.67743700	-49.73789400
H	-19.06933600	-17.57608900	-50.78204900
H	-20.24238800	-19.24432200	-48.47168100
H	-20.44385600	-19.61150400	-50.17509000
H	-21.45860800	-17.06184400	-48.80824300
H	-21.66793900	-17.44793100	-50.50738700
H	-22.82283700	-19.06454000	-48.16343400
H	-22.99932400	-19.49940700	-49.86255700
H	-24.17661200	-17.30494400	-50.27721000
H	-24.01315600	-16.90616300	-48.57298200
H	-25.84661100	-17.75453000	-52.68719200
H	-28.15811600	-25.11092300	-40.91868700
H	-28.86619300	-24.66933000	-42.47224400
H	-27.22773300	-25.33204600	-42.39851100
H	-25.38208700	-23.95194500	-41.30505400
H	-24.50143900	-21.69421500	-40.82330000
H	-26.00079300	-19.71206600	-40.96021500
H	-28.38788300	-20.02196400	-41.58896200
H	-29.26021400	-22.28252900	-42.07928500
H	-24.16643800	-22.19112800	-47.05617200
H	-23.24647900	-23.48763100	-46.29989000
H	-24.50604100	-25.30065300	-44.96306300
H	-26.26176600	-25.43561500	-45.14105600
H	-25.20489200	-25.85871400	-46.49007800
H	-25.72743100	-21.70918800	-45.33547900
H	-26.57519100	-22.98371000	-44.44302800
H	-24.83548700	-22.78915600	-44.24130400
H	-26.24967500	-23.60651200	-46.83437100
H	-21.88496000	-20.31227000	-42.64329400
H	-22.98648300	-18.93825900	-42.44288500
H	-23.57613200	-20.44304100	-43.17735400
H	-21.12511000	-20.99788400	-44.99068800
H	-22.78592200	-21.05533500	-45.60220900
H	-21.58466300	-20.01827200	-46.39541300
H	-21.43934700	-18.59380900	-44.38408300
H	-23.30216400	-17.57748800	-44.87057800
H	-30.64368000	-21.71482200	-39.62095500
H	-31.90292500	-21.14683300	-38.52578100
H	-32.31972000	-21.59176000	-40.18276100
H	-29.48465900	-19.47605700	-38.86692700
H	-29.14798000	-17.09790400	-39.45790200
H	-30.78837000	-15.92632400	-40.91199400
H	-32.74667600	-17.17738700	-41.81126500
H	-33.07035700	-19.55980800	-41.22640600
C	-30.33522500	-21.09615100	-46.95369600
C	-29.75895700	-21.20641900	-45.68917700
C	-28.71104000	-20.36403500	-45.31832300
C	-28.22035100	-19.38971200	-46.19965800
C	-28.80882800	-19.28263200	-47.46876800
C	-29.85254100	-20.12984500	-47.84017300
H	-31.15249100	-21.74941300	-47.24569700
H	-30.12070400	-21.95031600	-44.98554400
H	-28.28128200	-20.47966000	-44.33146500
H	-28.46651100	-18.53967200	-48.18227200
H	-30.28351400	-20.03086600	-48.83005000
C	-27.08677400	-18.48243700	-45.79739400
H	-25.06408300	-16.81730200	-46.22920000
C	-26.59447600	-18.57114300	-44.36967400
H	-25.65135900	-18.04304500	-44.24489900
H	-27.34373100	-18.09838500	-43.72516800
H	-26.43811100	-19.60045200	-44.05426100
N	-27.12161000	-17.25190000	-46.33508800
H	-25.48358500	-18.93929800	-47.77482900

H	-27.52598900	-17.12675900	-47.27943300
O	-25.67749900	-19.42345500	-46.64590500
H	-26.15305000	-17.71998400	-49.00988000
H	-24.88400900	-19.22328800	-46.11341100
H	-26.07268000	-15.89581900	-45.12573100
O	-23.44588300	-14.59889900	-45.58097000
H	-22.98685800	-14.43347500	-46.41601300
C	-23.99501900	-23.95086900	-48.28392000
H	-23.10660400	-23.59116100	-48.81467900
H	-23.90033500	-25.03832300	-48.19851600
H	-24.86450900	-23.74498500	-48.91675300
C	-31.77940200	-12.63992300	-48.11094600
H	-30.94950600	-11.99095200	-47.81483100
H	-32.13076500	-12.30311700	-49.09171000
H	-32.58969400	-12.49324900	-47.38929600

TS8:

Imaginary frequency -239 cm⁻¹

C	-31.55577100	-21.11102400	-39.56528800
C	-31.30558600	-19.68983400	-40.00056600
C	-30.25758300	-18.94069100	-39.44226800
C	-32.15425800	-19.05781300	-40.91891200
C	-30.07639400	-17.59945000	-39.77623900
C	-31.98142800	-17.71207100	-41.25397000
C	-30.94668600	-16.97376200	-40.67512900
C	-24.13430600	-23.27911600	-46.91359500
C	-25.43370300	-23.64804500	-46.17147200
C	-25.44323500	-25.11129900	-45.70507600
C	-25.67614600	-22.69068000	-45.00092600
C	-24.78500800	-21.39308100	-51.86129200
C	-26.19605900	-21.48902800	-51.33657700
C	-26.59139100	-21.64329600	-50.02810400
C	-27.40380400	-21.46788000	-52.12456500
C	-28.49764600	-21.61816800	-51.22879300
C	-27.66288200	-21.33765700	-53.50056300
N	-27.97231800	-21.72241700	-49.95714300
C	-29.82573700	-21.62331300	-51.66948300
C	-28.98024600	-21.34794400	-53.94137600
C	-30.05240700	-21.48499200	-53.03371000
C	-30.72295900	-13.75589800	-48.18496500
C	-30.33343800	-14.31635500	-46.83264700
C	-30.96813400	-15.44458900	-46.29989400
C	-29.32709300	-13.71369400	-46.06324300
C	-30.61477700	-15.96653500	-45.05443100
C	-28.96421000	-14.21434200	-44.81482200
C	-29.60541900	-15.35045000	-44.30695800
O	-29.17382400	-15.82937200	-43.09611500
C	-30.93555500	-17.83618700	-53.21865000
C	-31.83619100	-18.50513000	-52.21139400
O	-32.65932200	-19.36332200	-52.51972400
N	-31.63673500	-18.11060200	-50.92236400
C	-32.42873300	-18.65653100	-49.84294700
C	-33.71468000	-17.86731500	-49.57247400
H	-30.96979400	-17.38056600	-50.72473100
C	-25.47400100	-9.01406800	-53.29974500
C	-25.95359700	-9.11423000	-51.85655800
C	-26.17165400	-10.55039800	-51.41036200
O	-26.24721100	-11.49244000	-52.18365700
O	-26.28561300	-10.65169300	-50.08907300
C	-25.65783900	-17.19397000	-53.61265600
C	-26.92108900	-17.20516600	-54.48851400
C	-24.41366700	-17.78402200	-54.28696400
C	-26.82708600	-16.33502900	-55.74677600
C	-19.03389200	-18.01802900	-49.78011600
C	-20.28037600	-18.73547800	-49.24888500

