

Supporting Information:

Mechanistic insights into the non-bifunctional hydrogenation of ester by Co(II) pincer complexes: a DFT study

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Supporting Information

1. Energy profile diagram for the catalytic hydrogenation of ester (benzyl benzoate) to alcohol by Co^{II}(PNP) complex by using B3LYP/6-31+G**/LANL2DZ level of theory.
2. Optimized geometries of different possible intermediates and transition states by using B3LYP/6-31+G**/LANL2DZ level of theory.
3. Comparative energy profile diagram using different density functionals.
4. Effect of improved basis sets (LANL2TZ) for Co on energy profile diagram.
5. Comparison between electronic properties of Co(PNP) and Co(PNN) complexes.
6. Cartesian coordinates of the optimized geometries of different intermediates and transition states by using B3LYP/6-31+G**/LANL2DZ and M06L/6-31+G**/LANL2TZ levels of theories.

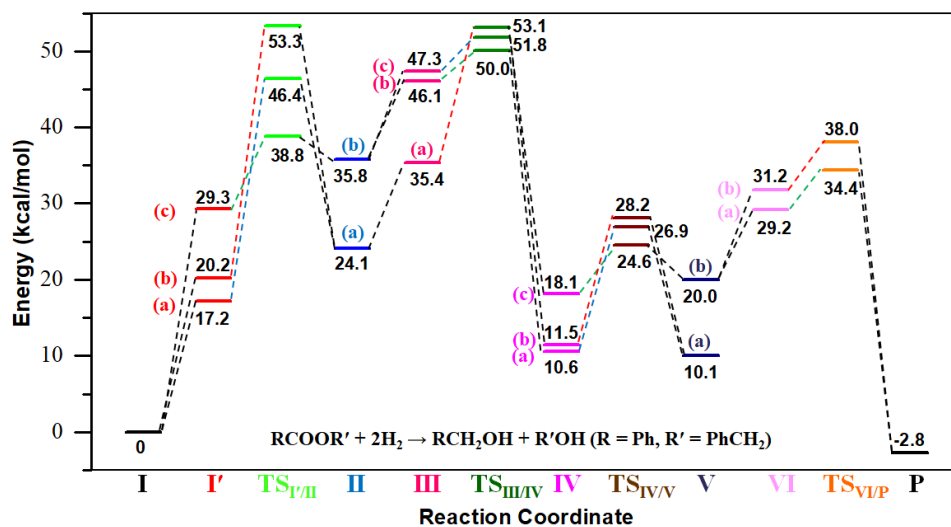


Figure S1: Energy profile diagram for the catalytic hydrogenation of benzyl benzoate ($\text{R} = \text{Ph}$, $\text{R}' = \text{PhCH}_2$) to benzyl alcohol by $\text{Co}^{II}(\text{PNP})$ complex. Labels of the intermediates and transition states are according to Figure 1 in the main paper. The calculations have been done by using B3LYP/6-31+G**/LANL2DZ level of theory in THF medium at 298.15 K.

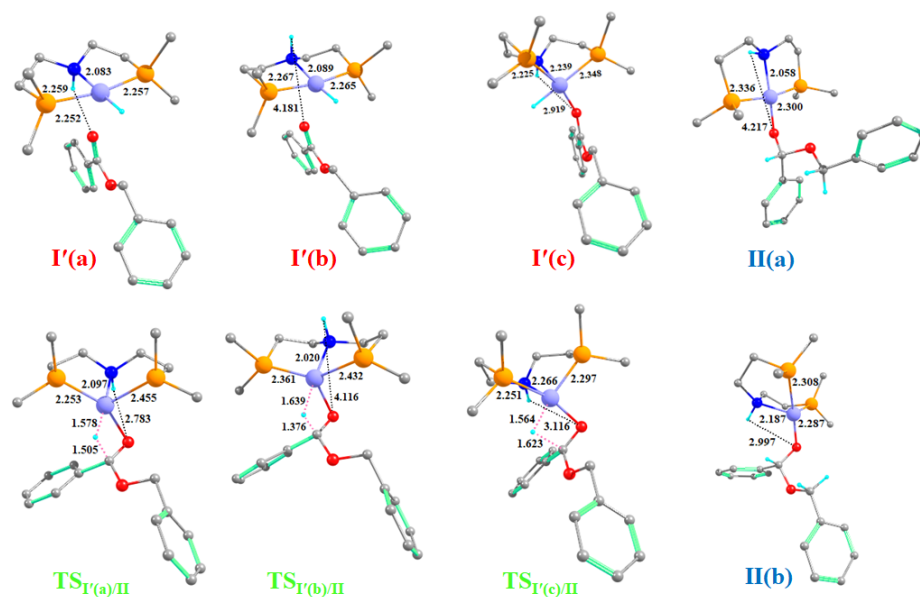


Figure S2: Optimized geometries of different conformations of the intermediate **I'** and the corresponding transition states to produce **II** during the catalytic hydrogenation of benzyl benzoate to benzyl alcohol by $\text{Co}^{\text{II}}(\text{PNP})$ complex using B3LYP/6-31+G**/LANL2DZ level of computation. Optimized geometries of two different conformations of the intermediate **II** are also shown. The bond lengths are shown in Å.

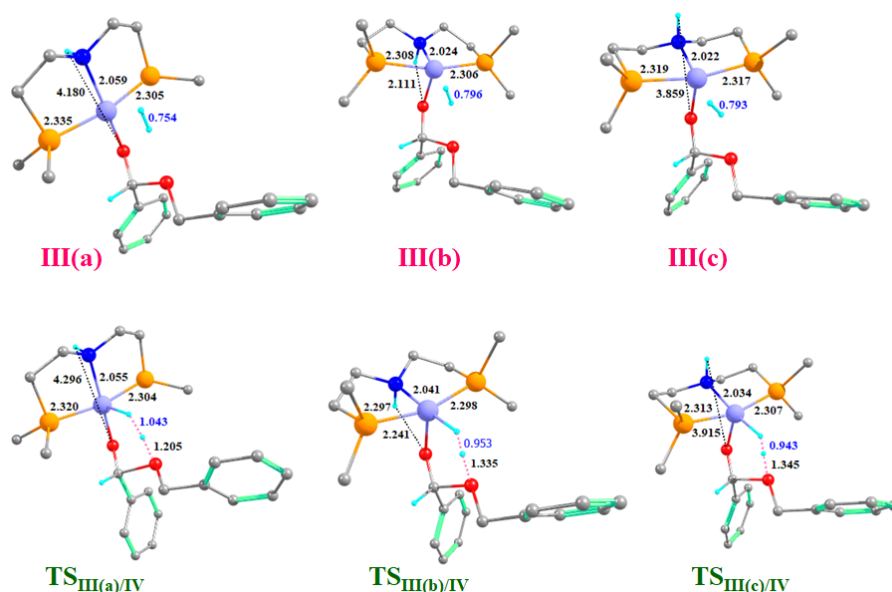


Figure S3: Optimized geometries of different conformations of the intermediate **III** and the corresponding transition states to produce **IV** during the catalytic hydrogenation of benzyl benzoate to benzyl alcohol by $\text{Co}^{\text{II}}(\text{PNP})$ complex using B3LYP/6-31+G**/LANL2DZ level of computation. The bond lengths are shown in Å.

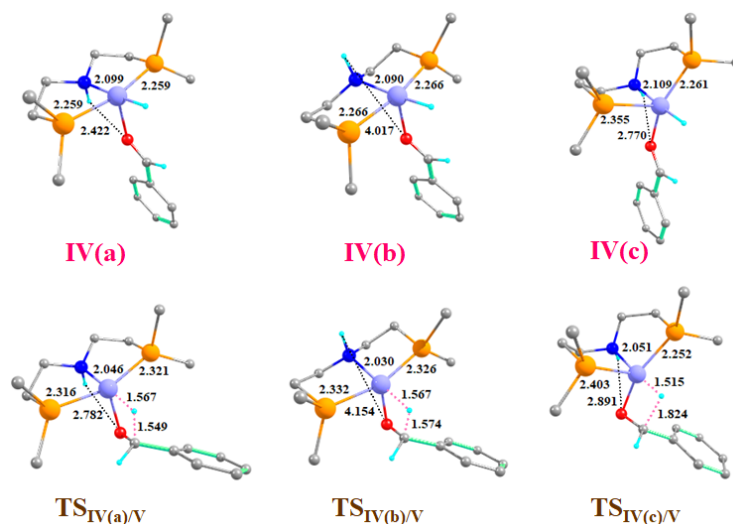


Figure S4: Optimized geometries of different conformations of the intermediate **IV** and the corresponding transition states to produce **V** during the catalytic hydrogenation of benzyl benzoate to benzyl alcohol by $\text{Co}^{II}(\text{PNP})$ complex using B3LYP/6-31+G**/LANL2DZ level of computation. The bond lengths are shown in Å.

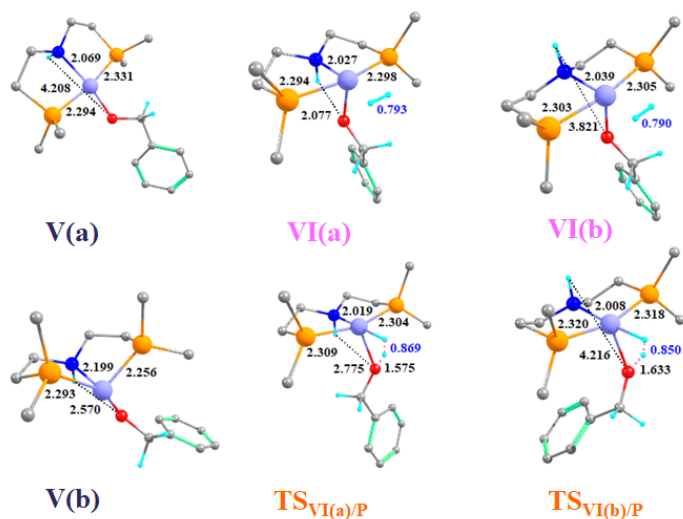


Figure S5: Optimized geometries of different conformations of the intermediate **V**, **VI** and the corresponding transition states to produce product **P** during the catalytic hydrogenation of benzyl benzoate to benzyl alcohol by $\text{Co}^{II}(\text{PNP})$ complex using B3LYP/6-31+G**/LANL2DZ level of computation. The bond lengths are shown in Å.

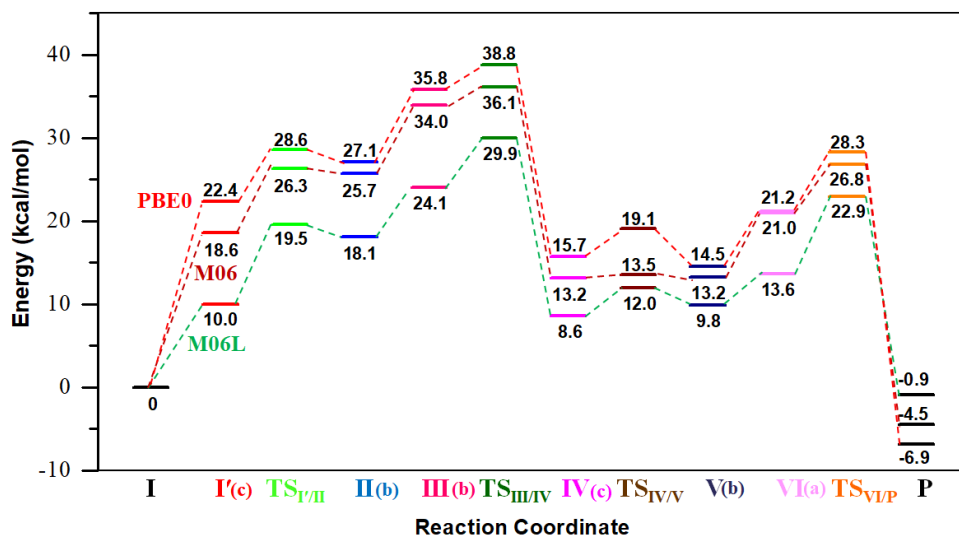


Figure S6: Comparative energy profile diagram, showing minimum energy pathway (labels of the intermediates and transition states are according to Figure 1 in the main paper) for the catalytic hydrogenation of benzyl benzoate to benzyl alcohol by $\text{Co}^{\text{II}}(\text{PNP})$ complex using PBE0, M06 and M06L functionals with 6-31+G**/LANL2DZ basis sets. The calculations have been done in THF medium at 298.15 K.

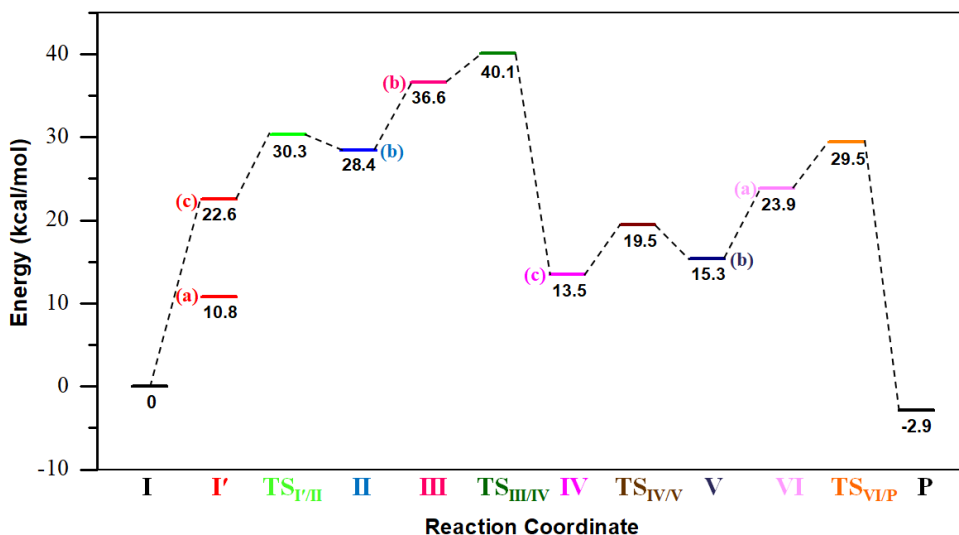


Figure S7: Energy profile diagram, showing minimum energy pathway (labels of the intermediates and transition states are according to Figure 1 in the main paper) for the catalytic hydrogenation of benzyl benzoate to benzyl alcohol by $\text{Co}^{\text{II}}(\text{PNP})$ complex using B3LYP/6-31+G**/LANL2TZ level of computation. The calculations have been done in THF medium at 298.15 K.

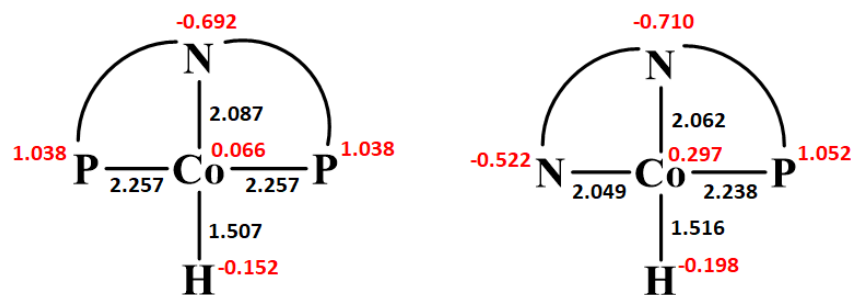


Figure S8: Comparison between electronic properties of Co(PNP) and Co(PNN) complexes. Numbers in black represent the corresponding bond lengths in Å; the red numbers represent the corresponding NBO charges over the elements.

Cartesian coordinates of the optimized geometries of the intermediates and transition states for the catalytic hydrogenation of benzyl benzoate by Co(PNP) and Co(PNN) complexes.

By using B3LYP/6-31+G/LANL2DZ level of theory:**

Co (PNP)

I

First vibrational frequency: 26.78 cm⁻¹

1	2	(Indicate Charge and Spin Multiplicity, respectively)		
Co	0.00000600	-0.60681300	-0.08108700	
P	2.25033900	-0.45547500	-0.00397400	
P	-2.25032600	-0.45550500	-0.00396600	
N	-0.00000200	1.46022600	-0.36878000	
H	0.00013400	1.55380200	-1.38774600	
C	1.24399100	2.11392800	0.13231600	
H	1.20088800	2.09452100	1.22577100	
H	1.27789500	3.16509300	-0.17916200	
C	2.47664000	1.35785200	-0.37309900	
H	3.39082100	1.76116500	0.07310500	
H	2.56602700	1.46469100	-1.46068200	
C	-1.24412300	2.11394700	0.13197700	
H	-1.27802100	3.16505700	-0.17968400	
H	-1.20122100	2.09473000	1.22544200	
C	-2.47664600	1.35772400	-0.37352900	
H	-2.56581900	1.46432700	-1.46115200	
H	-3.39093000	1.76109700	0.07241100	
C	-3.00573800	-0.70413100	1.65732200	
H	-4.05657100	-0.40016300	1.65961700	
H	-2.93448900	-1.76037000	1.92892300	
H	-2.45930000	-0.12058600	2.40281200	
C	-3.38287500	-1.34015900	-1.15035100	
H	-3.35202500	-2.40982100	-0.92822800	
H	-4.41003500	-0.98032200	-1.04152000	
H	-3.05306000	-1.19017300	-2.18128300	
C	3.00586600	-0.70457000	1.65718800	
H	2.93465200	-1.76089100	1.92848300	
H	4.05669400	-0.40058300	1.65950200	
H	2.45946300	-0.12125100	2.40288000	
C	3.38281800	-1.33979400	-1.15069000	
H	4.40998200	-0.97998000	-1.04182300	
H	3.35199400	-2.40952200	-0.92888100	
H	3.05293400	-1.18950800	-2.18155700	
H	0.00002700	-2.10302400	0.09588600	

I' (a)

First vibrational frequency: 7.52 cm⁻¹

1 2

Co	1.82976800	-1.03874300	-0.13400900
P	2.01692100	-1.37309700	2.09223700
P	2.04187300	-0.60579100	-2.33846500
N	2.93022500	0.70301600	0.17591100
H	2.15318200	1.35954500	0.28681200
C	2.85074500	0.21460200	2.60384200
H	2.06315400	0.94526100	2.82273100
H	3.44976000	0.09308600	3.51253200
C	3.71810700	0.70608400	1.43997100
H	4.57745000	0.04390500	1.29152700
H	4.10913100	1.71085200	1.64746900
C	2.87737600	1.05990300	-2.27699800
H	3.48727800	1.24996000	-3.16642900
H	2.08931000	1.82144700	-2.24789600
C	3.72984500	1.13254800	-1.00535600
H	4.11774500	2.14905400	-0.85826900
H	4.59135600	0.46083700	-1.07889500
C	0.59648700	-1.56323600	3.24631700
H	0.09404000	-2.51387400	3.04761600
H	0.93576400	-1.54851000	4.28677800
H	-0.11651600	-0.75004400	3.08903700
C	0.61808500	-0.38786100	-3.48319000
H	0.95175200	-0.01151000	-4.45519300
H	0.11868200	-1.35026700	-3.62447800
H	-0.09674400	0.31624000	-3.04991600
C	3.19770800	-1.68512800	-3.28646100
H	2.75666000	-2.68045300	-3.38848100
H	3.39092000	-1.27208100	-4.28147500
H	4.14422400	-1.78342200	-2.74791500
C	3.17846600	-2.70702700	2.61270900
H	3.37272200	-2.65992700	3.68876200
H	2.74245000	-3.67908700	2.36665800
H	4.12363500	-2.60861500	2.07189400
C	-1.18246000	1.25012600	0.13505600
O	-0.02929800	0.82047600	0.14712900
O	-2.25859100	0.46361800	0.02696600
C	-2.04423800	-0.98170800	-0.07213400
H	-1.45175300	-1.17738900	-0.96754300
H	-1.47118600	-1.29875100	0.80072900
C	-3.39356100	-1.64190500	-0.12976300
C	-4.06939300	-1.97759000	1.05296100
C	-3.99885000	-1.91937500	-1.36403800
C	-5.33195600	-2.57448400	1.00364000
H	-3.60467100	-1.77255900	2.01414800
C	-5.26127800	-2.51773700	-1.41647500
H	-3.47947800	-1.66894500	-2.28561100
C	-5.93023300	-2.84462000	-0.23220000
H	-5.84521300	-2.83212500	1.92553600
H	-5.71946100	-2.73079400	-2.37791700
H	-6.91003700	-3.31174400	-0.27184500
C	-1.53170000	2.69469400	0.23823600

C	-2.86631900	3.13304900	0.19640200
C	-0.49691300	3.63287900	0.38184700
C	-3.15628700	4.49460600	0.29436000
H	-3.66719800	2.41123400	0.08656300
C	-0.79093300	4.99264000	0.48007500
H	0.53145600	3.29117500	0.41658300
C	-2.12124800	5.42547800	0.43618100
H	-4.18868000	4.82888400	0.26040400
H	0.01366100	5.71309800	0.59111800
H	-2.35017000	6.48436800	0.51236200
H	1.04395800	-2.30897200	-0.35978100

I'(a) -TS

First vibrational frequency: -598.22 cm⁻¹

1 2

Co	1.15526200	-0.26171800	-0.09200000
P	2.62283200	0.44750800	1.46385600
P	0.82595300	-2.69413700	-0.07553400
N	2.81939900	-0.68142200	-1.29617300
H	2.54532600	-0.12221400	-2.10542300
C	3.91409800	0.98736100	0.24192900
H	3.53261100	1.89352300	-0.24273400
H	4.86403300	1.24255800	0.72491500
C	4.12184900	-0.13472300	-0.78016200
H	4.65362700	-0.96232300	-0.30450800
H	4.74305700	0.20921600	-1.61440300
C	1.63921600	-2.85983800	-1.74595000
H	1.81709800	-3.91013300	-2.00556800
H	0.94258700	-2.44802000	-2.48503800
C	2.96534600	-2.09959300	-1.76407100
H	3.41030900	-2.11632200	-2.76554500
H	3.67320000	-2.59005100	-1.09133000
C	2.23909900	1.93934200	2.46470500
H	1.52964700	1.67209300	3.25265000
H	3.14802100	2.34218700	2.92182200
H	1.78090600	2.70066600	1.82911700
C	-0.71853000	-3.68410800	-0.31227000
H	-0.47304400	-4.71191600	-0.59862900
H	-1.29543500	-3.70591700	0.61648400
H	-1.33434800	-3.23822400	-1.09615900
C	1.81664400	-3.83101300	0.99917300
H	1.35753700	-3.87600200	1.99113700
H	1.85340400	-4.84114300	0.57813300
H	2.83672100	-3.45809200	1.11709400
C	3.47771500	-0.66850100	2.65176700
H	4.28157100	-0.13138800	3.16462100
H	2.75680700	-1.02760000	3.39110100
H	3.89769300	-1.53228300	2.13184100
C	-0.73472000	0.88561900	-0.62428300
O	-0.16365500	0.13921100	-1.52281600
O	-2.04420200	0.68105200	-0.27239100

C	-2.53587400	-0.68000500	-0.30127200
H	-2.36806200	-1.09513700	-1.29781800
H	-1.95929000	-1.25705400	0.42914800
C	-3.99929700	-0.65783200	0.04995900
C	-4.40853400	-0.68682400	1.39151400
C	-4.97227900	-0.59655700	-0.95805500
C	-5.76628000	-0.65064900	1.72064800
H	-3.66148700	-0.74071700	2.17963800
C	-6.33150800	-0.56176900	-0.63216700
H	-4.66474800	-0.57891900	-2.00069700
C	-6.73040300	-0.58745000	0.70835400
H	-6.07149000	-0.67609500	2.76281500
H	-7.07609200	-0.51747500	-1.42175400
H	-7.78612300	-0.56332400	0.96282000
C	-0.43072000	2.37004600	-0.58114800
C	-0.98545600	3.19190500	0.41078900
C	0.40185400	2.92795700	-1.55943300
C	-0.70216700	4.55866400	0.42587600
H	-1.63464200	2.76157000	1.16633500
C	0.67972200	4.29845800	-1.54501400
H	0.81631000	2.29043200	-2.33312700
C	0.13108100	5.11567900	-0.55220300
H	-1.13288100	5.18959900	1.19785400
H	1.31904800	4.72617300	-2.31181800
H	0.34788700	6.17984800	-0.54072900
H	-0.07167200	0.40914100	0.63967300

I'(b)

First vibrational frequency: 13.96 cm⁻¹

1 2

Co	-1.76923300	-1.11303200	0.24889700
P	-1.64213100	-0.54281800	2.43712800
P	-2.23013600	-1.56890200	-1.92394000
N	-3.25050100	0.35294600	0.10171400
H	-4.11352600	-0.15234000	0.31870500
C	-2.95734500	0.78204400	2.51893900
H	-3.89799000	0.30198500	2.81466200
H	-2.72678300	1.54001900	3.27445500
C	-3.10240200	1.41916500	1.13205800
H	-2.20949700	1.99511100	0.87553400
H	-3.96280100	2.10068400	1.10723500
C	-3.55767400	-0.29572900	-2.26303700
H	-3.52960900	0.05533200	-3.29955700
H	-4.53022600	-0.77855300	-2.10841400
C	-3.38771100	0.87371200	-1.28690200
H	-4.23969200	1.56278400	-1.35772200
H	-2.47766200	1.43616500	-1.51066100
C	-2.10516800	-1.74916200	3.74893500
H	-1.32982400	-2.51687400	3.81970500
H	-2.21071500	-1.25488000	4.71975000
H	-3.04931600	-2.23368300	3.48595200

C	-2.98422400	-3.17569300	-2.41509000
H	-3.34197900	-3.14443500	-3.44898700
H	-2.23600800	-3.96722300	-2.31857200
H	-3.82086000	-3.40781900	-1.75067900
C	-0.95315800	-1.28425800	-3.22004100
H	-0.15758100	-2.02671000	-3.11201400
H	-1.39078400	-1.37086100	-4.21943600
H	-0.52063700	-0.28898600	-3.09604700
C	-0.12694200	0.25807400	3.11394800
H	-0.30534400	0.61439500	4.13328000
H	0.69418900	-0.46336700	3.12469800
H	0.16078500	1.10311100	2.48428700
C	1.02487300	1.20167500	-0.43015200
O	-0.09892000	0.70427100	-0.47678200
O	2.15267300	0.48346800	-0.37574000
C	2.04628600	-0.97595600	-0.44889500
H	1.29741700	-1.31017200	0.27031200
H	1.69744300	-1.22519300	-1.45418800
C	3.40882500	-1.54861700	-0.17292300
C	4.35837600	-1.65243900	-1.20077200
C	3.75261800	-1.97457000	1.11820500
C	5.63275200	-2.16316600	-0.94061900
H	4.09832900	-1.33232100	-2.20673800
C	5.02638700	-2.48748500	1.38123500
H	3.02118000	-1.90615200	1.91923500
C	5.96900700	-2.58090100	0.35207500
H	6.35960800	-2.23936900	-1.74412400
H	5.28059500	-2.81610000	2.38482500
H	6.95828600	-2.98106000	0.55461800
C	1.28043300	2.67047500	-0.43174000
C	2.56946800	3.19661500	-0.24019000
C	0.19931900	3.54173500	-0.64059600
C	2.76659100	4.57826200	-0.24806300
H	3.40701100	2.52712200	-0.08256800
C	0.40145100	4.92156600	-0.65459400
H	-0.79083400	3.12996100	-0.79842500
C	1.68538300	5.44199100	-0.45584500
H	3.76321400	4.98071900	-0.09473200
H	-0.43817400	5.58935500	-0.82166300
H	1.84293800	6.51649000	-0.46505700
H	-0.80722900	-2.26604000	0.39685100

I'(b) -TS

First vibrational frequency: -212.69 cm⁻¹

1 2

Co	-1.29459900	-0.61878300	-0.14713400
P	-0.48051500	-2.87624200	-0.54365900
P	-3.11529300	0.85524900	-0.44182700
N	-2.57158000	-1.61610100	1.05962800
H	-3.22858900	-2.14579800	0.48094000
C	-1.21903300	-3.67891600	0.98125800

H	-1.97839500	-4.40770700	0.67629400
H	-0.44201300	-4.22811900	1.52031300
C	-1.82450700	-2.60524600	1.88942500
H	-1.04648700	-2.05331200	2.42191700
H	-2.49818900	-3.05456300	2.62893700
C	-4.23111500	0.19074200	0.90154900
H	-4.72340600	1.00660800	1.43819200
H	-5.01670300	-0.41921800	0.44104900
C	-3.39037400	-0.65750700	1.85808800
H	-4.02864300	-1.20945500	2.55875100
H	-2.69805000	-0.03980000	2.43637800
C	-1.44128000	-3.60173800	-1.94840600
H	-1.02075100	-3.24098700	-2.89152900
H	-1.39753500	-4.69535100	-1.93235200
H	-2.48632000	-3.28433600	-1.89790500
C	-4.04965500	0.60247500	-2.01112800
H	-5.03116000	1.08437400	-1.96290000
H	-3.48068300	1.03210700	-2.84030800
H	-4.18146900	-0.46657800	-2.19757000
C	-3.16020900	2.67839000	-0.21256500
H	-4.19182900	3.03276000	-0.30395700
H	-2.77267800	2.93599700	0.77459300
H	-2.53793000	3.16591900	-0.96564800
C	1.14392000	-3.73429800	-0.73081200
H	0.97795200	-4.81551700	-0.77588300
H	1.63463600	-3.41413200	-1.65345500
H	1.79599900	-3.51015600	0.11582800
C	0.50413900	0.83398300	0.17705700
O	0.05233300	0.22381300	1.22853900
O	1.83624500	0.64335500	-0.22114300
C	2.45802300	-0.62995200	0.03598300
H	2.08279900	-1.02503500	0.98368800
H	2.18578200	-1.31008700	-0.77576500
C	3.95250200	-0.43231000	0.07300900
C	4.72914000	-0.65613800	-1.07261100
C	4.58648300	-0.01136700	1.25201200
C	6.11409600	-0.46247000	-1.04403400
H	4.24818400	-0.98643900	-1.99018600
C	5.96955400	0.18520600	1.28400000
H	3.99391200	0.16077000	2.14720500
C	6.73660000	-0.03969000	0.13471500
H	6.70421900	-0.64214400	-1.93821200
H	6.44888600	0.50870300	2.20361400
H	7.81225100	0.10957700	0.15982800
C	0.26408100	2.33220600	0.01331600
C	0.34031600	2.94918900	-1.24070900
C	0.06402800	3.10933500	1.15888400
C	0.21412500	4.33613400	-1.34969300
H	0.49953500	2.34589900	-2.13056000
C	-0.05548700	4.49890200	1.05089500
H	0.00951500	2.62238200	2.12737700

C	0.01732400	5.11479000	-0.20242200
H	0.27087800	4.80917600	-2.32590900
H	-0.20527300	5.09805000	1.94463400
H	-0.07721300	6.19361600	-0.28630200
H	-0.17354200	0.30989500	-0.89960500

I' (c)

First vibrational frequency: 11.27 cm⁻¹

1 2

Co	-1.25182400	-0.26582900	-0.20708900
P	-2.07833500	0.29303300	1.91854500
P	-2.63277600	-1.79293700	-1.05035600
N	-2.71498200	1.27038000	-0.92215900
H	-2.12542400	2.03669500	-1.24032100
C	-2.87743900	1.91766800	1.47395500
H	-3.55922600	2.25758600	2.26175100
H	-2.07622200	2.66093400	1.38792300
C	-3.61906700	1.78205900	0.13905100
H	-4.06090000	2.74483400	-0.15299000
H	-4.44801900	1.07631300	0.24797900
C	-3.94805200	-0.71214700	-1.81583500
H	-4.32525200	-1.16153200	-2.74072200
H	-4.78842900	-0.68318900	-1.11415400
C	-3.42502500	0.70732500	-2.09623300
H	-4.26244700	1.35133800	-2.40244500
H	-2.70976700	0.68251300	-2.92195500
C	-3.39230000	-0.59233800	2.87045400
H	-3.02117700	-1.57201700	3.18431100
H	-3.67834300	-0.01927300	3.75824600
H	-4.27947100	-0.74265300	2.24981400
C	-3.60184600	-3.01164700	-0.05280500
H	-4.33834700	-3.52567400	-0.67898000
H	-2.91978700	-3.75428100	0.37147600
H	-4.11880700	-2.50877800	0.76636000
C	-2.03121100	-2.86176400	-2.42841500
H	-1.61546800	-2.23567700	-3.22096700
H	-1.23905100	-3.51926700	-2.05824000
H	-2.84430500	-3.47391100	-2.83131600
C	-0.88216300	0.74198900	3.25098400
H	-1.37960200	1.27935100	4.06460100
H	-0.42816900	-0.16846200	3.65337700
H	-0.09052900	1.36910000	2.83433300
C	1.50433100	1.19569500	-0.08405500
O	0.28610200	1.08256900	0.09831500
O	2.36287500	0.18081300	-0.05139400
C	1.87975900	-1.16006900	0.30166000
H	1.43420900	-1.09890300	1.29728900
H	1.11558200	-1.44441200	-0.42574200
H	-0.71617400	-0.47983900	-1.59880800
C	3.05726700	-2.09320900	0.27246000
C	3.39760900	-2.76793100	-0.90925800

C	3.83292800	-2.29392000	1.42368100
C	4.50065600	-3.62540200	-0.94177800
H	2.79737000	-2.62280300	-1.80387300
C	4.93614000	-3.15132400	1.39334100
H	3.57155600	-1.77979700	2.34518700
C	5.27155100	-3.81792900	0.20983400
H	4.75514500	-4.14474600	-1.86106400
H	5.52915000	-3.30182300	2.29068900
H	6.12681300	-4.48702400	0.18612900
C	2.14412500	2.50731400	-0.35125700
C	3.53591100	2.62708400	-0.50802700
C	1.32885900	3.64753200	-0.44784100
C	4.10066700	3.87720100	-0.76168800
H	4.16549900	1.74823200	-0.43190100
C	1.89902100	4.89419900	-0.70111500
H	0.25659300	3.54560200	-0.32345300
C	3.28518900	5.01047400	-0.85861500
H	5.17563500	3.96772900	-0.88295900
H	1.26613500	5.77306900	-0.77589900
H	3.72874300	5.98184900	-1.05633600

I'(c) -TS

First vibrational frequency: -585.33 cm⁻¹

1 2

Co	0.93513500	-0.47332400	-0.06470800
P	2.31453500	-1.42590300	-1.63438700
P	1.57283400	-1.31529400	1.92296600
N	2.63598500	0.99525200	0.22997600
H	2.26188300	1.88709900	-0.08904300
C	3.40928300	0.04452000	-1.94086700
H	4.29165000	-0.23219500	-2.52842200
H	2.82836300	0.76207100	-2.53140100
C	3.82392300	0.66564000	-0.60198200
H	4.43950100	1.55903300	-0.76999700
H	4.44419500	-0.04213400	-0.04440600
C	3.04712600	-0.26440400	2.34888000
H	3.14340400	-0.15199500	3.43391800
H	3.93956400	-0.79720800	2.00395900
C	2.94022800	1.11577600	1.67816600
H	3.86926300	1.67923100	1.84443000
H	2.12671100	1.68839000	2.13228600
C	3.48787600	-2.82910100	-1.39421700
H	2.92891600	-3.74504900	-1.18399800
H	4.09028900	-2.97838500	-2.29582000
H	4.15757500	-2.62942900	-0.55372900
C	2.13878700	-3.04975900	2.18190000
H	2.49954000	-3.18639700	3.20619400
H	1.30227100	-3.73191800	2.00573400
H	2.94096700	-3.29724600	1.48414000
C	0.39694300	-1.07029100	3.32187100
H	0.11812500	-0.01576200	3.38676700

H	-0.50929500	-1.65488200	3.14044700
H	0.84599300	-1.38782300	4.26805000
C	1.55418400	-1.78930200	-3.27015500
H	2.32167900	-1.89484600	-4.04309200
H	0.98079700	-2.71852400	-3.20755300
H	0.87390600	-0.97698400	-3.53586500
C	-0.82521900	0.97065800	-0.54045900
O	-0.11836800	0.42710800	-1.47091300
O	-2.09432200	0.54148400	-0.29012300
C	-2.39075400	-0.84980300	-0.58339000
H	-2.11489700	-1.05934300	-1.61921000
H	-1.77708800	-1.47043800	0.08190500
H	-0.07942400	0.37341400	0.77162100
C	-3.85740700	-1.08028600	-0.33862500
C	-4.31607200	-1.46686400	0.92918900
C	-4.78564700	-0.90422500	-1.37521000
C	-5.67970900	-1.67004000	1.15959200
H	-3.60304100	-1.61249500	1.73687300
C	-6.14996500	-1.10616900	-1.14785300
H	-4.43856700	-0.61061800	-2.36270000
C	-6.59913600	-1.48915600	0.12068400
H	-6.02303200	-1.97222500	2.14480800
H	-6.85948300	-0.96912300	-1.95874400
H	-7.65870700	-1.65013200	0.29735200
C	-0.68684700	2.43855000	-0.23005400
C	-1.37624300	3.02077500	0.84344300
C	0.12733500	3.23263000	-1.04869900
C	-1.24852900	4.38767400	1.09459200
H	-2.00939800	2.40611000	1.47477000
C	0.25096400	4.60215800	-0.79527500
H	0.64036900	2.77779400	-1.88985100
C	-0.43370100	5.18103700	0.27758000
H	-1.78402400	4.83456100	1.92698500
H	0.87565900	5.21480500	-1.43856900
H	-0.33771500	6.24475900	0.47437900

II (a)

First vibrational frequency: 19.81 cm⁻¹

1 2

Co	-1.62008100	0.45733400	0.26881600
P	-1.44048400	-0.40085200	2.39560400
P	-2.13590900	1.08847200	-1.92033600
N	-3.49353200	-0.39490000	0.28255600
C	-0.20544900	-1.74426500	2.61166600
H	0.78887600	-1.34321900	2.40297200
C	-1.18988500	0.70736000	3.83626200
H	-0.20694600	1.17772400	3.75011400
C	-3.10691800	-1.19709800	2.60167700
H	-3.07210000	-2.07891600	3.24883400
H	-3.77902700	-0.46988400	3.07208000
C	-3.61606200	-1.56671500	1.20547400

H	-3.02526400	-2.38087600	0.77485900
H	-4.66034200	-1.89914900	1.24718600
C	-4.04714000	-0.69459000	-1.07319300
H	-5.09711600	-0.99993200	-0.98833900
H	-3.48624600	-1.54460300	-1.47424700
C	-3.90785800	0.53131600	-1.97677500
H	-4.53494300	1.35056300	-1.60549600
H	-4.23303600	0.30319800	-2.99667100
C	-2.15108100	2.85972100	-2.41342200
H	-1.12378500	3.23139100	-2.45507000
C	-1.34053500	0.22765800	-3.34343800
H	-0.29372200	0.53188100	-3.42075500
H	-4.07361200	0.35185500	0.67614200
H	-1.95270000	1.49015900	3.83655300
H	-1.24188200	0.14690100	4.77457000
H	-0.24085400	-2.14683200	3.62860700
H	-0.40552400	-2.54696300	1.89702800
H	-2.69997400	3.44145200	-1.66844400
H	-2.61979500	2.98938000	-3.39369600
H	-1.37557400	-0.85404800	-3.19007800
H	-1.85569000	0.47692200	-4.27636600
C	1.06677800	1.17737500	-0.32791000
O	0.00333500	1.41152700	0.48800100
O	1.42409300	-0.23215800	-0.21461600
C	2.37531000	-0.67954600	-1.18789900
H	2.00594900	-0.44815800	-2.19889900
H	3.33103700	-0.15506100	-1.05293100
H	0.84253400	1.34725400	-1.40275300
C	2.57212500	-2.16760300	-1.03151800
C	1.71260000	-3.07379400	-1.67108500
C	3.60608100	-2.67054400	-0.22834600
C	1.87784300	-4.45237300	-1.50791300
H	0.91330900	-2.69657300	-2.30458000
C	3.77624300	-4.04887600	-0.06233600
H	4.28404400	-1.97884300	0.26581200
C	2.91093300	-4.94327800	-0.70129000
H	1.20783500	-5.14200300	-2.01394900
H	4.58453200	-4.42299400	0.55977200
H	3.04436600	-6.01424300	-0.57748400
C	2.24094400	2.07472400	0.05766700
C	2.70501200	3.05355400	-0.82824500
C	2.85314900	1.94985400	1.31406900
C	3.76061700	3.90144800	-0.46923000
H	2.23990400	3.15491900	-1.80654100
C	3.90765500	2.79085900	1.67568000
H	2.50291200	1.18758100	2.00361500
C	4.36389500	3.77184500	0.78457700
H	4.10991700	4.65720800	-1.16743200
H	4.37625700	2.68309000	2.65028200
H	5.18448100	4.42564300	1.06642700

II (b)First vibrational frequency: 10.75 cm⁻¹

1 2

Co	1.23735700	-0.71078300	-0.00579900
P	2.16967400	-0.24562400	-2.04187800
P	2.80771200	-1.96615900	1.12787100
N	2.32517700	0.99405800	0.82775300
H	1.60704900	1.67608900	1.07139700
C	2.56956300	1.51701000	-1.62330700
H	3.25004700	1.95586000	-2.36123300
H	1.62613900	2.07096100	-1.65841500
C	3.19242400	1.60700900	-0.22164300
H	3.39762400	2.65466200	0.03039200
H	4.15349600	1.08661900	-0.21112900
C	3.88004000	-0.65343900	1.89027200
H	4.28143400	-0.98407000	2.85380300
H	4.73636300	-0.49761900	1.22559100
C	3.07302800	0.64346400	2.06729000
H	3.74130200	1.46217000	2.36594900
H	2.33387300	0.51942200	2.86390900
C	3.73693200	-0.95273800	-2.70304200
H	3.59139300	-2.00922300	-2.94383600
H	4.03940200	-0.41950900	-3.61003200
H	4.53790000	-0.87041800	-1.96420600
C	3.96198100	-3.22797200	0.45498700
H	4.62666900	-3.59644100	1.24223600
H	3.38523200	-4.06533800	0.05296300
H	4.56274500	-2.79997100	-0.35037300
C	2.00846300	-2.81684000	2.55685200
H	1.38593200	-2.10965600	3.11164200
H	1.36994100	-3.62452100	2.18882100
H	2.76488000	-3.23349200	3.22926800
C	1.05831600	-0.17772600	-3.49970300
H	1.49459300	0.43848100	-4.29195400
H	0.90032700	-1.19079800	-3.87996200
H	0.10000900	0.23733300	-3.18325600
C	-1.12838100	0.64226400	0.34363900
O	-0.30261300	0.13152800	-0.64681400
O	-2.49587400	0.29100000	0.09439800
C	-2.75760300	-1.11874900	0.18663900
H	-2.21547400	-1.65003400	-0.60356800
H	-2.39591200	-1.48583600	1.15971200
H	-0.86856800	0.22763000	1.34177600
C	-4.24335000	-1.34465500	0.05727500
C	-5.08824000	-1.18086200	1.16586700
C	-4.80700300	-1.70331900	-1.17541400
C	-6.46781400	-1.36829200	1.04484200
H	-4.66156600	-0.90705200	2.12781100
C	-6.18734900	-1.89272300	-1.30142000
H	-4.16156300	-1.83606000	-2.04032100
C	-7.02071900	-1.72432400	-0.19095600