C	-21.57768600	-17.97186000	-49.54112900	H	-25.38191900	-7.96858300	-53.61010900
C	-22.84861300	-18.66760100	-49.02931800	H	-24.49845500	-9.49354400	-53.42333800
C	-24.08846500	-17.83427900	-49.34578500	H	-25.25357700	-8.64207900	-51.15883800
N	-25.38481200	-18.44929300	-48.94199500	H	-26.90707100	-8.58593800	-51.72136300
H	-18.92664800	-17.02457200	-49.33044400	H	-26.36054300	-11.63187200	-49.82273400
N	-26.23224900	-13.08801000	-49.02664900	H	-18.12367600	-18.58353900	-49.55738400
C	-26.71807200	-14.29111500	-49.34758000	H	-19.08580600	-17.88503600	-50.86658800
C	-27.42449800	-14.44843100	-50.66499700	H	-20.18357900	-18.88379200	-48.16550100
C	-26.56953700	-15.41209700	-48.47880500	H	-20.34230400	-19.73932600	-49.69022400
O	-27.07100600	-16.58981000	-48.83785300	H	-21.51183400	-16.97026800	-49.09308400
C	-25.91064500	-15.20622900	-47.24000600	H	-21.66366300	-17.81232200	-50.62560600
C	-25.82307100	-16.33666800	-46.23569300	H	-22.78968100	-18.81280800	-47.94339900
C	-25.36042700	-13.94090800	-46.95750900	H	-22.93757900	-19.66170800	-49.48867200
C	-24.53678700	-13.68686600	-45.71579900	H	-24.15836100	-17.62085300	-50.41729100
C	-25.55195200	-12.92092200	-47.88178200	H	-24.02686700	-16.86935800	-48.83444600
H	-26.20281800	-17.59472300	-48.93985200	H	-25.86935600	-17.75799200	-52.69380000
H	-25.15039000	-11.92475400	-47.70781200	H	-28.13340200	-25.11666500	-40.91604700
H	-27.09431200	-15.36454900	-51.16360400	H	-28.88032400	-24.66823600	-42.44950600
H	-28.50681100	-14.55399400	-50.51680700	H	-27.23877000	-25.32729800	-42.41987900
H	-27.22957300	-13.58555200	-51.30496300	H	-25.36279700	-23.95956400	-41.42301100
H	-24.19027500	-12.64283000	-45.71551200	H	-24.47703300	-21.72623300	-40.84002800
H	-25.13365100	-13.82282800	-44.80633600	H	-25.99959800	-19.75941800	-40.77709900
C	-27.93593700	-24.66504500	-41.89616800	H	-28.40185400	-20.04955200	-41.34704000
C	-27.38276200	-23.28246300	-41.73930100	H	-29.27535300	-22.27932100	-41.96389800
C	-26.02807700	-23.09950400	-41.42261400	H	-24.10861300	-22.18942500	-47.04606400
C	-28.22163700	-22.16112800	-41.72344500	H	-23.27053400	-23.53083300	-46.28247600
C	-25.52830300	-21.84234100	-41.08698300	H	-24.63190300	-25.29430400	-44.98920400
C	-27.72877900	-20.90067600	-41.37920900	H	-26.38707500	-25.35719200	-45.20599100
C	-26.38160000	-20.73776600	-41.05271200	H	-25.31845700	-25.81355500	-46.53547400
C	-22.71704000	-19.76961000	-43.10283100	H	-25.71864100	-21.65346500	-45.34727100
C	-22.30902700	-19.25684000	-44.49869200	H	-26.61464000	-22.91428000	-44.48527000
C	-21.70602600	-20.38508800	-45.34161900	H	-24.87340200	-22.77146100	-44.25781700
O	-23.34959200	-18.57971600	-45.19237500	H	-26.26389700	-23.51969700	-46.88446400
H	-31.07430200	-21.45136800	-53.39600400	H	-21.84865300	-20.18486000	-42.58003900
H	-30.65580100	-21.72671100	-50.97700200	H	-23.12646000	-18.95387100	-42.49939600
H	-29.19374800	-21.24886000	-55.00153400	H	-23.47765600	-20.55532000	-43.17817500
H	-26.84475300	-21.23188900	-54.20766300	H	-20.84442900	-20.83812000	-44.83864000
H	-25.99586600	-21.73147100	-49.13021700	H	-22.44465500	-21.17546700	-45.51570700
H	-24.05427500	-21.45994700	-51.04956100	H	-21.37352800	-20.00871200	-46.31335400
H	-24.56745600	-22.20551300	-52.56461900	H	-21.53988000	-18.48653900	-44.35533300
H	-24.61165200	-20.45288600	-52.39839300	H	-24.09329700	-19.16846600	-45.43479900
H	-28.49625000	-21.85950600	-49.10788100	H	-30.63272000	-21.70031100	-39.56766600
H	-27.77083900	-16.34399400	-56.30179900	H	-31.95595100	-21.14227800	-38.54493000
H	-26.60306800	-15.29351500	-55.48950800	H	-32.27846600	-21.60961500	-40.21711300
H	-26.04469600	-16.68438100	-56.42837000	H	-29.58553800	-19.41366900	-38.73079700
H	-27.15373600	-18.24128900	-54.77041600	H	-29.26522900	-17.03486500	-39.32586600
H	-27.76749300	-16.86110200	-53.88075400	H	-30.82147200	-15.92098900	-40.90967000
H	-24.59166500	-18.81595300	-54.61306300	H	-32.66821900	-17.23646100	-41.94897300
H	-24.11610800	-17.20767400	-55.16852800	H	-32.97492900	-19.61954800	-41.35825300
H	-23.55747500	-17.79417100	-53.60324300	C	-30.80596200	-20.37956900	-46.26893000
H	-25.44753300	-16.16274000	-53.29827600	C	-30.42831500	-20.03316900	-44.97296200
H	-33.49472000	-16.82775500	-49.30525600	C	-29.14693900	-19.53293500	-44.72428100
H	-34.35030300	-17.86627500	-50.46197700	C	-28.21630700	-19.38511500	-45.76015500
H	-34.27780600	-18.31800200	-48.74796300	C	-28.60209700	-19.75500800	-47.05570500
H	-31.80779600	-18.69151800	-48.94139000	C	-29.88588100	-20.23374700	-47.31169200
H	-32.68247000	-19.68287900	-50.12114500	H	-31.80364500	-20.75960200	-46.46839900
H	-30.14550700	-18.53699400	-53.50656500	H	-31.12676400	-20.14706500	-44.14841600
H	-31.51438000	-17.60470700	-54.11542400	H	-28.87167700	-19.27692800	-43.70815000
H	-30.46922900	-16.91973800	-52.84616500	H	-27.88757600	-19.65762300	-47.86534100
H	-29.82819500	-13.36925100	-48.68573800	H	-30.17852800	-20.47946700	-48.32898100
H	-31.10453200	-14.56817000	-48.81618400	C	-26.80097200	-18.85177600	-45.52214700
H	-28.80466600	-12.84456000	-46.45415100	H	-25.04406700	-17.06318700	-46.49018600
H	-28.18551500	-13.74304300	-44.22366400	C	-26.44023500	-18.55275000	-44.06806500
H	-31.10229400	-16.86221000	-44.67838500	H	-25.44501800	-18.10807800	-44.03649700
H	-31.74707000	-15.94069400	-46.87396300	H	-27.15244500	-17.88694500	-43.57251500
H	-29.74202600	-16.55761000	-42.80414000	H	-26.40349400	-19.49602000	-43.51580700
H	-26.17017900	-9.51914800	-53.97342300	N	-27.09440100	-17.08666200	-46.13091900