H	-7.10977500	-1.24070000	1.91197500
H	-6.60982900	-2.17219100	-2.26249000
H	-8.09261500	-1.87304000	-0.28581600
C	-1.08490300	2.16223700	0.42904400
C	-0.86277800	2.79665700	1.65750600
C	-1.25959700	2.94698600	-0.72108800
C	-0.80928200	4.19438200	1.74111800
H	-0.73810300	2.19797900	2.55760000
C	-1.21456400	4.34011400	-0.63999600
H	-1.43080000	2.46095000	-1.67669100
C	-0.98602600	4.96869700	0.59180900
H	-0.63425700	4.67299900	2.70064200
H	-1.35645900	4.93833100	-1.53595500
H	-0.94803500	6.05264200	0.65207300

III (a)

First vibrational frequency: 14.46 cm⁻¹

1 2

Co	1.67982400	-0.19430900	0.18181300
P	1.63394100	0.54374400	2.36483600
P	2.14826200	-0.85650100	-2.00790200
N	3.55209800	0.66219000	0.13654100
C	0.36447100	1.78667500	2.83732300
H	-0.62630600	1.33446300	2.74678800
C	1.58536600	-0.69604100	3.71836700
H	0.62475100	-1.21647700	3.68309100
C	3.27931000	1.40343800	2.48933600
H	3.24230900	2.27291500	3.15249500
H	4.00161600	0.69712300	2.91468900
C	3.70995100	1.81458100	1.07805900
H	3.09104800	2.63337800	0.69917200
H	4.75177000	2.15703600	1.07419100
C	4.05947100	0.97670100	-1.23384000
H	5.11005000	1.28657200	-1.17919200
H	3.48449100	1.82793600	-1.61118800
C	3.90045600	-0.24499300	-2.14051800
H	4.56538400	-1.05118100	-1.80889200
H	4.16938800	-0.00174000	-3.17306100
C	2.21944500	-2.64678100	-2.42042400
H	1.20727800	-3.05957600	-2.41587600
C	1.27590100	-0.09315700	-3.44086400
H	0.23670400	-0.43090000	-3.46186400
H	4.14295900	-0.09257200	0.49738600
H	2.38401700	-1.42861900	3.57646700
H	1.70114500	-0.21579500	4.69473900
H	0.52056500	2.12150500	3.86728600
H	0.41361500	2.64735800	2.16595900
H	2.81045800	-3.17058100	-1.66477600
H	2.66726700	-2.80455800	-3.40622000
H	1.28293900	0.99562200	-3.34580900
H	1.76342200	-0.37648200	-4.37877500

C	-0.98796900	-1.17316600	-0.29925000
O	0.12165300	-1.23279200	0.48616900
O	-1.57016900	0.15862000	-0.16459800
C	-2.62827300	0.43891800	-1.09018700
H	-2.27596800	0.27160000	-2.11938100
H	-3.47237800	-0.24076500	-0.91041000
H	-0.77090200	-1.29922100	-1.38066900
C	-3.06598400	1.87217200	-0.91313400
C	-2.52813100	2.89174500	-1.71198700
C	-4.01009400	2.21005000	0.06861900
C	-2.91855200	4.22260400	-1.53094000
H	-1.80408700	2.64153500	-2.48355500
C	-4.40233600	3.53876800	0.25456700
H	-4.44220800	1.42664700	0.68646900
C	-3.85575100	4.54909400	-0.54510000
H	-2.49675500	5.00099400	-2.16072800
H	-5.13678700	3.78473900	1.01642100
H	-4.16360000	5.58149500	-0.40545900
C	-1.98571300	-2.25165800	0.11635000
C	-2.32001800	-3.28595900	-0.76497500
C	-2.55771700	-2.23878100	1.39773600
C	-3.20608900	-4.29899100	-0.37677200
H	-1.88658800	-3.30162100	-1.76273600
C	-3.44328700	-3.24526800	1.78849500
H	-2.30768400	-1.43558600	2.08453000
C	-3.76908500	-4.28092000	0.90204700
H	-3.45547100	-5.09605500	-1.07185700
H	-3.88133700	-3.22449500	2.78283500
H	-4.45801200	-5.06360300	1.20704200
H	0.35065900	1.43081900	-0.44346700
H	0.99917000	1.79965700	-0.55439500

III (a) -TS

First vibrational frequency: -1024.24 cm⁻¹

1 2

Co	-1.75113900	0.18368100	0.24302000
P	-1.41124200	-0.82086500	2.28789300
P	-2.54252400	1.10684800	-1.73226700
N	-3.43341700	-0.99393000	0.16161900
C	0.10735800	-1.82929700	2.52219600
H	0.98466300	-1.18045400	2.46657200
C	-1.53956500	0.16059500	3.83959000
H	-0.70065900	0.85988800	3.89154900
C	-2.83071700	-2.02186200	2.33139800
H	-2.56371600	-2.95577000	2.83536600
H	-3.64819400	-1.56403000	2.90050100
C	-3.26894400	-2.28656800	0.89001300
H	-2.51416600	-2.86445200	0.34953900
H	-4.20994400	-2.85008000	0.86602100
C	-3.94498400	-1.20052600	-1.22440300
H	-4.89213600	-1.75325100	-1.19506300

H	-3.21068300	-1.81742500	-1.75045000
C	-4.12499300	0.15100700	-1.91525200
H	-4.92635400	0.72162400	-1.43105700
H	-4.40301400	0.02047100	-2.96569400
C	-3.02964500	2.87975600	-1.83073500
H	-2.13315800	3.50462000	-1.79299800
C	-1.64252200	0.80721500	-3.31190200
H	-0.70133700	1.36346800	-3.32002900
H	-4.14730500	-0.45764000	0.66274100
H	-2.47019900	0.73423600	3.83751300
H	-1.51744200	-0.49059700	4.71901500
H	0.08583400	-2.33683100	3.49150900
H	0.17923400	-2.56950400	1.72201300
H	-3.66339300	3.13146400	-0.97626200
H	-3.57195700	3.08750400	-2.75842400
H	-1.41505800	-0.25757600	-3.40411000
H	-2.25073800	1.12614900	-4.16414400
C	0.67143000	1.59159500	-0.19917900
O	-0.30829200	1.47066800	0.61786200
O	1.33939400	-0.15735600	-0.30120400
C	2.15113200	-0.47592400	-1.44031900
H	1.51864600	-0.57224800	-2.33432200
H	2.84485800	0.35698600	-1.60248400
H	0.46644700	1.63247700	-1.27670500
C	2.92373300	-1.75627900	-1.20943100
C	2.44624700	-2.98037000	-1.69951100
C	4.12781300	-1.74002000	-0.48807700
C	3.15266700	-4.16605800	-1.47107200
H	1.51876200	-3.00535800	-2.26652700
C	4.83640600	-2.92213900	-0.25682600
H	4.51277700	-0.79609700	-0.10981100
C	4.34961200	-4.13933400	-0.74810100
H	2.77215200	-5.10618600	-1.86068000
H	5.76909700	-2.89376700	0.29962900
H	4.90204100	-5.05812600	-0.57297900
C	1.86356300	2.38109800	0.22074200
C	2.63421800	3.04203700	-0.74652200
C	2.20885100	2.49373900	1.57677400
C	3.74286900	3.80488500	-0.36522700
H	2.36132800	2.97093600	-1.79649900
C	3.31523200	3.25280000	1.95651400
H	1.60479100	1.98571900	2.32125000
C	4.08500700	3.90916200	0.98594700
H	4.33291100	4.31740400	-1.11921300
H	3.58048700	3.33580200	3.00652900
H	4.94538800	4.50109500	1.28453800
H	0.24722900	-0.65030400	-0.43276200
H	-0.72345800	-1.00133400	-0.58430300

III (b)

First vibrational frequency: 14.87 cm⁻¹

1 2

Co	1.51498900	-0.72537000	0.08412100
P	0.83967100	-1.56448700	-1.95472800
P	2.68423300	-0.07929500	1.96647300
N	2.98368800	0.19811000	-0.95786900
C	1.31275500	-3.31489100	-2.28684400
H	0.71163400	-3.97498300	-1.65544800
C	-0.86716200	-1.42793100	-2.60528800
H	-1.51533400	-2.12192600	-2.06431700
C	1.91716000	-0.54629200	-3.06444600
H	2.08202100	-1.03109800	-4.03177900
H	1.40239900	0.40338200	-3.24654000
C	3.24039500	-0.30538100	-2.33879600
H	3.81582700	-1.23218800	-2.25128100
H	3.85856100	0.41767000	-2.88474600
C	4.25287100	0.46223200	-0.21980200
H	4.87279600	1.16386500	-0.79107900
H	4.79916300	-0.48365600	-0.15317900
C	3.94732700	1.01792200	1.17046500
H	3.51333200	2.02079500	1.09563400
H	4.85822400	1.09139400	1.77272300
C	1.92223600	0.91480100	3.30758000
H	1.20446200	0.29891200	3.85558400
C	3.64249200	-1.38537600	2.84354300
H	2.94930600	-2.06272800	3.34998200
H	2.46286300	1.08071700	-1.03095400
H	-1.23781200	-0.41537700	-2.44220000
H	-0.88507000	-1.67232000	-3.67186500
H	1.14100700	-3.56905300	-3.33764400
H	2.36698900	-3.47436800	-2.04578800
H	1.39449300	1.76598400	2.87174000
H	2.68812000	1.27596400	4.00100100
H	4.22893400	-1.96524900	2.12559800
H	4.31550100	-0.94109500	3.58338500
H	0.00666700	-1.21836800	0.71201400
H	0.53459100	-1.67676600	1.09283800
C	-0.61079400	1.37977100	0.48717100
O	0.54189300	1.10132200	-0.15472000
O	-1.52237900	0.22833500	0.31626300
C	-2.67263600	0.24381300	1.16891800
H	-2.35734900	0.38140200	2.21481500
H	-3.32705900	1.08561700	0.90362100
H	-0.49468600	1.48190100	1.58961100
C	-3.41365300	-1.06227400	1.01327300
C	-3.11159800	-2.15953700	1.83384900
C	-4.40027900	-1.20975800	0.02669300
C	-3.77394400	-3.38021200	1.66877500
H	-2.35794800	-2.05513300	2.61092500
C	-5.06525500	-2.42805000	-0.14283300
H	-4.65052200	-0.36400400	-0.60919600
C	-4.75164500	-3.51764500	0.67732100

H	-3.53242800	-4.21916800	2.31558700
H	-5.82936600	-2.52542800	-0.90905700
H	-5.27043200	-4.46357100	0.54998200
C	-1.27852900	2.65415900	-0.03078700
C	-1.54411900	3.72061400	0.83592900
C	-1.61798100	2.78578900	-1.38619900
C	-2.13334600	4.90109500	0.36389700
H	-1.28703200	3.63025000	1.88939000
C	-2.21123400	3.95669600	-1.86172900
H	-1.41469800	1.96479600	-2.06697600
C	-2.46970000	5.02127800	-0.98681900
H	-2.32985900	5.72049800	1.05010200
H	-2.47289300	4.04296100	-2.91311800
H	-2.92975300	5.93312200	-1.35728400

III (b) -TS

First vibrational frequency: -890.05 cm⁻¹

1 2

Co	-1.50450700	-0.41632600	0.03458100
P	-1.20484400	-0.85429600	2.27004000
P	-2.38510300	-0.27180100	-2.08163100
N	-3.09547400	0.72187900	0.61785800
C	-1.79804800	-2.49312900	2.87018600
H	-1.12960200	-3.27413600	2.49736100
C	0.38211300	-0.60576300	3.15728900
H	1.10130800	-1.36044300	2.82857600
C	-2.39068900	0.38604500	2.97632500
H	-2.73096100	0.10838500	3.97923600
H	-1.85949700	1.34119700	3.05581700
C	-3.57414400	0.51037700	2.01567200
H	-4.17459200	-0.40472900	2.01937700
H	-4.23154800	1.33669700	2.31316400
C	-4.23300400	0.79549200	-0.34551000
H	-4.90783000	1.61359000	-0.06469800
H	-4.79509800	-0.13961200	-0.25820800
C	-3.71485500	0.98561600	-1.77154700
H	-3.26108100	1.97679700	-1.88426400
H	-4.53140100	0.90923500	-2.49690900
C	-1.49776900	0.32255100	-3.57856900
H	-0.70332200	-0.38222200	-3.83724900
C	-3.26748200	-1.78044500	-2.66837900
H	-2.53478900	-2.55972500	-2.89569200
H	-2.59176800	1.61406800	0.58513700
H	0.78194800	0.38130400	2.91825700
H	0.23720600	-0.69251800	4.23847400
H	-1.81381100	-2.52543100	3.96420100
H	-2.80342700	-2.69192800	2.48968900
H	-1.05043300	1.29922700	-3.38062700
H	-2.18898100	0.40894600	-4.42285300
H	-3.93233600	-2.15348900	-1.88488600
H	-3.85409500	-1.56534100	-3.56697500

H	0.35640900	-0.75643400	-0.33001200
H	-0.33784500	-1.40272400	-0.42179000
C	0.69897900	1.45236800	-0.62147700
O	-0.42120200	1.42952800	0.06051000
O	1.42747500	0.04015800	-0.30881300
C	2.43863100	-0.38960700	-1.24816400
H	2.00073400	-0.46951000	-2.25147900
H	3.21623300	0.38084200	-1.27087400
H	0.60620600	1.37907400	-1.72250600
C	3.00969800	-1.71551700	-0.80716600
C	2.65583900	-2.90288100	-1.46315800
C	3.90163200	-1.77735400	0.27553300
C	3.17831400	-4.13162300	-1.04450600
H	1.97255200	-2.86664200	-2.30799300
C	4.42236000	-3.00251500	0.69812000
H	4.18887300	-0.86146000	0.78575200
C	4.06084400	-4.18372000	0.03840400
H	2.89843200	-5.04345400	-1.56441700
H	5.11373100	-3.03651600	1.53535500
H	4.46946000	-5.13621900	0.36354500
C	1.69959900	2.53023800	-0.25281100
C	2.48713000	3.13208200	-1.24274000
C	1.83178500	2.95680400	1.07666500
C	3.40425700	4.13671300	-0.91130900
H	2.37883200	2.82183300	-2.27969900
C	2.74838200	3.95460100	1.41185700
H	1.20308500	2.50808400	1.83887000
C	3.53905000	4.54696100	0.41775600
H	4.00642200	4.59821100	-1.68888400
H	2.84498400	4.27654800	2.44514000
H	4.24933200	5.32634100	0.67882300

IIII (c)

First vibrational frequency: 12.48 cm⁻¹

1	2		
Co	-1.51381600	-0.90914100	-0.17645200
P	-2.84199400	-0.01902400	-1.85648400
P	-0.59657600	-2.03517400	1.62904400
N	-3.09355100	-0.56796000	1.03811100
C	-2.31721400	1.53264400	-2.68736600
H	-1.47087500	1.32960200	-3.34817900
C	-3.47331200	-1.07642400	-3.22344000
H	-2.65053200	-1.32100700	-3.90101600
C	-4.33161800	0.43708700	-0.84458900
H	-4.81314200	1.34269400	-1.22564500
H	-5.05930800	-0.37941000	-0.91958700
C	-3.88205400	0.62340900	0.60362200
H	-3.22549000	1.49023400	0.70594900
H	-4.74495900	0.75561400	1.26729200
C	-2.68789900	-0.47733500	2.47363400
H	-3.57692200	-0.32823600	3.09818600

H	-2.04587700	0.40184400	2.56427000
C	-1.94254700	-1.74938600	2.87642700
H	-2.61862500	-2.61242800	2.86188300
H	-1.54004200	-1.66343000	3.89029900
C	-0.37217000	-3.85922400	1.53827500
H	0.46513300	-4.08710600	0.87278500
C	0.94303200	-1.41442500	2.40245800
H	1.76837600	-1.51105500	1.69490200
H	-3.70470100	-1.38449700	0.94891100
H	-3.87724000	-2.00663600	-2.81531700
H	-4.25670500	-0.55814800	-3.78530800
H	-3.14365600	1.94110800	-3.27712900
H	-2.00854700	2.25850500	-1.93234200
H	-1.27549700	-4.32420900	1.13485100
H	-0.16338100	-4.27478100	2.52911600
H	0.82068400	-0.35460800	2.63053200
H	1.15640500	-1.97573100	3.31729800
H	-0.50970100	-1.49268800	-1.43285100
H	0.00681000	-1.16315900	-0.92975500
C	0.40557300	1.36445000	-0.34561400
O	-0.66715300	0.91252200	0.32753500
O	1.47928000	0.33994400	-0.26718900
C	2.56283700	0.53667100	-1.17893500
H	2.17789900	0.61848000	-2.20777300
H	3.08913400	1.47325400	-0.94599000
H	0.23204500	1.48995700	-1.43796100
C	3.51132600	-0.63308200	-1.06861800
C	3.41092600	-1.72538500	-1.94260700
C	4.49883600	-0.65606800	-0.07144400
C	4.27343000	-2.82033600	-1.82187300
H	2.65738500	-1.71534600	-2.72666100
C	5.36198800	-1.74827000	0.05473100
H	4.59219500	0.18878400	0.60663200
C	5.25038100	-2.83472600	-0.82085700
H	4.18649500	-3.65652400	-2.51020700
H	6.12367200	-1.74950900	0.82956500
H	5.92397200	-3.68192300	-0.72762800
C	0.92586200	2.69522200	0.20097600
C	1.13320100	3.78575500	-0.65212300
C	1.18923100	2.85248600	1.57066300
C	1.59199300	5.01250200	-0.15369700
H	0.93222600	3.67851400	-1.71612700
C	1.65088600	4.07042500	2.07323100
H	1.02444400	2.01405700	2.24024900
C	1.85270000	5.15758900	1.21120400
H	1.74429800	5.84925100	-0.83018800
H	1.85203800	4.17649300	3.13611700
H	2.20908600	6.10633000	1.60275500

III (c) -TS

First vibrational frequency: -848.03 cm⁻¹

1 2

Co	1.54712600	-0.61894100	0.00278100
P	2.53990300	-0.20160000	2.04994400
P	1.07332800	-1.34477500	-2.13561400
N	3.26918300	0.10261000	-0.80346700
C	1.83947200	1.01277800	3.24422200
H	0.89707200	0.63402300	3.64778200
C	3.04815600	-1.61263900	3.11831700
H	2.15961400	-2.06035100	3.57226300
C	4.12999300	0.57032200	1.46116000
H	4.47938700	1.34680400	2.14860400
H	4.90008300	-0.20948600	1.42853500
C	3.89129600	1.14453800	0.06353200
H	3.19437600	1.98525400	0.09713000
H	4.83168900	1.49061000	-0.38317500
C	3.05111100	0.57352300	-2.20306900
H	3.99203600	0.95358000	-2.62034400
H	2.33547800	1.39686300	-2.15034300
C	2.50464900	-0.57711900	-3.05085200
H	3.27292000	-1.34595400	-3.19425000
H	2.20621600	-0.22359900	-4.04235800
C	1.15419500	-3.14445700	-2.51642900
H	0.29376300	-3.64577600	-2.06443100
C	-0.44237500	-0.77740500	-3.00367800
H	-1.32396700	-1.16416200	-2.48675900
H	3.92351500	-0.68301100	-0.84808300
H	3.54834500	-2.37218400	2.51162300
H	3.72549300	-1.27986900	3.91106800
H	2.54144500	1.17826900	4.06765500
H	1.64885000	1.96223400	2.73820100
H	2.06706600	-3.57111900	-2.09253100
H	1.14165500	-3.31801700	-3.59704100
H	-0.48153600	0.31290900	-2.98323600
H	-0.44113900	-1.12613300	-4.04104200
H	0.31855100	-1.40452400	0.66881800
H	-0.33621300	-0.75849800	0.45910400
C	-0.48547700	1.46921800	0.47904200
O	0.59027600	1.27924000	-0.24148500
O	-1.36208000	0.10144100	0.32787800
C	-2.36832000	-0.13133300	1.33695400
H	-1.89043000	-0.23752100	2.32004000
H	-3.02003100	0.74815300	1.36573100
H	-0.35191500	1.47565800	1.57751200
C	-3.15971900	-1.36950800	0.99064200
C	-2.93913800	-2.57723800	1.66740800
C	-4.12815500	-1.32786200	-0.02548500
C	-3.66815200	-3.72462100	1.33480500
H	-2.19792400	-2.62026200	2.46163200
C	-4.85531000	-2.47177500	-0.36227000
H	-4.31311100	-0.39415400	-0.55066300
C	-4.62597500	-3.67442000	0.31766700