H	-25.64928500	-19.21406800	-49.56826400
H	-27.77498900	-16.58179300	-45.56359300
O	-25.86570300	-19.33105700	-46.26367700
H	-27.47724400	-17.16655400	-47.08478600
H	-25.38885600	-18.82923900	-47.97216300
H	-25.55230900	-15.96753400	-45.24807300
O	-23.44588400	-14.59890000	-45.58097000
H	-22.93025400	-14.54992900	-46.39715000
C	-23.99502800	-23.95087800	-48.28392600
H	-23.09000800	-23.61516300	-48.80231600
H	-23.93092600	-25.04056700	-48.19928600
H	-24.85046700	-23.72416200	-48.92869900
C	-31.77939900	-12.63992800	-48.11094300
H	-31.41676700	-11.79585800	-47.51555500
H	-32.02454900	-12.26736100	-49.11076000
H	-32.70260900	-13.00116000	-47.64586600

TS1':

Imaginary frequency -1012 cm⁻¹

C	-31.55570300	-21.11103500	-39.56537000
C	-31.30564100	-19.68982200	-40.00048600
C	-30.01581200	-19.14145100	-39.98848300
C	-32.37416000	-18.86305900	-40.37732700
C	-29.80354600	-17.80258300	-40.32280500
C	-32.16943100	-17.52457900	-40.71174300
C	-30.88116000	-16.98426800	-40.67727400
C	-24.13434300	-23.27918900	-46.91366000
C	-24.32822100	-24.27550700	-45.74977300
C	-23.13333900	-25.22860200	-45.58971700
C	-24.60343700	-23.54506000	-44.42932100
C	-24.78501600	-21.39302000	-51.86126700
C	-26.19604300	-21.48913700	-51.33661600
C	-26.60424400	-21.50204900	-50.02720100
C	-27.39629900	-21.49614400	-52.13508900
C	-28.50032100	-21.51102600	-51.23759500
C	-27.64470700	-21.47496400	-53.51916400
N	-27.98577500	-21.52853300	-49.95824700
C	-29.82502100	-21.48539800	-51.68811500
C	-28.95980100	-21.45464800	-53.96859200
C	-30.04051400	-21.45432300	-53.06152800
C	-31.46074700	-14.14361400	-48.17806000
C	-30.89706200	-14.70664100	-46.88870600
C	-31.61046000	-15.63237200	-46.11877900
C	-29.63579500	-14.30872200	-46.41804200
C	-31.09482000	-16.15561700	-44.93060500
C	-29.10557500	-14.81650700	-45.23379600
C	-29.83661600	-15.74637100	-44.48374200
O	-29.25699900	-16.22205800	-43.33748600
C	-30.93560000	-17.83619200	-53.21863100
C	-31.86742000	-18.49164500	-52.21747700
O	-32.65767100	-19.38311300	-52.53081500
N	-31.74817800	-18.01741500	-50.94980500
C	-32.42873500	-18.65651100	-49.84296100
C	-33.92302700	-18.32206000	-49.77642800
H	-30.95426000	-17.42398200	-50.72250900
C	-25.47400100	-9.01406700	-53.29974600
C	-25.97539900	-8.87051000	-51.86561900
C	-26.12396000	-10.20438700	-51.15438500
O	-25.84854500	-11.27723400	-51.66498700
O	-26.59195100	-10.06102900	-49.91153200
C	-25.65779700	-17.19395300	-53.61267700
C	-26.96970000	-16.71744000	-52.97111700
C	-25.82921300	-17.85058700	-54.98728600
C	-27.64468800	-15.55899500	-53.71342200
C	-19.03097600	-18.02626600	-49.77497900

C	-20.49450600	-18.32295300	-50.11986000
C	-21.49840200	-17.88744900	-49.04047300
C	-22.91679800	-18.39624600	-49.32894700
C	-23.96370300	-18.15009000	-48.23394100
N	-24.39047600	-16.74544500	-48.18508100
H	-18.72832500	-18.54333800	-48.85717900
N	-26.57105000	-12.45788100	-48.58097200
C	-27.02650000	-13.59118400	-49.13350700
C	-27.93190600	-13.47454300	-50.32692700
C	-26.62814800	-14.84916600	-48.61641200
O	-27.06223600	-16.00676500	-49.12391500
C	-25.72602200	-14.87957100	-47.52395100
C	-25.26404300	-16.27803500	-47.13461100
C	-25.30119900	-13.68104300	-46.93683300
C	-24.44242600	-13.59888900	-45.69062900
C	-25.74996300	-12.49642000	-47.52377700
H	-24.78922900	-16.48877200	-49.08432600
H	-25.43196400	-11.53271000	-47.13192700
H	-28.37822300	-14.43417900	-50.58674800
H	-28.72802100	-12.74936600	-50.12984500
H	-27.35974100	-13.09857200	-51.18206000
H	-23.99539700	-12.59557200	-45.63247400
H	-25.06623800	-13.71511100	-44.79552500
C	-27.93588100	-24.66498800	-41.89627700
C	-27.38284900	-23.28251800	-41.73911200
C	-26.20584600	-23.06242900	-41.00654300
C	-28.04204300	-22.17088900	-42.27839400
C	-25.70533400	-21.77537400	-40.81733100
C	-27.54737000	-20.87784500	-42.08973600
C	-26.37709300	-20.67501200	-41.35691000
C	-22.71705400	-19.76962500	-43.10278400
C	-22.30898300	-19.25678400	-44.49873300
C	-22.28558400	-20.36817200	-45.53311100
O	-23.22367900	-18.25413100	-44.96689000
H	-31.05927600	-21.39287600	-53.42919500
H	-30.66273000	-21.47781900	-50.99746800
H	-29.16348400	-21.43487400	-55.03533500
H	-26.81970900	-21.47296700	-54.22656600
H	-26.01352700	-21.49095400	-49.12215700
H	-24.05740200	-21.37480600	-51.04389900
H	-24.53227600	-22.24060900	-52.50999700
H	-24.64136700	-20.48184500	-52.45466100
H	-28.52229200	-21.48178600	-49.10547100
H	-28.54906900	-15.23012100	-53.19189200
H	-26.97345300	-14.69552000	-53.78685100
H	-27.93797200	-15.84039000	-54.73004200
H	-27.66253400	-17.56853400	-52.91334000
H	-26.76975500	-16.41137300	-51.93679800
H	-26.50552200	-18.71102500	-54.92624300
H	-26.24349200	-17.15369100	-55.72288600
H	-24.86992300	-18.20599600	-55.37882600
H	-24.96683200	-16.34337700	-53.69463900
H	-34.07599100	-17.24195400	-49.68145300
H	-34.41694200	-18.66536100	-50.68756400
H	-34.39226100	-18.81493300	-48.91730600
H	-31.93150300	-18.31962300	-48.92830800
H	-32.31111900	-19.74613200	-49.91752800
H	-30.27240700	-18.60286100	-53.63007600
H	-31.52437100	-17.43619000	-54.04917100
H	-30.33403300	-17.03612200	-52.78326200
H	-30.74950300	-14.32405300	-48.99380400
H	-32.36990800	-14.69535100	-48.44314300
H	-29.05445100	-13.58686300	-46.98492500
H	-28.14103400	-14.48321900	-44.86242900
H	-31.66851300	-16.87686100	-44.35337900
H	-32.59164400	-15.95939700	-46.45391200
H	-29.86440300	-16.82205300	-42.87767600

H	-26.16116000	-9.62113200	-53.89486300
H	-25.37670000	-8.03386300	-53.77637400
H	-24.50022400	-9.50993300	-53.32496800
H	-25.30146600	-8.24773600	-51.26411000
H	-26.94836400	-8.36530700	-51.82702600
H	-26.64559900	-10.96263900	-49.46419800
H	-18.36017700	-18.35114600	-50.57663400
H	-18.86614500	-16.95401000	-49.61871900
H	-20.60687000	-19.40239900	-50.29168900
H	-20.75405800	-17.83991500	-51.07126400
H	-21.16983700	-18.27732400	-48.06598300
H	-21.50345300	-16.79440000	-48.94518500
H	-22.87040100	-19.48201700	-49.48800400
H	-23.27914200	-17.97709000	-50.27883700
H	-23.55237400	-18.40881800	-47.25541200
H	-24.81119500	-18.82649100	-48.43587000
H	-25.17618400	-17.91276700	-52.93557800
H	-28.38784900	-25.02183500	-40.96241600
H	-28.70986200	-24.70568300	-42.66797400
H	-27.15620200	-25.38526200	-42.16631100
H	-25.67907300	-23.91188900	-40.57814600
H	-24.79295900	-21.62982000	-40.24592700
H	-25.99213900	-19.67072300	-41.20576700
H	-28.08213300	-20.03162200	-42.50927800
H	-28.95381900	-22.31638000	-42.85211300
H	-24.98924300	-22.58982800	-46.93140600
H	-23.24431900	-22.67067700	-46.71683200
H	-22.21098000	-24.66808300	-45.39111600
H	-23.29017000	-25.91298700	-44.74897400
H	-22.96710800	-25.83821400	-46.48226100
H	-25.48562100	-22.89930000	-44.49402500
H	-24.77858500	-24.25195000	-43.61191300
H	-23.75186900	-22.91808600	-44.14034800
H	-25.21296700	-24.88610800	-45.98736400
H	-22.00127200	-20.51386500	-42.73843900
H	-22.74309500	-18.94658400	-42.38005800
H	-23.71024000	-20.22780700	-43.13518600
H	-21.64516500	-21.19012900	-45.19951800
H	-23.29502600	-20.75948000	-45.68024500
H	-21.91025100	-20.00792100	-46.49435200
H	-21.30148500	-18.81836700	-44.42829000
H	-23.02215400	-17.41517400	-44.53095700
H	-30.74014400	-21.77359200	-39.87189900
H	-31.63407200	-21.17817600	-38.47324000
H	-32.48795100	-21.50129400	-39.98353100
H	-29.17076100	-19.76645500	-39.71358300
H	-28.79790700	-17.39220900	-40.29686100
H	-30.71754400	-15.93595000	-40.90976600
H	-33.01473700	-16.90053000	-40.98763700
H	-33.38072300	-19.27327000	-40.39888300
C	-29.65321700	-21.24890300	-46.87734400
C	-28.45378300	-21.60521500	-46.25271400
C	-27.45238100	-20.65241600	-46.08257900
C	-27.62152300	-19.33065000	-46.52801500
C	-28.81276600	-18.98836300	-47.17459500
C	-29.82003800	-19.94482000	-47.34383300
H	-30.44537600	-21.98123800	-47.00354700
H	-28.29931900	-22.61931800	-45.89650900
H	-26.52871900	-20.93406900	-45.58455000
H	-28.97016600	-17.99281200	-47.57557100
H	-30.73899200	-19.66409700	-47.84447800
C	-26.51615100	-18.33886800	-46.19647900
H	-25.55684600	-18.79644700	-46.43113600
C	-26.51831300	-18.01046100	-44.69210500
H	-25.68309600	-17.35567700	-44.43340300
H	-27.45731500	-17.53764000	-44.38752700
H	-26.39706700	-18.92841200	-44.11296800

N	-26.59414200	-17.06515700	-46.98105900
H	-26.94691600	-16.84917600	-48.13253200
H	-27.23450500	-16.44674700	-46.47206800
O	-29.20749000	-17.14535400	-50.18692300
H	-28.74711300	-17.86290000	-50.64036700
H	-28.49001800	-16.55882400	-49.85963700
H	-24.74729800	-16.31733100	-46.17989700
O	-23.44297000	-14.60713500	-45.57583300
H	-22.99429900	-14.67889800	-46.43082800
C	-23.99500400	-23.95084800	-48.28390800
H	-23.94876900	-23.20990800	-49.08811600
H	-23.08716200	-24.55787200	-48.34887900
H	-24.84911800	-24.60429000	-48.49467000
C	-31.77940500	-12.63991800	-48.11094800
H	-30.88441700	-12.05154600	-47.88444300
H	-32.17957700	-12.28485500	-49.06604900
H	-32.51988700	-12.42951000	-47.33239100