H	-3.48942900	-4.65275300	1.87028800
H	-5.60415200	-2.42489600	-1.14791200
H	-5.19449900	-4.56324100	0.05936700
C	-1.40173200	2.60259100	0.06166700
C	-2.05503500	3.37341600	1.03220800
C	-1.58632800	2.91473700	-1.29300600
C	-2.88887800	4.43433800	0.65873000
H	-1.90555400	3.15101900	2.08648000
C	-2.41957200	3.96907300	-1.67001100
H	-1.06384400	2.33149700	-2.04373800
C	-3.07498500	4.73196900	-0.69390600
H	-3.38616000	5.02671000	1.42164600
H	-2.55645900	4.20150500	-2.72257900
H	-3.72023600	5.55500200	-0.98780300

IV(a)

First vibrational frequency: 21.22 cm⁻¹

1 2

Co	1.25421800	0.00004900	-0.56812700
P	1.47310000	2.24613700	-0.46115500
P	1.47374200	-2.24596100	-0.46089000
N	1.64540900	0.00021400	1.49436300
C	3.01374000	2.97589500	-1.16488000
H	2.98211100	2.89778500	-2.25521900
C	0.16403100	3.43271600	-0.97800500
H	0.06204000	3.40438600	-2.06629600
C	1.63404300	2.47861800	1.38286400
H	2.18854000	3.38773300	1.63867300
H	0.62174000	2.58521500	1.79114700
C	2.31647100	1.24081500	1.97482200
H	3.36252500	1.18882600	1.65549300
H	2.30979900	1.28271700	3.07199200
C	2.31718000	-1.24002600	1.97477500
H	2.31081700	-1.28181800	3.07195200
H	3.36312800	-1.18757700	1.65517000
C	1.63518200	-2.47820700	1.38310700
H	0.62302100	-2.58522800	1.79163500
H	2.19014800	-3.38704000	1.63889400
C	0.16499300	-3.43305600	-0.97736200
H	0.06286100	-3.40496700	-2.06564500
C	3.01446900	-2.97522300	-1.16493200
H	2.98258300	-2.89704600	-2.25525800
H	1.04424500	-0.00022400	-2.06587100
H	0.69253500	-0.00008300	1.86509500
C	-3.62282100	-0.00000800	1.14303600
C	-4.95701200	0.00016900	1.53779200
C	-5.97492200	-0.00007000	0.57137700
C	-5.65995300	-0.00047600	-0.79176400
C	-4.32331100	-0.00063800	-1.19195700
C	-3.29881700	-0.00041400	-0.22816500
C	-1.90733900	-0.00065300	-0.68517700

H	-2.82438200	0.00016200	1.87811800
H	-5.21211700	0.00047200	2.59303900
H	-7.01471600	0.00006000	0.88498800
H	-6.45113700	-0.00065400	-1.53478200
H	-4.06766800	-0.00096700	-2.24840600
H	-0.79194700	3.14787200	-0.53120900
H	0.41629900	4.45187300	-0.66851400
H	3.11654000	4.02801100	-0.88117400
H	3.88516400	2.42051100	-0.80728300
H	-0.79103000	-3.14848000	-0.53049300
H	0.41767200	-4.45206400	-0.66771400
H	3.88580000	-2.41959500	-0.80748700
H	3.11765900	-4.02732600	-0.88132000
O	-0.92616400	-0.00044900	0.06307300
H	-1.75289000	-0.00106600	-1.77774100

IV(a) -TS

First vibrational frequency: -602.38 cm⁻¹

1 2

Co	-0.69038900	0.02465800	0.14211200
P	0.28568000	2.10184700	0.48551900
P	-2.21965200	-1.70677700	0.30817600
N	-2.13939100	1.02750900	-0.89726200
C	-0.06382900	2.82150400	2.14794200
H	0.54153500	2.30262800	2.89627200
C	2.01283000	2.62796800	0.14491100
H	2.69374700	2.12550300	0.83621600
C	-0.75559100	3.09258800	-0.69057100
H	-0.78048300	4.15463000	-0.42406300
H	-0.30017200	3.01018100	-1.68441500
C	-2.16802800	2.50984800	-0.69607500
H	-2.66284300	2.69424500	0.26236600
H	-2.77971100	2.97731400	-1.47707700
C	-3.51656000	0.45085800	-0.79966800
H	-4.15387900	0.87934300	-1.58252800
H	-3.92741300	0.76188400	0.16572000
C	-3.47960100	-1.07367100	-0.90087700
H	-3.16266400	-1.38608600	-1.90251900
H	-4.47348700	-1.49625000	-0.71989100
C	-1.87050400	-3.43217600	-0.22551800
H	-1.21821300	-3.91884300	0.50487200
C	-3.13650100	-1.91103300	1.89412600
H	-2.45550100	-2.30056400	2.65578500
H	0.49600300	-0.75204300	0.80922900
H	-1.80028300	0.85211400	-1.84687400
C	3.27088200	-0.38864600	-1.22154900
C	4.65111900	-0.24957100	-1.04675600
C	5.27879900	-0.81897700	0.06594200
C	4.52398700	-1.54033300	1.00039400
C	3.14834400	-1.68810900	0.81913100
C	2.51210100	-1.10271900	-0.28615100

C	1.04177900	-1.33173000	-0.51936100
H	2.77364200	0.03839200	-2.08651200
H	5.23614800	0.29854600	-1.77981400
H	6.35086700	-0.70946300	0.20191100
H	5.00896100	-1.98972800	1.86209300
H	2.56314700	-2.25395100	1.54087500
H	2.28923700	2.35269100	-0.87461800
H	2.10793500	3.71135600	0.26810300
H	0.17465200	3.88964100	2.16949300
H	-1.11737800	2.68191300	2.40416400
H	-1.36794800	-3.42186900	-1.19617000
H	-2.79976200	-4.00446100	-0.30695800
H	-3.51481800	-0.94366400	2.23521700
H	-3.97579100	-2.60309300	1.77308200
O	0.43208900	-0.77302000	-1.50746900
H	0.72822700	-2.34540200	-0.22134700

IV(b)

First vibrational frequency: 20.20 cm⁻¹

1	2		
Co	1.35328600	0.00005000	-0.56710600
P	1.50876500	-2.25743700	-0.45223000
P	1.50838600	2.25756300	-0.45224900
N	1.98042000	0.00011600	1.42669200
C	-0.00056400	-3.30040900	-0.63089400
H	-0.37338000	-3.22779500	-1.65640900
C	2.77360600	-3.18269800	-1.42087400
H	2.48950900	-3.18200500	-2.47689300
C	2.03296200	-2.46974900	1.33063100
H	1.63639300	-3.39236600	1.76675300
H	3.12698700	-2.54510200	1.34896000
C	1.57587100	-1.24653500	2.13433900
H	0.48641000	-1.22600800	2.22739300
H	2.00004200	-1.26982400	3.14699100
C	1.57565700	1.24669900	2.13433500
H	1.99983500	1.27006800	3.14698200
H	0.48620100	1.22598400	2.22740500
C	2.03252600	2.46999000	1.33061700
H	3.12653600	2.54554800	1.34895200
H	1.63578200	3.39253900	1.76672500
C	2.77309700	3.18300800	-1.42088800
H	2.48901100	3.18226300	-2.47691000
C	-0.00110600	3.30028900	-0.63097500
H	-0.37384000	3.22764300	-1.65651800
H	1.03085800	0.00003000	-2.04618900
H	3.00190700	0.00020300	1.37789900
C	-3.56482500	-0.00013100	1.09784100
C	-4.91609000	-0.00012600	1.43026800
C	-5.88814100	-0.00015600	0.41775200
C	-5.51066200	-0.00020000	-0.92938400
C	-4.15686300	-0.00022000	-1.26697900

C	-3.17803200	-0.00017100	-0.25672300
C	-1.76760100	-0.00017200	-0.65214800
H	-2.80103300	-0.00010100	1.86885600
H	-5.21998000	-0.00009000	2.47249400
H	-6.94137300	-0.00014900	0.68274300
H	-6.26658500	-0.00022500	-1.70829200
H	-3.85182800	-0.00025100	-2.31034200
H	3.74455600	-2.68947400	-1.32389200
H	2.85779800	-4.21699400	-1.07271900
H	0.22579500	-4.34705200	-0.40483500
H	-0.78090900	-2.94738800	0.04742000
H	3.74412000	2.68993200	-1.32389100
H	2.85712900	4.21732000	-1.07274000
H	-0.78144300	2.94712500	0.04727400
H	0.22506700	4.34696400	-0.40487500
O	-0.81797000	-0.00014500	0.13570700
H	-1.56772900	-0.00020200	-1.73729100

IV (b) -TS

First vibrational frequency: -603.86 cm⁻¹

1 2

Co	-0.73366400	0.08453500	0.26923400
P	-2.33208300	-1.61090600	0.37186100
P	0.33978800	2.12221600	0.59184800
N	-2.20586600	1.17860000	-0.59983800
C	-2.02562700	-3.22422800	-0.46163000
H	-1.31200000	-3.81232900	0.12179600
C	-3.13398300	-2.08793800	1.96022000
H	-2.41342700	-2.63256600	2.57671900
C	-3.68206600	-0.79814000	-0.62863100
H	-4.19825800	-1.52166700	-1.26658600
H	-4.42414300	-0.38940600	0.06694500
C	-3.06738900	0.32511700	-1.46832000
H	-2.43033600	-0.07611000	-2.26094000
H	-3.85129400	0.93523800	-1.93390600
C	-1.66394200	2.38065300	-1.29831500
H	-2.48540400	2.96032900	-1.73736600
H	-1.02604600	2.02503700	-2.11210300
C	-0.87060200	3.22899800	-0.30198300
H	-1.54555300	3.67321900	0.43891000
H	-0.35866500	4.05098800	-0.81131300
C	0.41107000	2.78173500	2.31074900
H	1.16882100	2.23091800	2.87491300
C	1.98328900	2.57039000	-0.10365700
H	2.76245100	1.97124800	0.37234200
H	0.44012100	-0.74218800	0.89716000
H	-2.79728200	1.52135800	0.16220200
H	-3.44399600	-1.19025800	2.50172100
H	-4.00726900	-2.72384400	1.78430000
H	-2.95877800	-3.78863100	-0.55185600
H	-1.60808800	-3.04931000	-1.45626000

H	-0.55647500	2.64005300	2.79960400
H	0.66590500	3.84607600	2.31322700
H	2.00071500	2.37064800	-1.17718300
H	2.18344600	3.63261500	0.06953800
C	3.18201500	-0.50851800	-1.26453000
C	4.57331400	-0.44503500	-1.14177600
C	5.20861700	-1.03396100	-0.04375500
C	4.44921500	-1.69877300	0.92828700
C	3.06176300	-1.77172200	0.79874100
C	2.41878800	-1.16647500	-0.29193500
C	0.93322300	-1.32327000	-0.47976900
H	2.67905500	-0.06550700	-2.11787100
H	5.16038400	0.05910500	-1.90419300
H	6.28939400	-0.98336100	0.05195600
H	4.93958500	-2.16252400	1.77926400
H	2.47285800	-2.29389200	1.54974000
O	0.31747100	-0.71689400	-1.43174400
H	0.58283100	-2.32539400	-0.18506100

IV(c)

First vibrational frequency: 19.84 cm⁻¹

1 2

Co	0.77682900	0.34039500	-0.36063800
P	2.69245300	1.54044500	-0.41032900
P	1.08188300	-1.98881100	-0.53090800
N	1.14698700	0.06831800	1.69820500
H	0.50003900	0.71940200	2.14523600
C	2.97952800	1.73539700	1.42061400
H	4.02517100	1.95919000	1.65856300
H	2.37475400	2.58640000	1.75683800
C	2.52763000	0.45082600	2.11995800
H	2.57056900	0.56422100	3.21083900
H	3.19726100	-0.37056000	1.85326800
C	1.40042900	-2.38834300	1.26729000
H	1.00324000	-3.37242200	1.53939700
H	2.48461000	-2.43119200	1.41675200
C	0.76659100	-1.30467200	2.15019500
H	1.05026300	-1.45074500	3.20123100
H	-0.32355700	-1.36370400	2.09208500
C	4.26118000	0.82961300	-1.06986000
H	4.15861400	0.66329800	-2.14570700
H	5.09927500	1.51026100	-0.88889800
H	4.46972200	-0.13036200	-0.59058100
C	2.43949100	-2.87221500	-1.42029200
H	2.45560800	-3.93720500	-1.16597400
H	2.29175900	-2.76744700	-2.49909700
H	3.40389800	-2.42787800	-1.16112400
C	-0.38633800	-3.03493000	-0.94967200
H	-0.64469800	-2.89419300	-2.00341600
H	-0.17887900	-4.09521900	-0.77135500
H	-1.24459300	-2.73312800	-0.34325900

C	2.70962900	3.26052700	-1.07148200
H	3.63624300	3.77754000	-0.80226500
H	2.62179600	3.22740800	-2.16094500
H	1.85657200	3.81627300	-0.67304100
C	-2.20601700	0.41778900	-0.73557800
O	-1.26206900	0.27350200	0.05535100
H	-1.99540300	0.51685400	-1.81091300
H	0.56719200	0.58779100	-1.81971300
C	-3.60730800	0.45908700	-0.33237400
C	-3.99021400	0.35305400	1.02034400
C	-4.58792800	0.60253500	-1.33207700
C	-5.33836000	0.38850400	1.36041200
H	-3.22591300	0.24402400	1.78286200
C	-5.93845900	0.63624300	-0.98562300
H	-4.28677200	0.68415300	-2.37309100
C	-6.31159600	0.52959700	0.35863900
H	-5.63947600	0.30719600	2.40018200
H	-6.69579700	0.74487200	-1.75537100
H	-7.36283200	0.55569000	0.63005500

IV(c) -TS

First vibrational frequency: -374.69 cm⁻¹

1 2

Co	-0.30237400	-0.07554400	-0.08454400
P	-0.44822900	2.06102900	0.61200600
P	-2.17931800	-1.40186100	0.61714800
N	-1.45636900	0.45664300	-1.69446300
H	-0.78092600	0.54301100	-2.45562600
C	-1.18935400	2.80847100	-0.92340700
H	-1.71521300	3.74630100	-0.71578100
H	-0.36457100	3.03525900	-1.60914600
C	-2.13620700	1.77989600	-1.54517800
H	-2.50401000	2.12226300	-2.52013000
H	-3.00543700	1.63567600	-0.89970500
C	-3.25509600	-1.09524100	-0.88121800
H	-3.82011000	-1.99264800	-1.15512700
H	-3.99089200	-0.32882700	-0.61599600
C	-2.39611100	-0.64515200	-2.07056200
H	-3.03400300	-0.32300100	-2.90378200
H	-1.77772700	-1.47358100	-2.42402900
C	-1.56583800	2.54797500	1.99127800
H	-1.21064000	2.09691900	2.92168700
H	-1.58515400	3.63666300	2.10193400
H	-2.57977700	2.18972200	1.79756700
C	-3.35106300	-1.18511300	2.02948100
H	-4.22831100	-1.83111400	1.91931700
H	-2.84078600	-1.43664000	2.96372000
H	-3.67929500	-0.14408200	2.08629300
C	-1.91954100	-3.23242300	0.60182500
H	-1.35476600	-3.52636800	1.49158400
H	-2.87389400	-3.76888700	0.59372100

H	-1.33876900	-3.51032600	-0.28134200
C	1.08312000	3.02731100	0.93504400
H	0.86170500	4.09688100	1.00379800
H	1.52923600	2.69269700	1.87551800
H	1.80167200	2.85598600	0.12967800
C	1.37986800	-1.56135000	-0.00864400
O	0.62894200	-1.55377500	-1.05044100
H	1.18747400	-2.30994600	0.77176500
H	0.57519100	-0.37071400	1.11411400
C	2.75914300	-1.00330300	-0.02726600
C	3.23471800	-0.28326400	-1.13478400
C	3.61369500	-1.25468800	1.05720800
C	4.54652600	0.19185500	-1.14705200
H	2.57538600	-0.11038000	-1.97950300
C	4.92571900	-0.77770300	1.04408900
H	3.24925800	-1.82256200	1.90997500
C	5.39283800	-0.05153600	-0.05743400
H	4.91321000	0.74631200	-2.00592100
H	5.58288000	-0.97492300	1.88573600
H	6.41411600	0.31775400	-0.07046300

V(a)

First vibrational frequency: 17.92 cm⁻¹

1 2

Co	0.94767600	0.03592300	-0.06588400
P	1.14041600	-2.28585700	-0.15535800
P	1.16310200	2.31672300	0.05552900
N	3.00843700	0.03548000	-0.24700700
C	0.83461000	-3.27070100	1.37286200
H	-0.23193100	-3.25540300	1.61123400
C	0.35210200	-3.26466500	-1.49857200
H	-0.73096200	-3.28143400	-1.35262500
C	2.96882200	-2.43262300	-0.45653300
H	3.37256200	-3.37315400	-0.06893400
H	3.13352200	-2.42513800	-1.54046100
C	3.66218500	-1.23424600	0.19272100
H	3.58460600	-1.27948300	1.28346600
H	4.72853900	-1.21431400	-0.06318200
C	3.66300600	1.23567800	0.36269600
H	4.73481100	1.23325700	0.13014000
H	3.55963600	1.14311600	1.44835000
C	2.99852500	2.52054600	-0.14137000
H	3.21097200	2.66659300	-1.20695400
H	3.38566500	3.39331100	0.39356800
C	0.36898200	3.39663000	-1.19801500
H	-0.71614600	3.30454700	-1.10472300
C	0.73194500	3.08110400	1.67136600
H	-0.34131400	2.96261500	1.84252200
H	3.14657400	0.10411600	-1.25908800
C	-3.61729500	0.56756800	-0.83434800
C	-4.96427700	0.84913600	-1.09510400

C	-5.96715700	0.31792400	-0.27842000
C	-5.61264700	-0.49499100	0.80572300
C	-4.26726600	-0.77155300	1.06393500
C	-3.25387800	-0.24735500	0.24534600
C	-1.79592500	-0.59942000	0.52054000
H	-2.83414000	0.98102000	-1.46113500
H	-5.22904700	1.48416500	-1.93674200
H	-7.01219200	0.53660400	-0.47965800
H	-6.38311800	-0.90834600	1.45124400
H	-4.00125500	-1.39965300	1.91224900
H	0.56521700	-2.79584200	-2.46274600
H	0.72862200	-4.29215700	-1.50328900
H	1.15762700	-4.30721100	1.23503000
H	1.38108600	-2.83168400	2.21195400
H	0.66204400	3.07264700	-2.19994400
H	0.65737900	4.44247800	-1.05505200
H	1.26934600	2.57388000	2.47697600
H	0.98542200	4.14556600	1.68094600
O	-0.91143600	0.24417300	-0.15266300
H	-1.64308600	-0.57222700	1.61569500
H	-1.65841900	-1.66070100	0.23082600

v(b)

First vibrational frequency: 20.71 cm⁻¹

1 2

Co	0.79166900	-0.54513900	-0.24236400
P	0.26817500	1.60802100	-0.66484800
P	3.05685700	-0.80625900	-0.48610200
N	1.31710200	0.05023300	1.80833300
C	1.46524400	2.86733300	-1.27399100
H	1.71272800	2.65929500	-2.31850700
C	-1.28130600	2.02354200	-1.56212200
H	-1.14699000	1.83400000	-2.63064900
C	-0.06850400	2.04017100	1.10929200
H	-0.16003300	3.12400300	1.24288100
H	-1.03258700	1.58422900	1.35573500
C	1.03729000	1.49885100	2.03047000
H	1.96545900	2.04436100	1.83933100
H	0.76904300	1.68744800	3.07748000
C	2.68343600	-0.36590200	2.24906500
H	2.65051000	-0.79917100	3.25467100
H	3.30738000	0.52969200	2.31258700
C	3.32412100	-1.36365200	1.26933500
H	2.84464200	-2.34607700	1.35608300
H	4.38799200	-1.49771400	1.49674500
C	3.58784400	-2.23319100	-1.52188200
H	3.50796000	-1.96306600	-2.57855400
C	4.34406300	0.46854900	-0.81710900
H	4.23247500	0.84028500	-1.83910900
H	-1.64903800	-1.09285600	-1.63815800
H	0.61710100	-0.49636800	2.30774300

C	-3.54650200	-0.46409400	1.05073200
C	-4.83810700	-0.04426900	1.39248900
C	-5.86956000	-0.09781600	0.45016800
C	-5.60017800	-0.57454300	-0.83887900
C	-4.30989500	-0.99204200	-1.17641400
C	-3.26829200	-0.94191800	-0.23596800
C	-1.87909900	-1.44142300	-0.61630800
H	-2.74261000	-0.42230500	1.77841700
H	-5.03721300	0.32405200	2.39554000
H	-6.87130700	0.22937200	0.71404900
H	-6.39317700	-0.61661900	-1.58071500
H	-4.10935100	-1.35774100	-2.18179600
H	-2.10097200	1.40362300	-1.19360600
H	-1.53226500	3.07897100	-1.41666200
H	1.03099200	3.86944500	-1.20107200
H	2.38555500	2.83438000	-0.68748300
H	2.93400600	-3.08838500	-1.33147300
H	4.62233800	-2.51429700	-1.30144300
H	4.24356200	1.31026800	-0.12834000
H	5.34201400	0.03457100	-0.70180600
O	-0.87633300	-1.07344600	0.29759200
H	-1.92117100	-2.54272300	-0.68616400