TS2':

Imaginary frequency -1173 cm⁻¹

C	-31.55570400	-21.11103600	-39.56537000
C	-31.30563900	-19.68982100	-40.00048500
C	-30.02123000	-19.13087900	-39.96578700
C	-32.38689200	-18.85126200	-40.31222800
C	-29.83031000	-17.76408000	-40.17990000
C	-32.20275300	-17.48714300	-40.53123000
C	-30.92329800	-16.93220300	-40.44064000
C	-24.13434300	-23.27918900	-46.91365700
C	-24.37498300	-24.26450000	-45.74966000
C	-23.22292500	-25.26752500	-45.58350100
C	-24.62242800	-23.51650100	-44.43311900
C	-24.78501800	-21.39302800	-51.86127300
C	-26.19604300	-21.48911800	-51.33661200
C	-26.59425700	-21.42867300	-50.02277400
C	-27.40498600	-21.55382600	-52.12045900
C	-28.50021500	-21.53066500	-51.21196700
C	-27.66867200	-21.60207000	-53.50107500
N	-27.97534600	-21.46671000	-49.93874300
C	-29.82968500	-21.53780900	-51.64794500
C	-28.98824500	-21.61180400	-53.93637400
C	-30.05959100	-21.57473800	-53.01855300
C	-31.17860100	-14.04550000	-47.95712900
C	-30.72475400	-14.35554800	-46.54636800
C	-31.36100500	-15.32995500	-45.77054700
C	-29.64641900	-13.66509000	-45.96929600
C	-30.93370500	-15.62812700	-44.47400900
C	-29.21229500	-13.94249900	-44.67779200
C	-29.84710100	-14.93947300	-43.92844700
O	-29.34421700	-15.21634800	-42.68625800
C	-30.93559500	-17.83619200	-53.21863000
C	-31.84262100	-18.50176000	-52.21498300
O	-32.66446600	-19.35959500	-52.52562400
N	-31.64947800	-18.10092400	-50.92536100
C	-32.42873800	-18.65651000	-49.84296300
C	-33.64658000	-17.80530300	-49.46777100
H	-30.98188900	-17.37063700	-50.72919700
C	-25.47400100	-9.01406700	-53.29974600
C	-25.91886100	-8.84008200	-51.84792200
C	-25.92940400	-10.14186800	-51.06102100
O	-25.49580100	-11.19732600	-51.48871400
O	-26.46957500	-9.98521300	-49.84690100
C	-25.65780000	-17.19395900	-53.61267200
C	-26.93582900	-16.34983300	-53.48892300
C	-25.63639600	-18.12852700	-54.82809800
C	-27.10166100	-15.28515200	-54.57912100

C	-19.03388700	-18.01802800	-49.78011500	H	-29.79718300	-15.99351800	-42.32692600
C	-20.45157500	-18.55764800	-49.99036800	H	-26.15125200	-9.68172900	-53.83938100
C	-21.49094500	-17.93467800	-49.04764600	H	-25.45625100	-8.04979900	-53.81652800
C	-22.86373700	-18.61848300	-49.13857400	H	-24.47564500	-9.45563500	-53.35027800
C	-23.87001000	-18.19392000	-48.06382500	H	-25.26287400	-8.14090300	-51.31297900
N	-24.53408000	-16.89873100	-48.37225400	H	-26.92220500	-8.40319500	-51.78255500
H	-18.68433200	-18.21177600	-48.75965100	H	-26.47472900	-10.85987000	-49.35089200
N	-26.54542500	-12.39077200	-48.44400900	H	-18.32403700	-18.48593800	-50.46933800
C	-27.07846400	-13.42255000	-49.10254600	H	-18.98973100	-16.93537400	-49.94451800
C	-27.92618900	-13.12673800	-50.30820800	H	-20.44784400	-19.64617000	-49.84174500
C	-26.83251700	-14.77841100	-48.71898100	H	-20.76071100	-18.39615000	-51.03117700
O	-27.46261800	-15.74453400	-49.37071500	H	-21.12644200	-18.00844200	-48.01286400
C	-25.94695100	-15.01105500	-47.63294000	H	-21.57640600	-16.85965500	-49.26347100
C	-25.51997600	-16.43710100	-47.28961800	H	-22.71360700	-19.70000600	-49.02327900
C	-25.47271100	-13.89855600	-46.89536200	H	-23.29899600	-18.47941900	-50.13627200
C	-24.74471300	-13.99233800	-45.56559400	H	-23.40083500	-18.13739000	-47.07962300
C	-25.79420000	-12.62389300	-47.35566600	H	-24.68373200	-18.92147300	-48.00180800
H	-23.84002400	-16.16309200	-48.50660600	H	-25.54345300	-17.77723700	-52.69444300
H	-25.43392300	-11.74377300	-46.82719700	H	-28.79597700	-24.82833100	-41.23429400
H	-28.59222600	-13.96192100	-50.52378400	H	-28.28157000	-24.84893800	-42.91846100
H	-28.50314000	-12.21138900	-50.15207200	H	-27.19227100	-25.42903400	-41.65055000
H	-27.28095200	-12.96012900	-51.17856400	H	-25.84711200	-23.85683600	-40.34212700
H	-24.68456700	-12.98258800	-45.13675500	H	-24.97795400	-21.56377900	-40.02845900
H	-25.32485800	-14.59725500	-44.86215500	H	-26.01609900	-19.65653800	-41.24472400
C	-27.93588300	-24.66499000	-41.89627600	H	-27.92795000	-20.08044400	-42.78619600
C	-27.38284600	-23.28251500	-41.73911400	H	-28.78241700	-22.37049800	-43.10248900
C	-26.30576800	-23.02933100	-40.87817600	H	-24.96717800	-22.56383100	-46.94472600
C	-27.95328500	-22.19804000	-42.42099900	H	-23.23004500	-22.69603400	-46.70363500
C	-25.81503200	-21.73501000	-40.69953100	H	-22.27794600	-24.74655100	-45.38356600
C	-27.46837000	-20.90183500	-42.24526700	H	-23.41207600	-25.94091900	-44.74067600
C	-26.39624600	-20.66468400	-41.38186500	H	-23.08051400	-25.88699600	-46.47349700
C	-22.71705500	-19.76962600	-43.10278400	H	-25.46427900	-22.82003600	-44.50754200
C	-22.30898300	-19.25678200	-44.49873300	H	-24.84541900	-24.20980500	-43.61590200
C	-22.30816300	-20.36084600	-45.54062100	H	-23.73815600	-22.93920500	-44.13829900
O	-23.22043300	-18.24167400	-44.94502700	H	-25.28420700	-24.83766700	-45.98936500
H	-31.08202200	-21.54519900	-53.38026500	H	-22.01631200	-20.53147900	-42.74546100
H	-30.65793400	-21.49944400	-50.94692500	H	-22.72002600	-18.94966500	-42.37607500
H	-29.20320700	-21.64382300	-55.00051500	H	-23.72094400	-20.20387300	-43.13175500
H	-26.85169300	-21.62463800	-54.21693800	H	-21.67745500	-21.19303700	-45.21439300
H	-25.99658700	-21.37172200	-49.12369700	H	-23.32375300	-20.73667000	-45.68485600
H	-24.06330000	-21.31621000	-51.04208900	H	-21.93072100	-20.00166600	-46.50149700
H	-24.51180000	-22.26927200	-52.46172000	H	-21.29605000	-18.82943800	-44.43378700
H	-24.65802200	-20.51244300	-52.50208200	H	-23.03781100	-17.41789900	-44.47327000
H	-28.50070200	-21.40532900	-49.07967900	H	-30.71865500	-21.76760600	-39.82286500
H	-28.01276200	-14.69707600	-54.42391200	H	-31.68568800	-21.16065800	-38.47752000
H	-26.25609100	-14.58747000	-54.57823000	H	-32.46250400	-21.52026300	-40.02078700
H	-27.16540700	-15.72711400	-55.57938400	H	-29.16686800	-19.76468500	-39.74486100
H	-27.80620100	-17.02136900	-53.49877200	H	-28.83050600	-17.34312300	-41.11691400
H	-26.93824900	-15.86647000	-52.50533500	H	-30.78560100	-15.85960400	-40.54617500
H	-26.47204000	-18.83758300	-54.79110100	H	-33.05791500	-16.85229600	-40.74535600
H	-25.70965000	-17.57898600	-55.77290500	H	-33.38926600	-19.27060600	-40.35216100
H	-24.70918300	-18.71215100	-54.86459700	C	-29.56623700	-21.39265400	-46.62852900
H	-24.78975600	-16.52001700	-53.65437100	C	-28.21795400	-21.64333000	-46.36120600
H	-33.34860000	-16.79756200	-49.15753300	C	-27.34002300	-20.57869200	-46.13995300
H	-34.32119000	-17.71412600	-50.32344700	C	-27.78543400	-19.25196000	-46.17784600
H	-34.19991500	-18.26495100	-48.64140300	C	-29.14287600	-19.01318000	-46.44222300
H	-31.77371900	-18.78923800	-48.97349700	C	-30.02348100	-20.07214300	-46.66745300
H	-32.75823000	-19.64515200	-50.17154500	H	-30.25567900	-22.21617000	-46.79118300
H	-30.17715100	-18.55942600	-53.53545100	H	-27.84955900	-22.66434800	-46.31781400
H	-31.51821000	-17.56354500	-54.10158200	H	-26.29555400	-20.78192000	-45.92028400
H	-30.42967100	-16.94723600	-52.83261000	H	-29.52307200	-17.99542700	-46.46016300
H	-30.32918200	-14.15275400	-48.64330200	H	-31.07281600	-19.86813500	-46.85947300
H	-31.92067100	-14.79134800	-48.26769600	C	-26.81215400	-18.10340700	-45.93410800
H	-29.12484300	-12.90699100	-46.54779100	H	-25.85053100	-18.53923700	-45.63933200
H	-28.37024200	-13.41495000	-44.24187000	C	-27.28416000	-17.19522900	-44.78625400
H	-31.43767800	-16.39587500	-43.89135800	H	-26.53214200	-16.43412800	-44.55899200
H	-32.20716400	-15.87348500	-46.18460400	H	-28.21170500	-16.67895500	-45.03890200

H	-27.44924100	-17.77567700	-43.87239200
N	-26.58416500	-17.40777900	-47.21084600
H	-25.20141300	-17.13347600	-49.40763400
H	-27.42898900	-17.07209100	-47.66378300
O	-25.99159800	-17.37681800	-50.32935300
H	-26.35781400	-18.26552800	-50.21072300
H	-26.77660300	-16.59476000	-49.91333500
H	-24.94951200	-16.43639000	-46.35857600
O	-23.44588100	-14.59889700	-45.58096900
H	-22.89379500	-14.07664800	-46.17890000
C	-23.99500300	-23.95084800	-48.28391000
H	-23.92172800	-23.20882300	-49.08536500
H	-23.10152800	-24.57961800	-48.33993300
H	-24.86203100	-24.58301300	-48.50683200
C	-31.77940500	-12.63992100	-48.11094900
H	-31.05452300	-11.86676100	-47.83764100
H	-32.08863100	-12.45633400	-49.14526400
H	-32.65542000	-12.51516800	-47.46618600

TS4':

Imaginary frequency -436 cm⁻¹

C	-31.55570800	-21.11104000	-39.56535600
C	-31.30563600	-19.68981600	-40.00050200
C	-30.02286300	-19.12808700	-39.94690400
C	-32.36908500	-18.87707800	-40.41842100
C	-29.81309100	-17.78983900	-40.28426800
C	-32.16633100	-17.53901100	-40.75572700
C	-30.88593400	-16.98559200	-40.68184500
C	-24.13432600	-23.27918400	-46.91366000
C	-24.37860000	-24.26969300	-45.75405800
C	-23.22651000	-25.27281600	-45.58808400
C	-24.63342000	-23.53116600	-44.43408600
C	-24.78501600	-21.39302500	-51.86127000
C	-26.19603600	-21.48912800	-51.33661600
C	-26.61088100	-21.51647100	-50.02884000
C	-27.39257200	-21.48847000	-52.13966200
C	-28.49882100	-21.51267100	-51.24619800
C	-27.63491800	-21.45616100	-53.52481100
N	-27.99046800	-21.54097400	-49.96523100
C	-29.82208900	-21.48461000	-51.70089500
C	-28.94822900	-21.43548600	-53.97816900
C	-30.03217500	-21.44361300	-53.07416500
C	-31.43464200	-14.13806200	-48.11803000
C	-30.89484900	-14.66623000	-46.80290700
C	-31.48405400	-15.75911300	-46.15782200
C	-29.76146500	-14.09636100	-46.20204300
C	-30.95800500	-16.28709400	-44.97530400
C	-29.23015200	-14.60132800	-45.02026400
C	-29.81972800	-15.71117600	-44.40780500
O	-29.22498800	-16.19128200	-43.26799000
C	-30.93557400	-17.83618300	-53.21865100
C	-31.83885200	-18.50522200	-52.20434200
O	-32.64271100	-19.38879400	-52.51052200
N	-31.68265400	-18.06001300	-50.93093400
C	-32.42874200	-18.65651400	-49.84294800
C	-33.90439800	-18.24083600	-49.81941500
H	-30.90861400	-17.42988900	-50.72249900
C	-25.47400100	-9.01406700	-53.29974600
C	-25.54382100	-8.90135000	-51.78086600
C	-25.69138500	-10.25690100	-51.11126800
O	-25.51767800	-11.31320000	-51.70026500
O	-26.02511900	-10.15686200	-49.82795500
C	-25.65782500	-17.19396100	-53.61265900
C	-27.16460100	-17.12559500	-53.90745200
C	-24.82299700	-17.84589900	-54.72116200