VI (a)

First vibrational frequency: 18.42 cm⁻¹

1 2

Co	-1.26759800	-0.11570300	-0.58505500
P	-0.80858200	-2.36686700	-0.52857400
P	-1.95555100	2.05556900	-0.30890800
N	-1.56461400	-0.29523700	1.41246600
C	-2.06022700	-3.50570700	-1.25461900
H	-2.06807800	-3.38979400	-2.34197600
C	0.80904100	-3.01928800	-1.09414500
H	0.87170800	-2.95333900	-2.18335100
C	-0.86738400	-2.65592300	1.30151000
H	-1.14231200	-3.68891500	1.53541200
H	0.13856200	-2.47799600	1.69662000
C	-1.85995100	-1.66697000	1.91039600
H	-2.88839900	-1.91155600	1.62614500
H	-1.80387400	-1.68635100	3.00592400
C	-2.42868400	0.73681900	2.04970400
H	-2.33022000	0.68081300	3.14099100
H	-3.46836800	0.50415900	1.79832100
C	-2.03153500	2.12142400	1.54159000
H	-1.03307900	2.38868200	1.90326600
H	-2.73231000	2.88718900	1.88798000
C	-0.85668500	3.42591200	-0.82923500
H	-0.85813000	3.50449500	-1.91961800
C	-3.63455000	2.53444500	-0.89438600
H	-3.65416300	2.52382800	-1.98760800
H	-0.58361500	-0.07394800	1.62707000

C	3.27059700	0.11079400	1.01671600
C	4.56490800	0.04367800	1.54986500
C	5.66904700	0.39170900	0.76660500
C	5.46871900	0.81310800	-0.55505000
C	4.17585800	0.88182300	-1.07997100
C	3.05951500	0.53111000	-0.30204400
C	1.65470200	0.59380000	-0.90266700
H	2.40684300	-0.15400700	1.61827500
H	4.70943200	-0.28149500	2.57727100
H	6.67313700	0.34049800	1.17860600
H	6.31929000	1.09033200	-1.17248000
H	4.02993200	1.21559700	-2.10619500
H	1.60949600	-2.41960500	-0.65561100
H	0.92493800	-4.06439400	-0.79104400
H	-1.82646600	-4.54532800	-1.00489700
H	-3.05475000	-3.25852200	-0.87351300
H	0.15728600	3.20488500	-0.48989900
H	-1.19418700	4.37436700	-0.40049400
H	-4.37530300	1.81854100	-0.52818100
H	-3.89551000	3.53636900	-0.53965100
O	0.63861500	0.40451400	0.01689500
H	1.57131000	1.56942300	-1.42928800
H	1.62536900	-0.16246600	-1.71797700
H	-0.98501300	-0.36314700	-2.25097300
H	-1.21322600	0.39526700	-2.21244000

VI (a) -TS

First vibrational frequency: -564.95 cm⁻¹

1 2

Co	1.16977500	0.02642300	-0.51146300
P	1.29915600	2.32703700	-0.50331500
P	1.66545600	-2.22405400	-0.36162500
N	1.68022100	0.12173500	1.44012700
C	2.81409200	3.09225300	-1.21764600
H	2.80249000	2.96756300	-2.30393700
C	-0.08310000	3.37597000	-1.09229400
H	-0.12505100	3.33537000	-2.18413200
C	1.42638100	2.59061800	1.32759700
H	1.89034600	3.55063700	1.57536200
H	0.40943800	2.59467000	1.73541200
C	2.23431000	1.43118900	1.90900500
H	3.27677200	1.47867300	1.57998500
H	2.23052500	1.45951800	3.00491000
C	2.48275700	-1.02584600	1.96792300
H	2.49717300	-0.99230900	3.06360000
H	3.51020100	-0.88786300	1.61847700
C	1.91560900	-2.35616600	1.47098400
H	0.93992200	-2.55413100	1.92908500
H	2.58089900	-3.18401100	1.73639000
C	0.57906600	-3.62679900	-0.83656400
H	0.42149400	-3.61123900	-1.91820100

C	3.29562800	-2.65381000	-1.10568200
H	3.21650800	-2.61211000	-2.19541100
H	0.73245900	0.04080900	1.82207900
C	-3.63365700	0.85391600	0.30068900
C	-4.97226500	1.21550000	0.49771300
C	-5.98739800	0.26389200	0.36016000
C	-5.65326200	-1.05297600	0.01924100
C	-4.31607700	-1.40812800	-0.17879900
C	-3.28914000	-0.46050900	-0.03765500
C	-1.83222100	-0.87800100	-0.21736600
H	-2.84120200	1.58817300	0.40071000
H	-5.22142800	2.24115500	0.75813700
H	-7.02635500	0.54347300	0.51123700
H	-6.43418300	-1.79983700	-0.09774000
H	-4.06765100	-2.43283600	-0.44986600
H	-1.01865900	2.98072300	-0.69218400
H	0.05473700	4.41435100	-0.77602700
H	2.85942900	4.15924300	-0.97831700
H	3.70547600	2.59682100	-0.82376200
H	-0.38900200	-3.53314500	-0.34050100
H	1.04209000	-4.57748400	-0.55469900
H	4.05510600	-1.93450900	-0.78810100
H	3.60276200	-3.66027400	-0.80479100
O	-0.96125400	0.20334800	-0.37018400
H	-1.55880400	-1.49197300	0.66492200
H	-1.79078300	-1.56948600	-1.08126100
H	-0.04447300	0.04056900	-1.64046800
H	0.68080400	-0.05428400	-2.11055200

VI (b)

First vibrational frequency: 22.97 cm⁻¹

1 2

Co	1.32022600	0.15006100	-0.54350700
P	2.00939900	-2.03618100	-0.32091600
P	0.85606300	2.40737300	-0.49408100
N	1.87003900	0.36716100	1.40752200
C	0.71416000	-3.32410600	-0.47506600
H	0.42153100	-3.42338200	-1.52342000
C	3.45503900	-2.70479000	-1.24123500
H	3.19558900	-2.81385800	-2.29787000
C	2.51759600	-2.01842700	1.46367600
H	2.34186400	-2.98806500	1.93967200
H	3.59472500	-1.81876700	1.50738400
C	1.73314200	-0.91265700	2.16499000
H	0.66645800	-1.14574600	2.18931900
H	2.08773500	-0.77330500	3.19359000
C	1.11211300	1.46998500	2.07055000
H	1.46527900	1.59444300	3.10152600
H	0.06640000	1.15591500	2.09119600
C	1.27508900	2.76407800	1.27806400
H	2.31172600	3.11835500	1.31827800

H	0.64008300	3.55658400	1.68586400
C	1.84290200	3.60124400	-1.48710300
H	1.58795500	3.49328400	-2.54499600
C	-0.88538000	2.93656600	-0.72577900
H	-1.16990900	2.81170700	-1.77367700
H	2.86030400	0.62511600	1.41425800
C	-3.23948500	-0.16154800	0.96370800
C	-4.55265500	-0.13183600	1.45234500
C	-5.62246800	-0.47173300	0.61940800
C	-5.36842100	-0.84627800	-0.70718000
C	-4.05693800	-0.87591300	-1.18813900
C	-2.97485000	-0.53206300	-0.36032000
C	-1.54737800	-0.54508800	-0.91004700
H	-2.40074400	0.09706900	1.60192300
H	-4.73866700	0.15730800	2.48388700
H	-6.64127700	-0.44938000	0.99643200
H	-6.19203300	-1.11627700	-1.36321800
H	-3.86964800	-1.17128000	-2.21946500
H	4.29859600	-2.01462500	-1.15736300
H	3.74646800	-3.68162900	-0.84260400
H	1.08621700	-4.28657100	-0.11114000
H	-0.15570400	-3.00871900	0.10417100
H	2.90882700	3.39339600	-1.36143800
H	1.63632600	4.62928900	-1.17329300
H	-1.53420000	2.31158900	-0.10895000
H	-0.99987100	3.98806500	-0.44530400
O	-0.57710600	-0.33476900	0.05033100
H	-1.41543100	-1.51127800	-1.44600900
H	-1.51736400	0.22180900	-1.71705900
H	1.22563200	-0.34816700	-2.19100800
H	0.97688100	0.40102500	-2.21359000

VI (b) -TS

First vibrational frequency: -453.05 cm⁻¹

1	2		
Co	1.17624500	-0.46308700	-0.41914000
P	-0.00175800	-2.44219900	-0.13885300
P	2.75157500	1.23202600	-0.28918600
N	1.04785000	-0.28095300	1.57622000
C	-1.64078000	-2.80640400	-0.88664700
H	-1.53892800	-2.88674200	-1.97192400
C	0.95932800	-3.98711900	-0.41970700
H	1.11147200	-4.12591300	-1.49359800
C	-0.28791100	-2.35710800	1.70008200
H	-1.25637200	-2.78465800	1.97552000
H	0.48709500	-2.95179600	2.19698400
C	-0.19892400	-0.89263400	2.13089700
H	-1.04244500	-0.31492900	1.74432400
H	-0.19642600	-0.80479400	3.22398900
C	1.22735500	1.14019500	2.00598400
H	1.15455800	1.20729500	3.09800300

H	0.40419000	1.71023400	1.57023900
C	2.57798900	1.66211900	1.51368700
H	3.39700700	1.18054000	2.06024800
H	2.66192300	2.74010900	1.68076300
C	4.54014100	0.87961800	-0.53744800
H	4.72386100	0.66785600	-1.59437400
C	2.44016300	2.77260500	-1.23309000
H	2.64490400	2.58990900	-2.29161400
H	1.83581500	-0.81124200	1.95930800
C	-2.47148100	1.85737200	0.25871300
C	-3.55028000	2.10509800	1.11549900
C	-4.79060900	1.50232200	0.87948700
C	-4.94201500	0.65244900	-0.22244000
C	-3.85935300	0.40744000	-1.07352400
C	-2.60885400	1.00452500	-0.84497500
C	-1.45073000	0.77399900	-1.81362700
H	-1.50934200	2.32786000	0.43437700
H	-3.42354300	2.77045800	1.96585800
H	-5.62863000	1.69200800	1.54437800
H	-5.90033100	0.17760300	-0.41623700
H	-3.98904600	-0.25426000	-1.92816200
H	1.93684800	-3.90674200	0.06287500
H	0.42770100	-4.85542100	-0.01807800
H	-2.02753100	-3.75087300	-0.49118800
H	-2.34358500	-2.00279400	-0.65719800
H	4.83058800	0.00442500	0.04965800
H	5.14962100	1.73648200	-0.23340200
H	1.38542100	3.03285700	-1.12909800
H	3.08101300	3.58332300	-0.87371500
O	-0.18028800	0.98816000	-1.27707900
H	-1.56761500	-0.24128800	-2.23953600
H	-1.61132800	1.46032700	-2.66982200
H	1.39964300	-0.69765400	-2.07654500
H	0.84071400	-0.06171400	-1.99891900

Co (PNN)

I' (a)

First vibrational frequency: 5.38 cm⁻¹

1 2

Co	1.88915300	-1.06289700	0.23389800
P	2.01232400	-1.13774800	-1.99941700
N	3.02076700	0.65091000	0.09877400
H	2.29625000	1.37136700	0.06816900
C	2.82626000	0.39799400	2.50444900
H	2.00099400	1.11446500	2.55216300
H	3.34654800	0.42185500	3.47164300
C	3.76682900	0.79111400	1.37035800
H	4.63931300	0.13268800	1.32624800
H	4.13454100	1.81382200	1.52308000
C	2.96691100	0.42792400	-2.35488300
H	3.57256800	0.34461900	-3.26314700

H	2.23562300	1.22800400	-2.51954400
C	3.84085200	0.75149800	-1.13630700
H	4.28892400	1.74918900	-1.23055800
H	4.65864900	0.02931100	-1.04589300
C	1.01919100	-1.11154700	3.10916000
H	0.59353700	-2.10161700	2.94335400
H	1.27455600	-1.00024300	4.17255300
H	0.28216200	-0.35556700	2.83537900
C	0.55143300	-1.07395400	-3.11548100
H	0.86306700	-0.94762600	-4.15707500
H	-0.01429200	-2.00499600	-3.02239300
H	-0.09571000	-0.24096700	-2.83003500
C	3.03682900	-2.49557900	-2.70893000
H	2.52242400	-3.44892900	-2.56032900
H	3.20527800	-2.33872400	-3.77887700
H	4.00111600	-2.54196800	-2.19559300
C	3.19533600	-2.02568500	2.60405600
H	3.49816600	-1.95343100	3.65785000
H	2.72721500	-2.99481100	2.42736700
H	4.08482600	-1.95151800	1.97510600
C	-1.09220600	1.24781500	0.16509800
O	0.03723900	0.78912300	0.33355600
O	-2.19351100	0.49057400	0.11399600
C	-2.04073200	-0.95451000	0.29676300
H	-1.35719800	-1.32641100	-0.46796200
H	-1.59053600	-1.12237100	1.27699200
C	-3.40494500	-1.57735900	0.19222400
C	-4.20856000	-1.72179500	1.33285200
C	-3.89476200	-2.01356500	-1.04768000
C	-5.48320800	-2.28684100	1.23566200
H	-3.83420900	-1.39334600	2.29922300
C	-5.16903900	-2.57921900	-1.14779400
H	-3.27617400	-1.91222800	-1.93579200
C	-5.96548000	-2.71584500	-0.00568700
H	-6.09600000	-2.39601500	2.12573700
H	-5.53732300	-2.91595100	-2.11252000
H	-6.95456200	-3.15826900	-0.08175700
C	-1.38239600	2.70025700	0.00301800
C	-2.68246700	3.16788000	-0.25484600
C	-0.32535800	3.61732400	0.11853800
C	-2.91519300	4.53632700	-0.39932100
H	-3.50121400	2.46329800	-0.34272400
C	-0.56261400	4.98424100	-0.02257100
H	0.67486400	3.25406700	0.32580100
C	-1.85808300	5.44570200	-0.28309800
H	-3.92063600	4.89294100	-0.60086100
H	0.25865000	5.68810000	0.07152900
H	-2.04310500	6.51014000	-0.39346500
H	1.08372800	-2.34794400	0.32533100
N	2.22559800	-0.95192400	2.26167100

I'(a) -TSFirst vibrational frequency: -654.61 cm⁻¹

1 2

Co	1.33266000	-0.14167200	0.06235500
P	1.12937600	-2.61843400	-0.06178400
N	3.01036700	-0.43516500	-1.10319700
H	2.80963100	0.20903200	-1.86852300
C	3.73783600	1.07903100	0.70258300
H	3.35488900	1.98514300	0.22331800
H	4.58079800	1.37077800	1.34422700
C	4.19497200	0.08245500	-0.35440700
H	4.69566500	-0.76814600	0.11197400
H	4.92045400	0.55454500	-1.02578900
C	1.94749200	-2.62235500	-1.73700700
H	2.17510300	-3.64004800	-2.07475600
H	1.22627400	-2.18984800	-2.43904000
C	3.23219900	-1.79179800	-1.70619100
H	3.65012500	-1.68585300	-2.71303100
H	3.98610000	-2.30289800	-1.10196000
C	2.02342400	1.60069900	2.34540500
H	1.20964500	1.19168800	2.94543200
H	2.78054300	2.03426300	3.01224300
H	1.62738800	2.38209200	1.69593300
C	-0.38318900	-3.63506900	-0.38250600
H	-0.10418700	-4.63579300	-0.72816900
H	-0.97075300	-3.73189700	0.53470900
H	-1.00145900	-3.15983600	-1.14624700
C	2.14334300	-3.82413600	0.91675900
H	1.68801900	-3.95675600	1.90265100
H	2.18580100	-4.79537600	0.41279500
H	3.16289300	-3.46029100	1.06333500
C	3.10722100	-0.54412600	2.44727300
H	3.81809300	-0.12266000	3.17071700
H	2.25560600	-0.96530500	2.98342600
H	3.60006900	-1.34212200	1.89554200
C	-0.65179700	0.85461800	-0.53235500
O	-0.01666100	0.12038300	-1.38962900
O	-1.95369300	0.59897900	-0.20817300
C	-2.40684100	-0.77541200	-0.26185500
H	-2.17540700	-1.18150300	-1.24883500
H	-1.85566800	-1.33860000	0.49848800
C	-3.88729200	-0.78770700	0.00989400
C	-4.36896600	-0.88162400	1.32377600
C	-4.80416500	-0.68954800	-1.04696700
C	-5.74329300	-0.87299300	1.57876900
H	-3.66552100	-0.96415400	2.14867600
C	-6.17917800	-0.68111900	-0.79535900
H	-4.44009500	-0.62184000	-2.06913800
C	-6.65085200	-0.77174600	0.51872300
H	-6.10472600	-0.94870200	2.60028200
H	-6.87991600	-0.60715500	-1.62200300

H	-7.71916100	-0.76823800	0.71505900
C	-0.40892300	2.34740900	-0.48375800
C	-1.00888000	3.14546000	0.50182900
C	0.41011400	2.94091300	-1.45326700
C	-0.78192800	4.52243700	0.52095100
H	-1.64697500	2.68745200	1.25049100
C	0.63118400	4.32157800	-1.43505400
H	0.85711000	2.32165800	-2.22387100
C	0.03899000	5.11409900	-0.44731500
H	-1.24630700	5.13437700	1.28864300
H	1.26024200	4.77618200	-2.19479200
H	0.21205600	6.18618900	-0.43239800
H	0.02436700	0.37589100	0.78739600
N	2.62118700	0.51203900	1.52452200

I'(c)

First vibrational frequency: 11.20 cm⁻¹

1 2

Co	-1.37243100	-0.21677600	-0.01116800
P	-2.81277900	-1.73743300	-0.83619500
N	-2.74319400	1.31913300	-0.76969300
H	-2.15879300	2.05868100	-1.15201800
C	-2.61783400	1.78612800	1.64589500
H	-3.17072300	2.17979300	2.51224500
H	-1.73303200	2.41240300	1.50331700
C	-3.49012900	1.85029400	0.39384400
H	-3.81700200	2.88568400	0.23077100
H	-4.39630900	1.25503000	0.52860600
C	-4.14358700	-0.61638700	-1.51244800
H	-4.61666600	-1.06144600	-2.39451100
H	-4.92277300	-0.53803600	-0.74593800
C	-3.58467600	0.77385500	-1.86166000
H	-4.41478200	1.45276900	-2.10497000
H	-2.94788000	0.70488900	-2.74769800
C	-3.23781000	-0.42545300	2.47577400
H	-2.87686400	-1.44218500	2.64062500
H	-3.58847100	-0.01453100	3.43396900
H	-4.08310800	-0.46256000	1.78945900
C	-3.76995500	-3.03136000	0.08069700
H	-4.49962300	-3.50687600	-0.58277300
H	-3.07800200	-3.79542800	0.44714400
H	-4.29560000	-2.60303900	0.93552300
C	-2.24502800	-2.71088900	-2.29824600
H	-1.85503100	-2.03215600	-3.05972100
H	-1.43782200	-3.38332100	-1.99324200
H	-3.06508500	-3.30234900	-2.71741400
C	-1.06324300	0.44326400	2.94200000
H	-1.43930000	0.85787700	3.88850300
H	-0.69973600	-0.57075600	3.12649400
H	-0.23817900	1.05844800	2.58618300
C	1.44450200	1.18743200	0.02730600

O	0.23437800	1.07984500	0.25976900
O	2.30403400	0.17286600	0.03664200
C	1.84384900	-1.16943800	0.41545400
H	1.48501700	-1.11703700	1.44605400
H	1.01856700	-1.44089000	-0.24643600
H	-0.77120900	-0.54267500	-1.33980900
C	3.01021100	-2.10664600	0.27660600
C	3.28537600	-2.71342700	-0.95812000
C	3.84020400	-2.37926300	1.37356000
C	4.37780600	-3.57336200	-1.09627900
H	2.64254600	-2.51224600	-1.81132900
C	4.93227400	-3.24135700	1.23812200
H	3.63035700	-1.91791800	2.33533000
C	5.20292900	-3.83855000	0.00246400
H	4.58202200	-4.03876400	-2.05612400
H	5.56763500	-3.44809900	2.09435800
H	6.05007700	-4.51004800	-0.10315500
C	2.07926400	2.49558600	-0.27236600
C	3.46810500	2.61364400	-0.45529400
C	1.26343600	3.63565600	-0.36518800
C	4.02901100	3.86138200	-0.72854200
H	4.09881800	1.73542900	-0.38167100
C	1.82937300	4.87995500	-0.63897800
H	0.19355600	3.53649100	-0.22079900
C	3.21266200	4.99443600	-0.82053300
H	5.10188800	3.95037500	-0.86812800
H	1.19543200	5.75837500	-0.71013400
H	3.65323800	5.96412700	-1.03264600
N	-2.13874600	0.39940400	1.92094000

I'(c) -TS

First vibrational frequency: -549.03 cm⁻¹

1 2

Co	1.03345100	-0.55744500	-0.26786000
P	1.72790900	-1.45278600	1.71171600
N	2.78302000	0.78737400	-0.05319500
H	2.47054400	1.71930400	-0.31711800
C	3.06283200	-0.35374700	-2.22425300
H	3.79915000	-0.72435100	-2.95195800
H	2.42814700	0.37761200	-2.73153100
C	3.77428500	0.31563600	-1.05060400
H	4.39276800	1.14046000	-1.42580900
H	4.45484100	-0.38524300	-0.56205100
C	3.33368600	-0.55193800	1.98511800
H	3.55631700	-0.46788700	3.05419300
H	4.13280800	-1.15866600	1.54449500
C	3.28669100	0.84424700	1.34140300
H	4.28254500	1.30655300	1.38779900
H	2.60304800	1.48881400	1.90131100
C	2.97806500	-2.65239700	-1.38577700
H	2.30829100	-3.44704500	-1.05364600

H	3.56682100	-3.01785500	-2.23855900
H	3.66233200	-2.40480600	-0.57520100
C	2.12231500	-3.21909100	2.07304200
H	2.53545200	-3.31313300	3.08207800
H	1.20613500	-3.81283400	2.00903600
H	2.84370600	-3.61469400	1.35636800
C	0.69311900	-0.99221500	3.16737000
H	0.53229400	0.08844700	3.17939300
H	-0.28083300	-1.48324700	3.08903600
H	1.17720700	-1.29862100	4.09986500
C	1.29125400	-1.87500900	-2.90164800
H	1.88933300	-2.23914700	-3.74807800
H	0.63044100	-2.67766400	-2.56600500
H	0.68654700	-1.02659000	-3.21825300
C	-0.70296900	0.97122200	-0.55999200
O	-0.06100400	0.46970700	-1.55790200
O	-1.97916500	0.58027200	-0.28165400
C	-2.35597700	-0.76937000	-0.66189200
H	-2.15557000	-0.90584600	-1.72688300
H	-1.73149400	-1.46744700	-0.08968400
H	0.05871400	0.24704900	0.64356100
C	-3.81355700	-0.95553500	-0.33697300
C	-4.20748800	-1.42183400	0.92583900
C	-4.79757200	-0.65317100	-1.28952300
C	-5.56170200	-1.57911400	1.23429800
H	-3.45160900	-1.66505900	1.66850400
C	-6.15266800	-0.80904600	-0.98399400
H	-4.50167400	-0.29707400	-2.27311600
C	-6.53686500	-1.27136800	0.27943500
H	-5.85471200	-1.94351500	2.21471700
H	-6.90584800	-0.57376500	-1.73039500
H	-7.58949900	-1.39563500	0.51680400
C	-0.48699600	2.40564800	-0.14873000
C	-1.08429400	2.92659600	1.00804800
C	0.30910600	3.23070100	-0.95408800
C	-0.88109300	4.26286600	1.35642500
H	-1.70311800	2.28785100	1.62977000
C	0.50727700	4.56981100	-0.60422700
H	0.74997000	2.82495900	-1.85892700
C	-0.08454000	5.08717400	0.55216600
H	-1.34414700	4.66180100	2.25408300
H	1.11735700	5.20743600	-1.23721900
H	0.07021500	6.12707400	0.82438900
N	2.17492200	-1.46946700	-1.77633500

III (b)

First vibrational frequency: 14.53 cm⁻¹

1 2

Co	1.65306900	-0.63203600	0.25304100
P	1.12271700	-1.27658700	-1.87926000
N	3.06927100	0.46018100	-0.59986900

C	1.66645000	-2.97938800	-2.32460300
H	1.05101400	-3.70733400	-1.78892000
C	-0.54855400	-1.12512000	-2.61170900
H	-1.20638100	-1.87353700	-2.16305900
C	2.23628300	-0.14029400	-2.83445100
H	2.49813500	-0.55487700	-3.81283500
H	1.69152700	0.79517500	-3.00175800
C	3.48433200	0.11195700	-1.98553500
H	4.11047500	-0.78376500	-1.93020400
H	4.09341200	0.91980800	-2.40851200
C	4.19432700	0.65446900	0.34825400
H	4.78866300	1.53597300	0.08080100
H	4.84830200	-0.21933500	0.28389100
C	3.59689100	0.81652000	1.73774000
H	3.00852600	1.73647500	1.77503300
H	4.38292300	0.87828200	2.50157500
C	1.78512500	0.06429000	3.17077200
H	1.10835000	-0.76130200	3.39838100
C	3.41482500	-1.54669000	2.38827900
H	2.70776200	-2.34928500	2.60672300
H	2.50856800	1.32045000	-0.62608200
H	-0.95475000	-0.13706100	-2.39210000
H	-0.50226500	-1.28509700	-3.69330500
H	1.56353200	-3.14550800	-3.40154600
H	2.71004300	-3.12884600	-2.03562400
H	1.20282200	0.94243000	2.89415100
H	2.38578300	0.28577000	4.06293200
H	4.05309300	-1.85974000	1.56024200
H	4.04061200	-1.37498000	3.27389600
H	0.12830400	-1.20651400	0.84591400
H	0.63270400	-1.78598200	1.02899800
C	-0.60943000	1.37863300	0.76222800
O	0.63694200	1.19078800	0.28655800
O	-1.41635100	0.18412900	0.42397000
C	-2.66928800	0.08915900	1.11197200
H	-2.50323100	0.18078100	2.19656100
H	-3.33129500	0.91000800	0.80469100
H	-0.66014400	1.43928800	1.87340200
C	-3.30639500	-1.24095500	0.79007600
C	-3.01144200	-2.37942700	1.55551400
C	-4.18948900	-1.36691600	-0.29268100
C	-3.57892900	-3.61850600	1.24262300
H	-2.33939100	-2.29273900	2.40606100
C	-4.76058200	-2.60357100	-0.60941400
H	-4.43370100	-0.49028800	-0.88785700
C	-4.45472000	-3.73339400	0.15727400
H	-3.34479000	-4.48985300	1.84799500
H	-5.44573900	-2.68405500	-1.44877000
H	-4.90071800	-4.69396600	-0.08464400
C	-1.28046300	2.63510100	0.20128400
C	-1.91425400	3.54584800	1.05497000

C	-1.26402600	2.90255600	-1.17624000
C	-2.52525400	4.70082200	0.54888700
H	-1.92779000	3.35460700	2.12609600
C	-1.87546900	4.04862400	-1.68784600
H	-0.75834200	2.21150800	-1.84339700
C	-2.50956400	4.95360300	-0.82512200
H	-3.00968600	5.39864200	1.22655500
H	-1.85622000	4.24164200	-2.75731600
H	-2.98246300	5.84727700	-1.22272300
N	2.66240800	-0.31211600	2.03468200

III (b) -TS

First vibrational frequency: -930.98 cm⁻¹

1 2

Co	-1.63537200	-0.40104100	-0.20119700
P	-1.30445300	-0.89034500	2.00257400
N	-3.18709200	0.70302700	0.43088600
C	-1.83835600	-2.57414800	2.52774800
H	-1.14892200	-3.31486500	2.11343800
C	0.27731900	-0.62990700	2.89486400
H	1.02146800	-1.33932500	2.52410400
C	-2.53168200	0.27592900	2.76971600
H	-2.87238000	-0.06877500	3.75123900
H	-2.02724000	1.23870300	2.91059600
C	-3.70534900	0.42528700	1.79851500
H	-4.28759200	-0.49995100	1.74733200
H	-4.38304700	1.22648000	2.11775100
C	-4.23297300	0.73356900	-0.62093500
H	-4.90193100	1.59348100	-0.49653000
H	-4.83782900	-0.17195200	-0.52272600
C	-3.53290200	0.79776900	-1.97050500
H	-3.00010000	1.74856200	-2.05788200
H	-4.25879000	0.73824000	-2.79262500
C	-1.59539400	0.02197900	-3.20750800
H	-0.83954000	-0.76083800	-3.28564800
C	-3.16087100	-1.60110400	-2.35217300
H	-2.38866400	-2.36754700	-2.43879000
H	-2.71010800	1.60942500	0.43963500
H	0.64170000	0.38167900	2.70780700
H	0.13918100	-0.77922200	3.97004800
H	-1.84258200	-2.65795000	3.61905800
H	-2.84073500	-2.78582700	2.14645900
H	-1.10689000	0.97771800	-3.02008200
H	-2.14834400	0.08033300	-4.15529600
H	-3.82951300	-1.87381500	-1.53366600
H	-3.73838300	-1.56569500	-3.28590300
H	0.26681300	-0.72523100	-0.56469700
H	-0.44756400	-1.35857100	-0.70996600
C	0.62328400	1.49468100	-0.80430800
O	-0.56616300	1.45875100	-0.25915200
O	1.31397600	0.05617900	-0.44883400

C	2.41034600	-0.36571500	-1.29111600
H	2.06269000	-0.47155400	-2.32668600
H	3.16891900	0.42292200	-1.26002400
H	0.66671600	1.44624400	-1.90951500
C	2.97507200	-1.66901500	-0.77918100
C	2.72871500	-2.87330500	-1.45287600
C	3.75604300	-1.69078200	0.38771600
C	3.24832000	-4.07957800	-0.96970800
H	2.13141400	-2.86840400	-2.36127900
C	4.27342000	-2.89327100	0.87434300
H	3.96043200	-0.76111000	0.91268500
C	4.01962600	-4.09194500	0.19603900
H	3.05249900	-5.00490000	-1.50403000
H	4.87927000	-2.89589900	1.77605300
H	4.42587500	-5.02687800	0.57125800
C	1.58358700	2.55184700	-0.29562600
C	2.50929700	3.14036000	-1.16714400
C	1.53872300	2.97694200	1.03990900
C	3.38960600	4.12871200	-0.71101600
H	2.53640700	2.83450000	-2.21068300
C	2.41649900	3.96024200	1.49942900
H	0.80009800	2.54260400	1.70576200
C	3.34723700	4.53721600	0.62486500
H	4.10024500	4.57990400	-1.39772700
H	2.37414200	4.28265600	2.53619600
H	4.02759200	5.30493200	0.98235100
N	-2.51338800	-0.28885700	-2.08613100

IV(a)

First vibrational frequency: 20.94 cm⁻¹

1 2

Co	1.31284400	-0.19637900	-0.55095500
P	1.56306800	2.01989800	-0.38262500
N	1.66361800	-0.25356800	1.48738400
C	3.09750000	2.73583500	-1.11236600
H	3.03705900	2.67956100	-2.20275700
C	0.26368100	3.23965100	-0.84252500
H	0.13267000	3.23384700	-1.92809800
C	1.77706900	2.21043100	1.46308100
H	2.38430500	3.08411000	1.72166300
H	0.78124200	2.36271900	1.89633400
C	2.40279900	0.92307800	2.01525600
H	3.44264600	0.82980300	1.68586400
H	2.40300600	0.92771000	3.11300900
C	2.27143700	-1.56973000	1.79335300
H	2.18935800	-1.82634700	2.85729800
H	3.33646600	-1.51357700	1.55099000
C	1.56439000	-2.62142500	0.94455200
H	0.51530400	-2.68595700	1.24935300
H	2.01564600	-3.61203300	1.09496400
C	0.56037300	-3.03119300	-1.23270400

H	0.58060000	-2.75368800	-2.28704400
C	2.91578400	-2.53139500	-1.09951500
H	2.89753800	-2.25713800	-2.15504300
H	1.12082200	-0.14896700	-2.05918900
H	0.71817500	-0.23944500	1.87472400
C	-3.58006600	-0.10211400	1.13110400
C	-4.91263000	-0.02800200	1.52429300
C	-5.92433200	0.08295100	0.55773900
C	-5.60490900	0.11956300	-0.80388100
C	-4.26988300	0.04547600	-1.20251300
C	-3.25153500	-0.06632200	-0.23855600
C	-1.86140800	-0.14025300	-0.69342700
H	-2.78617400	-0.18757300	1.86616200
H	-5.17122500	-0.05498900	2.57833400
H	-6.96287700	0.14102100	0.87010000
H	-6.39142700	0.20567300	-1.54685800
H	-4.01102200	0.07350000	-2.25780800
H	-0.68529700	2.96528400	-0.37484400
H	0.54500800	4.24752900	-0.52159800
H	3.22496900	3.78031400	-0.81113700
H	3.96738200	2.15890800	-0.78654600
H	-0.42746700	-2.81042100	-0.82652200
H	0.75543700	-4.10896100	-1.13726000
H	3.69140500	-1.94468100	-0.60330100
H	3.16273400	-3.59828200	-1.00509700
O	-0.88521600	-0.24397500	0.05435700
H	-1.70317600	-0.09657800	-1.78464900
N	1.58441200	-2.24572900	-0.50368200

IV(a) -TS

First vibrational frequency: -652.59 cm⁻¹

1 2

Co	-0.81571700	-0.17232300	0.15068900
P	0.00124000	1.94303700	0.45842000
N	-2.23990100	0.69002300	-0.99289400
C	-0.43023300	2.66023500	2.10170200
H	0.18185000	2.18227900	2.87146000
C	1.70609700	2.55708400	0.16047800
H	2.39541000	2.08299400	0.86334200
C	-1.06275600	2.85824500	-0.76081600
H	-1.17750500	3.91452000	-0.49614900
H	-0.56181200	2.81234000	-1.73481400
C	-2.42294700	2.16150800	-0.82350600
H	-2.97506500	2.31204100	0.10913300
H	-3.03592700	2.56235900	-1.63952000
C	-3.51090800	-0.07357900	-0.87596600
H	-4.15160600	0.08500800	-1.75099500
H	-4.04884700	0.30459800	-0.00307800
C	-3.17842800	-1.54983900	-0.72588800
H	-2.70582800	-1.91424200	-1.64275200
H	-4.09466600	-2.13491000	-0.56318600

C	-1.69060100	-3.15588500	0.29083000
H	-1.00144600	-3.34558700	1.11547400
C	-2.86027000	-1.60136900	1.71065700
H	-2.12735600	-1.80029300	2.49455100
H	0.36465400	-0.82286300	0.94028600
H	-1.85743000	0.52486400	-1.92671300
C	3.06780200	-0.34829800	-1.27856100
C	4.42327400	-0.02131700	-1.17992800
C	5.14916400	-0.37568800	-0.03793800
C	4.51898800	-1.07021000	1.00325100
C	3.16879900	-1.40674800	0.89871300
C	2.43282200	-1.03810300	-0.23785500
C	1.00542300	-1.48288900	-0.38955100
H	2.49598500	-0.08956200	-2.16412900
H	4.91305100	0.50546600	-1.99398000
H	6.20218200	-0.12061800	0.03878100
H	5.08151000	-1.35274100	1.88837500
H	2.68130300	-1.95323300	1.70318100
H	2.01934300	2.30607700	-0.85443800
H	1.74144800	3.64268600	0.29519200
H	-0.24749400	3.73929600	2.11481500
H	-1.48167200	2.47016500	2.33290100
H	-1.16951500	-3.28531800	-0.65902400
H	-2.51430800	-3.88083900	0.34934400
H	-3.22765900	-0.58111400	1.83451900
H	-3.70309400	-2.29777600	1.82185600
O	0.30193100	-1.12473300	-1.40288700
H	0.82572200	-2.47517600	0.05126300
N	-2.20699500	-1.77063500	0.38557700

IV(c)

First vibrational frequency: 18.88 cm⁻¹

1 2

Co	-0.81198100	-0.21909600	-0.34382900
P	-2.71909900	-1.38817300	-0.20079500
N	-1.17377000	0.37813000	1.63095900
H	-0.45398800	-0.07976000	2.18930100
C	-2.92406100	-1.39553000	1.65107100
H	-3.94672600	-1.63964500	1.95870500
H	-2.26337300	-2.17621200	2.04662900
C	-2.50483000	-0.02185400	2.18095700
H	-2.47813900	-0.01423800	3.27752500
H	-3.23532100	0.73158100	1.87420300
C	-1.61089000	2.53290700	0.49899200
H	-1.43499100	3.61848100	0.54972700
H	-2.69308500	2.38674600	0.55586100
C	-0.93450400	1.84629800	1.68481900
H	-1.30478400	2.27655800	2.62479500
H	0.14642800	2.00275300	1.65560100
C	-4.34509300	-0.82331200	-0.86556900
H	-4.28909600	-0.75471700	-1.95536500

H	-5.13419800	-1.53041900	-0.59097800
H	-4.59850900	0.16243100	-0.46750100
C	-2.14245600	2.20606500	-1.85402000
H	-2.32237400	3.28166800	-2.00927400
H	-1.78266200	1.77224000	-2.78935500
H	-3.08630000	1.72701500	-1.58976900
C	0.13100400	2.60275700	-1.20185400
H	0.49831800	2.12065700	-2.11051100
H	-0.00769500	3.67699800	-1.40000700
H	0.88445600	2.48335800	-0.42280100
C	-2.67648100	-3.16602600	-0.67814000
H	-3.56448800	-3.69208900	-0.31371000
H	-2.63420300	-3.24566000	-1.76781600
H	-1.78133000	-3.63610400	-0.26243000
C	2.13318300	-0.45642600	-0.67602600
O	1.20433200	-0.00117700	0.00920400
H	1.90782900	-0.89876600	-1.65741000
H	-0.60399200	-0.69134200	-1.76210700
C	3.53213600	-0.43672500	-0.26538100
C	3.93038600	0.09271900	0.97921300
C	4.49626000	-0.95732000	-1.14943000
C	5.27694400	0.09962300	1.32705600
H	3.17894200	0.49059400	1.65331600
C	5.84527300	-0.94697100	-0.79597000
H	4.18378700	-1.36428600	-2.10744200
C	6.23354200	-0.41929100	0.44037700
H	5.58956800	0.50595800	2.28387700
H	6.58982000	-1.34662100	-1.47699700
H	7.28368700	-0.41062700	0.71703600
N	-1.14262200	1.97180900	-0.79352800

IV(c) -TS

First vibrational frequency: -358.86 cm⁻¹

1 2

Co	0.44419100	-0.22075100	0.05633200
P	0.80997900	1.90555300	-0.56150000
N	1.71067600	0.10748400	1.62615600
H	1.11667100	0.06547800	2.45399600
C	1.51298400	2.52454300	1.04777800
H	2.06524300	3.46261400	0.92658000
H	0.66675600	2.72125400	1.71647900
C	2.41198400	1.43007400	1.62849800
H	2.73051700	1.67990300	2.64702600
H	3.31714600	1.33126000	1.02433100
C	3.16867400	-1.35593700	0.26716100
H	3.86095500	-2.20997200	0.30798000
H	3.74268400	-0.50241600	-0.10330700
C	2.64114600	-1.05636500	1.66869000
H	3.47901400	-0.86488300	2.35074400
H	2.08101900	-1.90749900	2.06233200
C	2.00077000	2.43808300	-1.86257800

H	1.66153000	2.07691800	-2.83703000
H	2.06401800	3.53046200	-1.88690500
H	2.99475300	2.02963100	-1.66526000
C	2.51018600	-1.36333600	-2.07558200
H	3.33660000	-2.03440900	-2.35651300
H	1.67599400	-1.53080900	-2.76035200
H	2.84691900	-0.33137900	-2.18229800
C	1.61032300	-3.01805900	-0.58958900
H	0.79646500	-3.18807700	-1.29781300
H	2.43140300	-3.70934700	-0.83211000
H	1.24244800	-3.23075300	0.41395000
C	-0.66496600	2.95560700	-0.88314100
H	-0.39472100	4.01607800	-0.88268400
H	-1.08875300	2.69334400	-1.85623300
H	-1.42037100	2.77274800	-0.11486200
C	-1.39316800	-1.52828800	0.00421700
O	-0.62426800	-1.59077200	1.02936400
H	-1.28547900	-2.28517700	-0.78425200
H	-0.48771500	-0.38154000	-1.13539500
C	-2.71527900	-0.84849100	0.04654500
C	-3.10376800	-0.08700400	1.16008600
C	-3.60932700	-1.02574100	-1.02071900
C	-4.36941600	0.49912800	1.19710700
H	-2.41523800	0.03018200	1.99090300
C	-4.87464700	-0.43702300	-0.98323400
H	-3.31236100	-1.62377900	-1.87897300
C	-5.25532900	0.32773500	0.12545800
H	-4.66957500	1.08444900	2.06127900
H	-5.56299700	-0.57764600	-1.81116200
H	-6.24075700	0.78315900	0.15792800
N	2.06048700	-1.61122600	-0.68986100

VI (a)

First vibrational frequency: 7.73 cm⁻¹

1 2

Co	1.34598000	-0.13945900	-0.53095100
P	1.00888800	2.12046500	-0.48390800
N	1.58432500	0.02576200	1.43458600
C	2.34799200	3.17417500	-1.18129800
H	2.37929900	3.05189800	-2.26748000
C	-0.55118000	2.86637100	-1.09246700
H	-0.59079100	2.79670900	-2.18267600
C	1.04552800	2.41348600	1.34977400
H	1.38374000	3.42622100	1.58855100
H	0.02098500	2.30599700	1.72174600
C	1.95466000	1.35694300	1.97982100
H	3.00506300	1.53969000	1.73322300
H	1.86192200	1.35736800	3.07278900
C	2.40043600	-1.10568300	1.93447500
H	2.25440400	-1.25598900	3.01091400
H	3.45468300	-0.86541100	1.77137700