C	-27.53660500	-16.22621600	-55.09146700
C	-19.03388700	-18.01802900	-49.78011500
C	-20.51082800	-18.10055600	-50.21111000
C	-21.54590000	-17.84149500	-49.09588100
C	-22.99501700	-17.92464700	-49.61908400
C	-24.13113000	-17.59748800	-48.63700200
N	-24.31744700	-18.61750800	-47.54827100
H	-18.80232600	-18.75292200	-49.00091100
N	-26.23580600	-12.52803200	-48.60110700
C	-26.91914800	-13.58834000	-49.03474300
C	-27.68439300	-13.45557000	-50.32086100
C	-26.94204700	-14.82043700	-48.29516800
O	-27.58890600	-15.86778200	-48.71278300
C	-26.21053600	-14.85640700	-47.05948900
C	-26.23556100	-16.04450100	-46.25354100
C	-25.46950800	-13.71228500	-46.65427400
C	-24.58083300	-13.71934100	-45.43594100
C	-25.52167900	-12.58710900	-47.45816400
H	-24.15538000	-19.55958400	-47.90490800
H	-24.97669700	-11.68385700	-47.19088100
H	-27.87725900	-14.42943100	-50.77035600
H	-28.65992300	-12.98435900	-50.14029800
H	-27.12720300	-12.82725800	-51.01952700
H	-24.24485700	-12.69583500	-45.22170300
H	-25.10582500	-14.07920100	-44.54533400
C	-27.93588900	-24.66499000	-41.89626600
C	-27.38284000	-23.28251500	-41.73912800
C	-26.21349500	-23.05824900	-40.99808400
C	-28.05191100	-22.17237500	-42.27173700
C	-25.72897700	-21.76659400	-40.78959300
C	-27.57552500	-20.87764600	-42.06182600
C	-26.41151000	-20.66936500	-41.31840400
C	-22.71706800	-19.76963100	-43.10279400
C	-22.30896800	-19.25677700	-44.49872300
C	-22.29662000	-20.38878900	-45.51436700
O	-23.15759200	-18.22332900	-45.02002500
H	-31.04957500	-21.37794500	-53.44482500
H	-30.66158900	-21.47827400	-51.01314200
H	-29.14880400	-21.40645400	-55.04526700
H	-26.80757100	-21.44612000	-54.22960300
H	-26.02790300	-21.53049000	-49.11876700
H	-24.05317100	-21.41297800	-51.04594800
H	-24.54234400	-22.22403000	-52.53460700
H	-24.62926100	-20.46740300	-52.42930700
H	-28.53146000	-21.51000500	-49.11290600
H	-28.62275000	-16.17955600	-55.21951800
H	-27.17689300	-15.20239500	-54.93651900
H	-27.11172200	-16.58933200	-56.03327500
H	-27.54079700	-18.14264400	-54.08455900
H	-27.68017800	-16.75876000	-53.01169700
H	-25.17242200	-18.86423000	-54.92914500
H	-24.87869100	-17.28142300	-55.65731400
H	-23.76545100	-17.90706200	-54.44085900
H	-25.28156500	-16.17952100	-53.42115900
H	-34.00040100	-17.15368500	-49.73131800
H	-34.39230100	-18.56139400	-50.74181400
H	-34.42184300	-18.70348600	-48.97124000
H	-31.94559200	-18.34434600	-48.91237000
H	-32.36588500	-19.75008700	-49.91214500
H	-30.19939100	-18.56684900	-53.56833500
H	-31.53664500	-17.54432700	-54.08418200
H	-30.41564800	-16.96472700	-52.81799400
H	-30.69851100	-14.33293000	-48.90943200
H	-32.32756900	-14.71202300	-48.39236100
H	-29.27097300	-13.24876200	-46.67258700
H	-28.35104500	-14.15581400	-44.56634100
H	-31.42809200	-17.14574400	-44.50158900

H	-32.37025700	-16.21811100	-46.58960100
H	-29.77501300	-16.88713300	-42.87942500
H	-26.39573500	-9.44304800	-53.70295000
H	-25.32426700	-8.03183200	-53.75909300
H	-24.65404200	-9.67014300	-53.60103000
H	-24.63833300	-8.43006000	-51.37555500
H	-26.37651900	-8.26826700	-51.45478900
H	-26.12790900	-11.08944200	-49.42581200
H	-18.37368000	-18.21299500	-50.62996800
H	-18.78834700	-17.02571400	-49.38618200
H	-20.70242500	-19.09108000	-50.64512000
H	-20.68645400	-17.38060400	-51.02113700
H	-21.38846800	-18.56393600	-48.28183800
H	-21.37456700	-16.84741600	-48.65971200
H	-23.17676300	-18.91867600	-50.05302700
H	-23.10620800	-17.22088200	-50.45343800
H	-25.07959400	-17.52412400	-49.17417600
H	-23.97226200	-16.64034500	-48.13332100
H	-25.50892100	-17.75612000	-52.68003800
H	-28.63088600	-24.90826000	-41.08255200
H	-28.48993200	-24.77624000	-42.83335200
H	-27.14675200	-25.42298500	-41.87982000
H	-25.68118400	-23.90681000	-40.57491800
H	-24.82270300	-21.61777900	-40.20904000
H	-26.04246700	-19.66147800	-41.15269200
H	-28.11602400	-20.03285200	-42.47515500
H	-28.95638000	-22.32160600	-42.85573200
H	-24.96722300	-22.56313300	-46.94055500
H	-23.22485200	-22.70403700	-46.70015300
H	-22.28220300	-24.75320100	-45.38095600
H	-23.41959900	-25.95005500	-44.74952500
H	-23.07985200	-25.88864300	-46.47967200
H	-25.47907200	-22.83955100	-44.50590300
H	-24.85661100	-24.23140300	-43.62340700
H	-23.75254800	-22.95342600	-44.12921600
H	-25.28644000	-24.84045100	-46.00130300
H	-21.98901300	-20.51050700	-42.76008000
H	-22.73536000	-18.95268200	-42.37378500
H	-23.70753200	-20.23337800	-43.12200900
H	-21.67030700	-21.21065700	-45.15827000
H	-23.30738400	-20.77976000	-45.65532300
H	-21.89741000	-20.06038600	-46.47924900
H	-21.28834600	-18.85245500	-44.42302700
H	-22.93400800	-17.36057500	-44.64312300
H	-30.72825400	-21.76892600	-39.84953100
H	-31.66039800	-21.17539500	-38.47522300
H	-32.47433300	-21.50996300	-40.00496000
H	-29.18177300	-19.74294000	-39.63855900
H	-28.81310600	-17.36861200	-40.23009400
H	-30.72225100	-15.94116400	-40.92873900
H	-33.00687800	-16.92643400	-41.06900200
H	-33.36987000	-19.29835200	-40.47245100
C	-29.78242000	-21.35827400	-47.03068400
C	-28.56400500	-21.72556300	-46.44781200
C	-27.59607700	-20.76157400	-46.18766500
C	-27.80443900	-19.39462500	-46.48187800
C	-29.02959600	-19.04504500	-47.08145100
C	-29.99727800	-20.01524100	-47.34801000
H	-30.55066300	-22.10089800	-47.22388700
H	-28.36849800	-22.76451600	-46.19644000
H	-26.65832200	-21.06767800	-45.73397900
H	-29.25128600	-18.00495800	-47.30069900
H	-30.94119300	-19.71587000	-47.78724700
C	-26.75297100	-18.42238600	-46.11141400
H	-25.36263000	-18.64102100	-47.04030200
C	-26.33501400	-18.43293000	-44.64932200
H	-25.32274700	-18.05990500	-44.48783300