C	1.96834900	-2.34206700	1.16127400
H	0.92936300	-2.57591300	1.40677000
H	2.58662600	-3.21126000	1.41866900
C	1.17174800	-3.07723100	-1.01043800
H	1.26286100	-2.94213000	-2.09024700
C	3.41876400	-2.18056800	-0.81384200
H	3.43183300	-1.98070300	-1.88705700
H	0.59490500	-0.15872000	1.64447900
C	-3.19067100	-0.10866700	1.01121200
C	-4.47131200	0.06195800	1.55471900
C	-5.60578200	-0.14285300	0.76453900
C	-5.45020300	-0.52443700	-0.57524200
C	-4.17153200	-0.69618000	-1.11055700
C	-3.02452300	-0.48898000	-0.32560200
C	-1.63569100	-0.66745400	-0.94023300
H	-2.30437500	0.04425500	1.61879200
H	-4.58100300	0.35521800	2.59591900
H	-6.59920900	-0.01123500	1.18441100
H	-6.32489400	-0.69029200	-1.19889700
H	-4.06112100	-0.99735500	-2.15119600
H	-1.39908500	2.32187800	-0.67123800
H	-0.60796100	3.91908300	-0.79893600
H	2.17527900	4.22807900	-0.94263400
H	3.31314400	2.86570200	-0.77031400
H	0.13582300	-2.92147700	-0.70937700
H	1.48932300	-4.09713100	-0.75739400
H	4.05743700	-1.44936800	-0.31485200
H	3.82043200	-3.18610200	-0.63410000
O	-0.59525000	-0.58516000	-0.03003500
H	-1.64739500	-1.64093100	-1.47828200
H	-1.54926500	0.09286500	-1.74686400
H	1.40495500	0.02426900	-2.27818200
H	0.90517300	-0.56015400	-2.15338100
N	2.02218600	-2.07979400	-0.31126800

VI (a) -TS

First vibrational frequency: -554.44 cm⁻¹

1 2

Co	1.23319600	0.15813400	-0.44730100
P	0.34156200	2.24738800	-0.12009900
N	0.62053600	-0.22966600	1.40579500
C	1.65434800	3.51017500	0.15679200
H	2.16039600	3.71727300	-0.78995200
C	-0.89554100	3.11336600	-1.16334300
H	-0.47132600	3.29807600	-2.15358100
C	-0.45639500	1.99235100	1.53734500
H	-0.52115700	2.92441500	2.10732800
H	-1.47708700	1.63468100	1.36272700
C	0.36064300	0.94231900	2.29335900
H	1.33254000	1.34665900	2.59171300
H	-0.15871400	0.61662600	3.20195400

C	1.51128500	-1.25428400	2.01829500
H	0.99757800	-1.79207400	2.82293800
H	2.36546600	-0.73526700	2.46024800
C	1.94835500	-2.21690500	0.92421700
H	1.08812000	-2.78440300	0.56052600
H	2.68885200	-2.93174100	1.30773200
C	2.57252000	-2.36746700	-1.41937000
H	3.02569300	-1.83081100	-2.25472600
C	3.85628800	-0.93499900	0.05086600
H	4.22311500	-0.39178400	-0.82196900
H	-0.27972600	-0.67519500	1.19995200
C	-2.32552200	-1.79417100	0.03004100
C	-3.29204200	-1.96362600	1.02802400
C	-4.40559000	-1.11776500	1.08033300
C	-4.54553600	-0.10716800	0.12283500
C	-3.57480600	0.05871700	-0.87134800
C	-2.44963800	-0.77787400	-0.93037800
C	-1.40572100	-0.61637600	-2.03244100
H	-1.46887000	-2.46011100	-0.02184800
H	-3.17899500	-2.75902800	1.76021300
H	-5.15623300	-1.24633900	1.85496500
H	-5.40680400	0.55496600	0.15252600
H	-3.69755500	0.84729700	-1.61128600
H	-1.78909500	2.49570400	-1.27131500
H	-1.17056700	4.06856300	-0.70549200
H	1.22026300	4.43689400	0.54484600
H	2.39403800	3.13364800	0.86823500
H	1.56266100	-2.66662000	-1.69813500
H	3.18756800	-3.24657200	-1.18558500
H	3.83046300	-0.25047000	0.90051800
H	4.54874100	-1.75647300	0.27746600
O	-0.11873600	-1.01292000	-1.65631500
H	-1.73946400	-1.22173800	-2.89736400
H	-1.43759700	0.43146700	-2.38272400
H	1.69541900	0.48272700	-2.04237300
H	1.02090100	-0.06144500	-2.10366300
N	2.49741600	-1.46372600	-0.24238200

By using M06L/6-31+G/LANL2TZ level of theory:**

Co (PNP)

I' (c)

First vibrational frequency: 22.76 cm⁻¹

1 2			
Co	-1.28320400	-0.12392700	-0.39329200
P	-1.44862000	0.37555900	1.82461400
P	-2.99622500	-1.38055200	-0.81850100
N	-2.61304000	1.61807600	-0.66166700

H	-2.03345600	2.30060100	-1.14331600
C	-1.99195400	2.13215000	1.66215000
H	-2.33510400	2.53910100	2.61981700
H	-1.11610600	2.71469400	1.35123800
C	-3.08284300	2.21303800	0.60749000
H	-3.41872900	3.24776300	0.45963900
H	-3.96216700	1.64622700	0.93624600
C	-4.31460900	-0.11295400	-1.09501000
H	-5.05849900	-0.47254500	-1.81381400
H	-4.84136700	0.01896200	-0.14187800
C	-3.70765100	1.20462000	-1.56115500
H	-4.48653500	1.97785300	-1.62922800
H	-3.27484500	1.08454700	-2.55875000
C	-2.65555100	-0.32113600	3.00831500
H	-2.46565400	-1.38560500	3.16502800
H	-2.59234000	0.19391600	3.97144700
H	-3.67317000	-0.20798800	2.62441200
C	-3.76951700	-2.54342000	0.36256200
H	-4.70663500	-2.93606400	-0.04369700
H	-3.09435600	-3.38098800	0.55390600
H	-3.97939200	-2.05017300	1.31311900
C	-2.98982600	-2.37499100	-2.34956900
H	-2.77752900	-1.72538500	-3.20116200
H	-2.20254700	-3.13106100	-2.29768100
H	-3.95109500	-2.87456100	-2.50124900
C	0.06533000	0.48970500	2.84327500
H	-0.12963800	1.02146800	3.77929400
H	0.43454000	-0.51118400	3.08205700
H	0.84768100	1.02414000	2.29794700
C	1.55062700	1.06333900	-0.46991000
O	0.31500700	1.12841200	-0.45723500
O	2.24314600	-0.07050300	-0.42080000
C	1.51004200	-1.32578600	-0.33082700
H	0.79356600	-1.23792300	0.49898300
H	0.95017400	-1.46981100	-1.26037500
H	-1.17965000	-0.32498600	-1.89723300
C	2.50259500	-2.41518000	-0.09463600
C	2.65567100	-3.44426800	-1.02556300
C	3.28826100	-2.41389300	1.06388900
C	3.58175400	-4.46273000	-0.80354400
H	2.04853200	-3.44544700	-1.92788000
C	4.22030700	-3.42385300	1.28068600
H	3.17089100	-1.61262000	1.79112200
C	4.36725300	-4.45140600	0.34695400
H	3.69433600	-5.25932100	-1.53316200
H	4.83041600	-3.41344800	2.17912700
H	5.09367400	-5.24065700	0.51754400
C	2.39231900	2.26734000	-0.51769100
C	3.78973600	2.18268800	-0.44383000
C	1.77302200	3.52040500	-0.62683400
C	4.55541300	3.34232900	-0.47801300

H	4.26616900	1.21205000	-0.35557600
C	2.54486000	4.67493600	-0.66380300
H	0.69000100	3.57341400	-0.68671300
C	3.93589000	4.58748100	-0.58838500
H	5.63722500	3.27575700	-0.41872900
H	2.06409600	5.64427500	-0.75232100
H	4.53761400	5.49105600	-0.61580700

I'(c) -TS

First vibrational frequency: -611.85 cm⁻¹

1 2

Co	0.78523200	-0.53394900	-0.11604200
P	2.21502100	-1.73022700	-1.34509900
P	1.02510000	-1.26740200	1.92892100
N	2.50684700	0.78023400	0.30937400
H	2.31070500	1.66024400	-0.16473900
C	3.49899900	-0.42974700	-1.58289700
H	4.41771000	-0.84310600	-2.01286300
H	3.09668500	0.29815300	-2.29774400
C	3.76652900	0.23751600	-0.24420400
H	4.52668200	1.02382900	-0.33482400
H	4.16128800	-0.49753700	0.46664100
C	2.44308500	-0.25813400	2.54654300
H	2.34286000	-0.05751200	3.61789300
H	3.34964600	-0.86199300	2.42678400
C	2.55233800	1.04312000	1.76166400
H	3.46790100	1.58168000	2.04396000
H	1.70512100	1.69943200	1.99253200
C	3.16624700	-3.18721300	-0.79689700
H	2.49396500	-4.01625700	-0.56491400
H	3.86270000	-3.50379600	-1.57861500
H	3.74149200	-2.94756400	0.10125100
C	1.45518600	-2.97872100	2.38862100
H	1.56827300	-3.06602100	3.47299600
H	0.66609100	-3.65918700	2.06092500
H	2.38982400	-3.28195800	1.91344000
C	-0.35225800	-0.88718200	3.06457900
H	-0.58447700	0.18014500	3.01423600
H	-1.24348900	-1.44206200	2.76055300
H	-0.10140800	-1.15619500	4.09460200
C	1.67598700	-2.16950700	-3.02732400
H	2.52975000	-2.44695500	-3.65201900
H	0.98081700	-3.01091100	-2.98661100
H	1.16046600	-1.31748000	-3.47473900
C	-0.59956000	1.07424300	-0.84587000
O	0.12064800	0.43026800	-1.70062800
O	-1.93954900	0.81827400	-0.74533500
C	-2.29794700	-0.55919900	-0.94588100
H	-2.13170500	-0.84233800	-1.99053200
H	-1.61499600	-1.16826500	-0.32218900

H	-0.18663400	0.46327800	0.57311900
C	-3.71814100	-0.74691500	-0.52454200
C	-4.11559800	-0.41135900	0.77577500
C	-4.65807100	-1.27909200	-1.40874700
C	-5.43157800	-0.60752400	1.18188200
H	-3.38603300	0.01212700	1.46392100
C	-5.97630300	-1.48181500	-1.00143200
H	-4.35503500	-1.53563600	-2.42153000
C	-6.36475600	-1.14623700	0.29386300
H	-5.73146100	-0.34294900	2.19208300
H	-6.69941100	-1.89625900	-1.69772900
H	-7.39176400	-1.30139200	0.61222300
C	-0.29658600	2.50081000	-0.51486300
C	-0.97357200	3.15373000	0.52014400
C	0.70076700	3.17100100	-1.22757300
C	-0.65155600	4.46881100	0.83867600
H	-1.74420000	2.62310600	1.07434800
C	1.02191200	4.48815300	-0.90431000
H	1.20909000	2.65423400	-2.03795900
C	0.34967800	5.13647900	0.13069000
H	-1.17656200	4.97343300	1.64421200
H	1.79511700	5.00775000	-1.46250000
H	0.60237000	6.16173000	0.38431400

II (b)

First vibrational frequency: 10.85 cm⁻¹

1	2			
Co	0.81358500	-0.54213400	-0.13370000	
P	2.23459200	-1.64436900	-1.40144600	
P	1.03129200	-1.41293100	1.87267000	
N	2.49217700	0.76702100	0.44108900	
H	2.28940400	1.68213100	0.03998700	
C	3.49893600	-0.31452300	-1.53451200	
H	4.42748300	-0.68630000	-1.98072000	
H	3.08972500	0.44941900	-2.20614300	
C	3.75355700	0.27343100	-0.15559300	
H	4.50258500	1.07352400	-0.20045300	
H	4.15983000	-0.49554800	0.51072500	
C	2.44561200	-0.46341200	2.58087600	
H	2.34179600	-0.35663400	3.66513500	
H	3.35367900	-1.05350200	2.41351400	
C	2.55104200	0.90203500	1.91212600	
H	3.47003100	1.41256200	2.23109200	
H	1.71071100	1.53881500	2.21072000	
C	3.16963500	-3.14176200	-0.95067700	
H	2.48672900	-3.97122400	-0.75411300	
H	3.84332300	-3.42367600	-1.76490600	
H	3.76947200	-2.96647500	-0.05387700	
C	1.40080100	-3.15387200	2.25596900	
H	1.48175700	-3.29783200	3.33701900	

H	0.60220200	-3.79315300	1.87346400
H	2.33975700	-3.45971500	1.79064700
C	-0.37958100	-1.04134900	2.97289800
H	-0.61713900	0.02535200	2.93646900
H	-1.26083900	-1.59684300	2.64249400
H	-0.15269000	-1.32157700	4.00556200
C	1.67339200	-1.94923100	-3.10310200
H	2.51951100	-2.17347700	-3.75872800
H	0.97944100	-2.79236700	-3.12002500
H	1.15194500	-1.06226500	-3.46837300
C	-0.54724500	1.12909300	-0.66066500
O	0.21937800	0.55802500	-1.58877100
O	-1.93305500	0.87849300	-0.74129200
C	-2.22826500	-0.50457100	-0.91464300
H	-2.01440600	-0.82124600	-1.94322500
H	-1.54439900	-1.08457800	-0.25570400
H	-0.28003100	0.62722400	0.42775300
C	-3.65108800	-0.76688100	-0.53673400
C	-4.16533300	-0.27554500	0.66902800
C	-4.47072300	-1.54089300	-1.36096600
C	-5.47719000	-0.55405600	1.04081800
H	-3.52979700	0.33296000	1.30916600
C	-5.78286300	-1.82806500	-0.98577200
H	-4.07834100	-1.91818900	-2.30293100
C	-6.28847000	-1.33510600	0.21545800
H	-5.86807900	-0.16564500	1.97716300
H	-6.41121000	-2.43058500	-1.63548000
H	-7.31174400	-1.55415800	0.50696000
C	-0.32821100	2.60106200	-0.40038400
C	-1.04743300	3.25586600	0.60314100
C	0.63792700	3.29532500	-1.12968800
C	-0.81067300	4.60265300	0.86309900
H	-1.79411900	2.70717200	1.17349200
C	0.87389200	4.64435600	-0.86702600
H	1.18877600	2.77058700	-1.90644100
C	0.15178700	5.29859800	0.12938600
H	-1.37264200	5.10997300	1.64191800
H	1.62180400	5.18346100	-1.44155300
H	0.33756600	6.34871000	0.33557300

III (b)

First vibrational frequency: 19.74 cm⁻¹

1 2			
Co	-1.36713800	-0.86297500	-0.27111400
P	-0.19198200	-2.09608700	1.21887300
P	-2.89159400	0.20609800	-1.52897400
N	-2.70017000	-0.62688500	1.24613000
C	-0.32141500	-3.88796000	0.90948800
H	0.27743600	-4.14504700	0.03226700
C	1.53510400	-1.84821000	1.70637600

H	2.19458800	-2.14299800	0.88702200
C	-1.17365300	-1.79844500	2.74192400
H	-1.04781600	-2.60703900	3.46796200
H	-0.79337100	-0.87852300	3.20232700
C	-2.62161800	-1.62615900	2.33769100
H	-3.04782900	-2.56195100	1.95953900
H	-3.24106700	-1.30284200	3.18307900
C	-4.09671300	-0.34569600	0.83607900
H	-4.68627500	-0.04005700	1.70889400
H	-4.52508800	-1.28210500	0.46160300
C	-4.08100000	0.72701900	-0.23120300
H	-3.71534000	1.67210000	0.18562900
H	-5.07762000	0.90579900	-0.64459500
C	-2.43282200	1.73112800	-2.39947300
H	-1.76462600	1.50764000	-3.23365200
C	-3.87439200	-0.74949300	-2.72855300
H	-3.23498800	-1.08911500	-3.54580400
H	-2.29087000	0.25045200	1.58565700
H	1.71044900	-0.79108000	1.91036100
H	1.75678300	-2.45476800	2.58929800
H	0.04386300	-4.45877500	1.76788500
H	-1.35806000	-4.16746300	0.70833500
H	-1.91657100	2.39214200	-1.69937100
H	-3.32650100	2.23123900	-2.78332000
H	-4.30677600	-1.62888300	-2.24595400
H	-4.68136400	-0.13648700	-3.13964300
H	-0.03297100	-1.16189800	-1.15133600
H	-0.62270300	-0.97260800	-1.71720300
C	0.32911800	1.49529200	-0.29441100
O	-0.73258600	1.01770500	0.36542000
O	1.41713600	0.51381000	-0.17976000
C	2.47710000	0.70972900	-1.10428300
H	2.05971300	0.87256300	-2.11479500
H	3.06510300	1.60558800	-0.84445200
H	0.16770900	1.59663000	-1.40016100
C	3.32877900	-0.52169500	-1.06933600
C	2.95790200	-1.65567000	-1.80118900
C	4.44939200	-0.59267500	-0.23758500
C	3.68493000	-2.83956800	-1.69690500
H	2.09175000	-1.60598500	-2.45943300
C	5.18182400	-1.77416800	-0.13132100
H	4.74059900	0.28408300	0.33758700
C	4.79883700	-2.90121200	-0.85810900
H	3.38814100	-3.71168100	-2.27326600
H	6.05092800	-1.81581900	0.51945800
H	5.36920900	-3.82230600	-0.77658100
C	0.80517700	2.82962200	0.23967300
C	1.04361000	3.90242600	-0.61917200
C	1.02885700	2.99327400	1.61110000
C	1.49352100	5.12697300	-0.12136100
H	0.87406700	3.77405100	-1.68842800

C	1.48073400	4.21003100	2.11187000
H	0.84264900	2.15257000	2.27715600
C	1.71285800	5.28231800	1.24564500
H	1.67343100	5.95646900	-0.80029200
H	1.65338400	4.32830100	3.17865800
H	2.06440900	6.23284800	1.63730300

III (b) -TS

First vibrational frequency: -989.75 cm⁻¹

1 2

Co	1.98256200	-0.03653800	-0.53237400
P	1.73414600	2.17254200	-0.86107100
P	2.68059800	-2.13414600	-0.18337900
N	3.25995500	0.47739900	0.97023700
C	2.63040500	2.97072800	-2.23389500
H	2.21410800	2.64057200	-3.18783400
C	0.08223300	2.92464100	-0.89751400
H	-0.41244500	2.66660100	-1.83679400
C	2.55665800	2.79868100	0.66039100
H	2.87456100	3.84123300	0.56291500
H	1.82413300	2.74735600	1.47473900
C	3.73144800	1.88352600	0.95058800
H	4.49713300	1.95986300	0.17012000
H	4.21225000	2.13265800	1.90455300
C	4.35387600	-0.49267300	1.21312900
H	4.88958700	-0.23610600	2.13574200
H	5.06560800	-0.39542400	0.38559400
C	3.77251300	-1.89167900	1.28155900
H	3.14990200	-1.99899100	2.17761200
H	4.55833000	-2.65077200	1.33771400
C	1.57496400	-3.50493600	0.27903000
H	0.88392300	-3.72006500	-0.53936500
C	3.75747100	-2.85829500	-1.46450500
H	3.17242000	-3.05909700	-2.36449300
H	2.58268900	0.38959200	1.73335000
H	-0.51493200	2.51528900	-0.07948600
H	0.14466000	4.01275900	-0.80816800
H	2.55083400	4.05969000	-2.16999500
H	3.68578300	2.69030200	-2.20940000
H	0.99321100	-3.23117800	1.16182600
H	2.15284300	-4.40690000	0.50084100
H	4.55493600	-2.15921200	-1.72623900
H	4.20373700	-3.79298000	-1.11338400
H	0.28206300	-0.29024500	-1.31145100
H	1.09026700	-0.46327700	-1.78751400
C	-0.57120000	-0.54307700	0.80268900
O	0.52299200	0.09472100	1.03702200
O	-0.95758000	-0.16264400	-0.82508900
C	-1.81963400	-1.08202500	-1.47475800
H	-1.46779400	-1.18363800	-2.51268600

H	-1.72009000	-2.08383200	-1.02060800
H	-0.51434000	-1.64293400	0.64817500
C	-3.26165400	-0.65131300	-1.45540200
C	-4.26897700	-1.60973800	-1.60124000
C	-3.61894100	0.69061400	-1.30434200
C	-5.61066200	-1.23588100	-1.60098700
H	-3.99836400	-2.65985600	-1.70082400
C	-4.96148200	1.06620700	-1.30052400
H	-2.83813800	1.43391100	-1.16592000
C	-5.96159300	0.10574600	-1.44991100
H	-6.38273700	-1.99269900	-1.70957500
H	-5.22775800	2.11261500	-1.17430100
H	-7.00737700	0.39941200	-1.44239900
C	-1.79409600	-0.16139300	1.57392300
C	-2.82033500	-1.09003300	1.76133100
C	-1.92305100	1.12218700	2.11097800
C	-3.97434400	-0.73694800	2.45701100
H	-2.71513600	-2.09322100	1.34899000
C	-3.07417100	1.47836200	2.80724700
H	-1.10553200	1.82843700	1.98305500
C	-4.10398100	0.55039400	2.97745200
H	-4.77086800	-1.46359200	2.59225100
H	-3.17123100	2.47811400	3.22183300
H	-5.00224700	0.82919700	3.52135000

IV(c)