H	-27.02742400	-17.81408900	-44.05515900
H	-26.36750200	-19.44451100	-44.24589100
N	-26.85557900	-17.13992600	-46.65701700
H	-23.67890800	-18.44993000	-46.75313800
H	-27.32792000	-16.94650900	-47.58680700
O	-29.14258400	-16.66039100	-50.74644800
H	-28.63568300	-17.44638100	-50.98481900
H	-28.63878000	-16.26374400	-49.99474100
H	-25.69450700	-16.08159600	-45.31708800
O	-23.44588200	-14.59889800	-45.58097000
H	-22.98648900	-14.31188800	-46.38226100
C	-23.99502200	-23.95084500	-48.28390700
H	-23.91186700	-23.21168800	-49.08717800
H	-23.10713800	-24.58736100	-48.33573200
H	-24.86704900	-24.57391700	-48.51005100
C	-31.77940400	-12.63992000	-48.11094900
H	-30.90096600	-12.02398700	-47.89411300
H	-32.16802200	-12.32811600	-49.08576100
H	-32.53767800	-12.41375500	-47.35407000

TS6':

Imaginary frequency -912 cm⁻¹

C	-31.55571400	-21.11103900	-39.56535000
C	-31.30562700	-19.68981800	-40.00051000
C	-30.23189900	-18.95616200	-39.47159600
C	-32.16576100	-19.04780100	-40.90063300
C	-30.03582100	-17.61982900	-39.81760600
C	-31.97639400	-17.70842800	-41.24918300
C	-30.91475000	-16.98524200	-40.70152700
C	-24.13432500	-23.27915600	-46.91363600
C	-25.10296800	-24.00402300	-45.96328700
C	-24.57557200	-25.38045300	-45.53104600
C	-25.40907400	-23.13582000	-44.74185500
C	-24.78501700	-21.39301800	-51.86126900
C	-26.19603400	-21.48913900	-51.33661700
C	-26.58907300	-21.63533700	-50.03084700
C	-27.40421300	-21.46370800	-52.12349300
C	-28.49666200	-21.59710200	-51.22219100
C	-27.66903600	-21.33861400	-53.49891900
N	-27.96757200	-21.72010500	-49.95371500
C	-29.82716500	-21.58093600	-51.65706100
C	-28.98890600	-21.32945900	-53.93336700
C	-30.05913200	-21.44228600	-53.02059600
C	-30.58523700	-13.60880900	-48.13851800
C	-30.21279200	-14.15860400	-46.77727200
C	-30.75171100	-15.35988800	-46.30158500
C	-29.31521900	-13.47486800	-45.94436100
C	-30.40059400	-15.87513800	-45.05235500
C	-28.95549400	-13.97080800	-44.69428200
C	-29.49155600	-15.18178400	-44.24928700
O	-29.06675400	-15.65251700	-43.02827500
C	-30.93557400	-17.83618200	-53.21865100
C	-31.86670800	-18.47545900	-52.20895600
O	-32.75060300	-19.27196900	-52.53222500
N	-31.64530700	-18.09726300	-50.92335200
C	-32.42874200	-18.65651400	-49.84294800
C	-33.84166100	-18.06699000	-49.75553800
H	-30.79377100	-17.58038300	-50.70319600
C	-25.47400100	-9.01406700	-53.29974600
C	-25.61449700	-9.05357800	-51.78284100
C	-25.82845300	-10.46234900	-51.25476700
O	-25.83029000	-11.45024200	-51.97332600
O	-26.01287900	-10.48549800	-49.93928300
C	-25.65782500	-17.19396100	-53.61265900
C	-27.16767700	-17.05408800	-53.86052200

C	-24.84237100	-17.56633100	-54.85647500	H	-30.81745800	-16.82108500	-44.71328600
C	-27.54850500	-15.89951900	-54.79379200	H	-31.44896600	-15.91601400	-46.92368000
C	-19.03388600	-18.01802900	-49.78011500	H	-29.57547500	-16.44142200	-42.79129400
C	-20.46878100	-18.20224400	-50.27787100	H	-26.37038500	-9.40923500	-53.78484900
C	-21.50286500	-17.55272200	-49.35221100	H	-25.31394400	-7.98973600	-53.65117500
C	-22.94905300	-17.72004500	-49.83295700	H	-24.63277000	-9.62921500	-53.62928100
C	-23.98223100	-17.01534400	-48.95558400	H	-24.72721100	-8.64204400	-51.28506900
N	-24.09258500	-17.57795400	-47.58081700	H	-26.45389700	-8.43778300	-51.43759400
H	-18.89561000	-18.46508500	-48.78887300	H	-26.13174200	-11.45037400	-49.61676400
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C	-26.78106600	-14.02530100	-49.18422100	H	-18.77463200	-16.95625900	-49.70286200
C	-27.41042100	-14.08623700	-50.54738700	H	-20.69181600	-19.27288300	-50.37793000
C	-26.79029600	-15.17225600	-48.34557600	H	-20.56853100	-17.77549200	-51.28427900
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C	-24.63207400	-13.77732400	-45.49932300	H	-24.98703900	-17.06870300	-49.38298600
C	-25.55445000	-12.81871000	-47.62326200	H	-23.73819100	-15.95619700	-48.83709000
H	-24.37148900	-18.55870200	-47.60006900	H	-25.49986500	-17.96140700	-52.84176200
H	-25.08075700	-11.86739800	-47.38645900	H	-28.30562100	-25.04667800	-40.93653900
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