First vibrational frequency: 14.88 cm⁻¹

1 2			
Co	-0.78389600	-0.57068700	-0.34972200
P	-2.76670500	-1.49875200	-0.37144700
P	-0.96000300	1.69071500	-0.57092100
N	-1.09452600	-0.23540300	1.69971300
H	-0.48803300	-0.90940000	2.16512000
C	-3.04736300	-1.72390200	1.43911700
H	-4.10460800	-1.87270200	1.68402000
H	-2.50964100	-2.62824000	1.74728200
C	-2.48848400	-0.50234100	2.14295600
H	-2.52672400	-0.60791700	3.23407900
H	-3.08692400	0.37852500	1.88779600
C	-1.23872400	2.18370300	1.19037100
H	-0.80890300	3.16637800	1.41108400
H	-2.31859900	2.27108600	1.35450800
C	-0.63025200	1.12089600	2.09358200
H	-0.86774600	1.31560600	3.14802700
H	0.46079000	1.11957900	1.99817200
C	-4.21256500	-0.53459400	-0.93066000
H	-4.10284400	-0.27532700	-1.98634000
H	-5.13867100	-1.10123500	-0.79573300
H	-4.28167900	0.39323200	-0.35664800
C	-2.19844200	2.65750600	-1.50398700

H	-2.09830700	3.72822700	-1.30139500
H	-2.06325000	2.48899300	-2.57495700
H	-3.20910800	2.34192100	-1.23664200
C	0.59601100	2.56599200	-0.98625500
H	0.91317400	2.31355800	-2.00163700
H	0.46992500	3.65049900	-0.91556400
H	1.38941000	2.26286400	-0.29713800
C	-3.05724800	-3.14543300	-1.09544200
H	-4.04509800	-3.52895700	-0.82361800
H	-2.98942200	-3.08387500	-2.18368100
H	-2.29451400	-3.84429400	-0.74577600
C	2.12564100	-0.46478000	-0.74211600
O	1.17056600	-0.52417000	0.05454400
H	1.92840200	-0.49753500	-1.82743300
H	-0.60514200	-0.88205200	-1.80428900
C	3.50254000	-0.33388000	-0.32456500
C	3.85552800	-0.27181900	1.03640500
C	4.50067700	-0.25998700	-1.31098000
C	5.18790400	-0.14719500	1.39621600
H	3.07334500	-0.32653500	1.78864900
C	5.83398500	-0.13040200	-0.94382200
H	4.21742700	-0.30397100	-2.36001000
C	6.17686000	-0.07725300	0.40787000
H	5.46684500	-0.10314200	2.44440000
H	6.60589700	-0.07132900	-1.70455700
H	7.21948200	0.02044500	0.69615700

IV(c) -TS

First vibrational frequency: -636.95 cm⁻¹

1 2			
Co	0.28988200	-0.35322600	0.08482400
P	0.28391300	1.72220600	-0.62727400
P	2.20458900	-1.40182600	-0.61993400
N	1.33391700	0.28310500	1.71000200
H	0.66017800	0.22709400	2.47336000
C	0.75136700	2.55739100	0.94823800
H	1.11804700	3.57692700	0.79005200
H	-0.15173900	2.62508000	1.56695500
C	1.80105900	1.69577900	1.62432300
H	2.05072300	2.06608700	2.62507300
H	2.72806400	1.70117700	1.04180100
C	3.29328500	-0.93613100	0.80003100
H	4.03219400	-1.71426300	1.01684100
H	3.85692400	-0.04147100	0.51174900
C	2.43295200	-0.67124500	2.02522400
H	3.03554300	-0.28592000	2.85737700
H	1.95510500	-1.59536400	2.36335700
C	1.49080500	2.31723600	-1.85600700
H	1.35331500	1.78440700	-2.79969300
H	1.37142900	3.39024200	-2.03052300

H	2.50814200	2.13106300	-1.50217400
C	3.25379000	-1.10731200	-2.08481100
H	4.18872600	-1.67150900	-2.01629800
H	2.72256800	-1.41844500	-2.98725200
H	3.48989200	-0.04520500	-2.17832300
C	2.13008600	-3.22561800	-0.53730600
H	1.49810600	-3.60392600	-1.34487000
H	3.12516100	-3.67073100	-0.62854600
H	1.68031700	-3.53083900	0.41009700
C	-1.28772200	2.48056000	-1.14462300
H	-1.19077300	3.56610200	-1.23455200
H	-1.58936800	2.06988000	-2.11121400
H	-2.06834600	2.24554900	-0.41605300
C	-1.30810000	-1.65772200	-0.10291000
O	-0.57743900	-1.85497300	0.96638700
H	-1.30720800	-2.45031500	-0.87070700
H	-0.49800300	-0.77685500	-1.14093800
C	-2.58866600	-0.89728300	-0.00729500
C	-2.91512100	-0.17980900	1.14952500
C	-3.46631900	-0.88518600	-1.09555600
C	-4.10261600	0.54342200	1.21161300
H	-2.22877200	-0.20018600	1.99381100
C	-4.65210800	-0.15852200	-1.03461400
H	-3.21187900	-1.44523600	-1.99374700
C	-4.97138700	0.55895000	0.11876700
H	-4.35331400	1.09599700	2.11277200
H	-5.32882600	-0.15303200	-1.88428400
H	-5.89664000	1.12587200	0.16767600

v(b)

First vibrational frequency: 22.37 cm⁻¹

1 2			
Co	0.81334400	-0.54712600	-0.40653900
P	0.14027800	1.54396400	-0.40729500
P	3.01882000	-0.47094500	-0.55354200
N	1.18770200	-0.42859700	1.71034100
C	1.22644000	2.98407300	-0.67328600
H	1.58022300	3.00678700	-1.70626800
C	-1.40824400	2.03061000	-1.23094900
H	-1.27423100	2.03309900	-2.31484600
C	-0.25655600	1.57468700	1.39030800
H	-0.44326800	2.59415700	1.74574600
H	-1.18315600	1.00043500	1.51174000
C	0.87912800	0.94240800	2.18237600
H	1.79250200	1.53648800	2.05332200
H	0.65348800	0.94749100	3.25592300
C	2.53798600	-0.90025100	2.12638000
H	2.45720300	-1.61849500	2.94711100
H	3.09309800	-0.04154100	2.51770300
C	3.29067300	-1.50848300	0.94792700

H	2.89727700	-2.50499200	0.71413600
H	4.35623500	-1.62651100	1.17668600
C	3.84300300	-1.37695500	-1.90095700
H	3.79226600	-0.79620700	-2.82415800
C	4.09308400	0.98155600	-0.29979200
H	4.01089500	1.66566400	-1.14684700
H	-1.59280700	-0.92935100	-1.92610700
H	0.47395100	-1.06299800	2.06401200
C	-3.29785900	-0.72109700	0.93520500
C	-4.50716200	-0.23231400	1.43087100
C	-5.56549000	0.03288000	0.56371200
C	-5.40741100	-0.19667500	-0.80436800
C	-4.19836100	-0.68212900	-1.29597000
C	-3.12895100	-0.94710900	-0.43260000
C	-1.82105300	-1.46496900	-0.98469500
H	-2.46704900	-0.92956200	1.60495600
H	-4.62226000	-0.05861100	2.49784300
H	-6.50610300	0.41674100	0.94828000
H	-6.22567200	0.01020600	-1.48913200
H	-4.07490400	-0.84670600	-2.36566600
H	-2.20663600	1.32871800	-0.97913600
H	-1.70439800	3.03333600	-0.90925400
H	0.68222200	3.90961800	-0.46451700
H	2.09607600	2.93599700	-0.01482900
H	3.34160500	-2.33247000	-2.06668300
H	4.89306700	-1.56261300	-1.65780500
H	3.80619800	1.51983900	0.60735200
H	5.13553100	0.66614600	-0.20027500
O	-0.76709000	-1.39967700	-0.07458300
H	-1.96066300	-2.51732100	-1.29087100

VI (a)

First vibrational frequency: 16.74 cm⁻¹

1 2			
Co	1.26583300	0.17020700	-0.62198100
P	0.44898600	2.26038100	-0.59400500
P	2.15054400	-1.85575600	-0.26061400
N	1.63282400	0.48393100	1.35659800
C	1.38635700	3.58514300	-1.42052400
H	1.37254700	3.43192000	-2.50152900
C	-1.28348000	2.53289400	-1.05547000
H	-1.41820200	2.39741400	-2.13055700
C	0.54372300	2.64767700	1.20069800
H	0.61681600	3.72501100	1.37426900
H	-0.38875400	2.29863800	1.65877700
C	1.72477600	1.89895800	1.78094100
H	2.67800100	2.29763300	1.41691200
H	1.73997900	1.96063200	2.87620900
C	2.67491600	-0.37543100	1.96208200
H	2.67057000	-0.25684500	3.05271300

H	3.64853400	-0.02867600	1.59857700
C	2.40268900	-1.80969800	1.56091400
H	1.47766000	-2.16443700	2.02910800
H	3.20897100	-2.48062400	1.87036100
C	1.11713100	-3.31358900	-0.56934600
H	0.97192000	-3.45287700	-1.64251300
C	3.77932200	-2.26519800	-0.96496200
H	3.70925500	-2.32398200	-2.05298300
H	0.71438500	0.12696600	1.64826700
C	-3.17623200	-0.15817200	1.00816800
C	-4.48243800	-0.06824900	1.49337300
C	-5.54383000	-0.58032000	0.74987400
C	-5.29019300	-1.18555800	-0.48355300
C	-3.98625300	-1.27500900	-0.96228200
C	-2.91305000	-0.76316400	-0.22256700
C	-1.50075000	-0.84617200	-0.76229900
H	-2.33491000	0.23029100	1.57757900
H	-4.67085100	0.40180200	2.45570000
H	-6.56078800	-0.51280900	1.12679300
H	-6.11171900	-1.59036200	-1.06946900
H	-3.79287900	-1.75171300	-1.92286100
H	-1.90244000	1.80434800	-0.52419100
H	-1.59365000	3.54529100	-0.78272400
H	0.95146900	4.56288700	-1.19468600
H	2.42645400	3.57380600	-1.08722900
H	0.14360900	-3.15557800	-0.10065500
H	1.58425900	-4.21071400	-0.15375900
H	4.50679600	-1.49135500	-0.71018900
H	4.13208600	-3.22559900	-0.57908100
O	-0.54186800	-0.46230400	0.14346600
H	-1.34647400	-1.88237100	-1.14265600
H	-1.47592400	-0.22408100	-1.68946700
H	0.84605700	0.32411200	-2.18758400
H	1.21582300	-0.42746100	-2.13452900

VI (a) -TS

First vibrational frequency: -839.05 cm⁻¹

1 2			
Co	1.13301400	0.01545300	-0.50666600
P	1.48139400	2.23580500	-0.41698600
P	1.35373900	-2.23266900	-0.45959600
N	1.84564600	-0.03511400	1.39084200
C	2.95168600	2.94767600	-1.22438600
H	2.84738800	2.87781000	-2.30875600
C	0.12271600	3.37137200	-0.81110900
H	-0.05568400	3.37041600	-1.88872800
C	1.79533900	2.41510100	1.38566200
H	2.33626900	3.33578600	1.62383100
H	0.82310000	2.46156700	1.89019400
C	2.56577100	1.18982100	1.83241900

H	3.56259900	1.15855400	1.37879200
H	2.70097600	1.16879300	2.92014900
C	2.58253200	-1.27123200	1.76463600
H	2.75853900	-1.28815400	2.84657200
H	3.56169500	-1.21944500	1.27590700
C	1.80352800	-2.48749500	1.30759800
H	0.87553600	-2.58742300	1.88268600
H	2.37958800	-3.40620500	1.45508900
C	0.13710200	-3.53161500	-0.84009200
H	-0.18663900	-3.44612800	-1.87950900
C	2.84067500	-2.74986000	-1.38145600
H	2.65370700	-2.66932100	-2.45421100
H	0.95072000	-0.04847000	1.88854400
C	-3.66270500	1.06607800	0.02097100
C	-5.01570400	1.40497300	0.07649200
C	-5.98349000	0.41200900	0.21256600
C	-5.58998900	-0.92559100	0.29204100
C	-4.23966600	-1.25988500	0.23767600
C	-3.26107500	-0.26769500	0.10002100
C	-1.80096600	-0.65225900	0.04097500
H	-2.90013500	1.83167500	-0.08961800
H	-5.31393500	2.44851400	0.01343400
H	-7.03681300	0.67501500	0.25413100
H	-6.33763000	-1.70759500	0.39618500
H	-3.93670900	-2.30491000	0.29792300
H	-0.78067400	3.01350300	-0.31299400
H	0.35208200	4.39043900	-0.48826900
H	3.07389700	3.99820500	-0.94564500
H	3.84789200	2.39587500	-0.93232200
H	-0.73849900	-3.43352200	-0.19523900
H	0.58214100	-4.51900900	-0.68771300
H	3.68153900	-2.09701900	-1.13567800
H	3.10887700	-3.78283100	-1.14248800
O	-0.95049800	0.43456900	-0.14208000
H	-1.55136200	-1.20193100	0.97332300
H	-1.68305200	-1.39956300	-0.76962300
H	-0.24624600	0.26290200	-1.39736800
H	0.44589600	0.07975000	-1.98262700

Co (PNP)

I' (c)

First vibrational frequency: 12.95 cm⁻¹

1 2			
Co	-1.27105100	-0.23762900	-0.06977100
P	-2.64546100	-1.76230000	-0.80377800
N	-2.65991800	1.25227300	-0.80929100
H	-2.10083700	1.98966300	-1.22864100
C	-2.48974600	1.75342000	1.57441300
H	-3.01653700	2.14159700	2.45915400
H	-1.60432300	2.37671300	1.41297100

C	-3.38249300	1.80190500	0.35306300
H	-3.72354500	2.82955500	0.17755000
H	-4.28418000	1.20281000	0.51240900
C	-4.03851300	-0.70580400	-1.41154000
H	-4.57776300	-1.19409100	-2.23041500
H	-4.75542500	-0.60928300	-0.58625700
C	-3.52838800	0.66252400	-1.84636700
H	-4.37261500	1.32377100	-2.08879800
H	-2.92112500	0.56564400	-2.75140500
C	-3.09433800	-0.45793000	2.37280000
H	-2.72246400	-1.47000400	2.54473300
H	-3.46389700	-0.04833600	3.32435300
H	-3.93017900	-0.50919000	1.67210100
C	-3.51517500	-3.07811500	0.13226600
H	-4.22668400	-3.59299000	-0.52085300
H	-2.79120300	-3.80828900	0.50160300
H	-4.05860500	-2.67188900	0.98625000
C	-2.11855600	-2.69820500	-2.28217300
H	-1.80507400	-2.00149800	-3.06225800
H	-1.26150800	-3.32835400	-2.03142400
H	-2.92682600	-3.33102200	-2.66034000
C	-0.93736800	0.41225300	2.84685500
H	-1.31814800	0.80645100	3.79963300
H	-0.56119300	-0.59996200	3.01598600
H	-0.12146900	1.04856100	2.50278400
C	1.38917600	1.29393500	-0.00109200
O	0.16389900	1.19525900	0.14895400
O	2.23943200	0.27558400	0.08348000
C	1.71014100	-1.02519000	0.48629400
H	1.38357600	-0.93712100	1.52797800
H	0.84183400	-1.24654200	-0.14920700
H	-0.69323800	-0.54883100	-1.42115500
C	2.79107500	-2.03826700	0.31862100
C	2.98668200	-2.65313600	-0.92265000
C	3.62011600	-2.38029900	1.39082100
C	3.99950200	-3.59352700	-1.09063800
H	2.33770300	-2.39220000	-1.75660900
C	4.63218900	-3.32334100	1.22506600
H	3.46737200	-1.90773400	2.35863100
C	4.82304000	-3.92997600	-0.01585000
H	4.14342700	-4.06801600	-2.05692500
H	5.26922300	-3.58669900	2.06442500
H	5.60985700	-4.66757500	-0.14461600
C	2.03466900	2.58718600	-0.26947900
C	3.42666700	2.70430700	-0.39057800
C	1.22578400	3.72618200	-0.38947200
C	3.99723000	3.94956100	-0.62811100
H	4.05163100	1.82263900	-0.29645200
C	1.80240200	4.96774300	-0.62430400
H	0.14898400	3.62226200	-0.29374300
C	3.18861100	5.08089700	-0.74304000

H	5.07504300	4.03951500	-0.72055400
H	1.17397100	5.84847500	-0.71345300
H	3.63929700	6.05223400	-0.92438600
N	-2.00437500	0.37060500	1.83076000

I'(c) -TS

First vibrational frequency: -484.13 cm⁻¹

1 2			
Co	0.95348900	-0.52975900	-0.59406000
P	1.42511200	-1.18359600	1.45306700
N	2.68065400	0.78388600	-0.41801000
H	2.42952500	1.67034700	-0.85015700
C	3.12660600	-0.63555600	-2.35495600
H	3.90049800	-1.12311300	-2.96489400
H	2.55637200	0.03532200	-3.00576500
C	3.74810400	0.15326900	-1.22106100
H	4.45025800	0.89454400	-1.61985800
H	4.33220200	-0.50243500	-0.56797900
C	2.99670700	-0.26971500	1.78837600
H	3.11272900	-0.07405400	2.85945100
H	3.82805400	-0.92639300	1.50406100
C	3.03389900	1.02896200	0.99301800
H	4.02000900	1.50478200	1.08651200
H	2.29645900	1.73796600	1.38648500
C	2.89269700	-2.77048600	-1.21373200
H	2.17017000	-3.49808400	-0.83982700
H	3.55040700	-3.26204300	-1.94363000
H	3.50114900	-2.41902600	-0.37793300
C	1.75896800	-2.87628500	2.05440900
H	2.03677400	-2.84740600	3.11206900
H	0.86149700	-3.48923400	1.94546200
H	2.56813800	-3.34690200	1.49409300
C	0.26962800	-0.55810100	2.72123500
H	0.16520700	0.52518100	2.62247900
H	-0.71603000	-1.00738800	2.57708600
H	0.62506000	-0.79375900	3.72835100
C	1.35888600	-2.18276300	-2.94861400
H	1.99627100	-2.69335700	-3.68290500
H	0.63472800	-2.89767800	-2.55013700
H	0.82296300	-1.36544900	-3.43193100
C	-0.54636000	1.00392000	-1.16567700
O	0.18797000	0.48271500	-2.09325500
O	-1.87023600	0.65556500	-1.07024800
C	-2.13687300	-0.71736700	-1.40936100
H	-1.87399700	-0.89939500	-2.45683800
H	-1.47107500	-1.34170000	-0.78156200
H	-0.07529400	0.33985300	0.14804300
C	-3.57524100	-1.01094900	-1.13365500
C	-4.08332000	-0.91091500	0.16715700
C	-4.42748600	-1.40254900	-2.16928600

C	-5.42148500	-1.19600300	0.42477600
H	-3.42220500	-0.60640100	0.97678200
C	-5.76734400	-1.69462300	-1.91217100
H	-4.03695800	-1.48009500	-3.18194300
C	-6.26630700	-1.58960900	-0.61543200
H	-5.80752300	-1.11480900	1.43702700
H	-6.42043700	-1.99856300	-2.72581600
H	-7.31005900	-1.81506700	-0.41312200
C	-0.32906700	2.42045500	-0.72856900
C	-0.96100200	2.91868800	0.41505000
C	0.55683800	3.22882600	-1.44413000
C	-0.69883300	4.21565000	0.84405300
H	-1.64590100	2.27989000	0.96855900
C	0.81287700	4.53013800	-1.01506400
H	1.03066400	2.83180100	-2.33915200
C	0.19188400	5.02182800	0.13218100
H	-1.18391300	4.59748000	1.73798400
H	1.49736100	5.15941400	-1.57667800
H	0.39872600	6.03289500	0.47125500
N	2.16990800	-1.64866300	-1.83499900

II (b)

First vibrational frequency: 6.48 cm⁻¹

1 2			
Co	-1.31691000	-0.74996200	0.25270400
P	-2.89778300	-1.82519900	-0.91173500
N	-2.13355400	0.96998500	-0.52588600
H	-1.35862900	1.59325100	-0.75334800
C	-2.31492300	1.22125800	1.92760300
H	-2.90712700	1.67654600	2.73479200
H	-1.28673600	1.58902000	2.00002000
C	-2.89939100	1.60108600	0.58167100
H	-2.89495600	2.69109300	0.46972800
H	-3.94251900	1.28277000	0.50083400
C	-3.86894600	-0.41912200	-1.59759800
H	-4.34170800	-0.67774700	-2.55009300
H	-4.68047800	-0.19759200	-0.89403500
C	-2.93857200	0.77234900	-1.75818200
H	-3.49902200	1.68410900	-1.99988700
H	-2.22946000	0.59971500	-2.57452700
C	-3.58211900	-0.82283600	2.31550700
H	-3.49788900	-1.90874300	2.39159200
H	-4.03083000	-0.43448900	3.24096500
H	-4.24753600	-0.58177600	1.48292400
C	-4.13516600	-3.06015500	-0.40398300
H	-4.73094100	-3.37503500	-1.26488000
H	-3.63535900	-3.93483800	0.01744400
H	-4.80392400	-2.64582100	0.35281300
C	-2.10330500	-2.57969400	-2.37369900
H	-1.40381500	-1.87107000	-2.82484400

H	-1.54007500	-3.46559800	-2.07326200
H	-2.84940400	-2.86771600	-3.11995500
C	-1.38978800	-0.57998800	3.24528200
H	-1.80483800	-0.16393300	4.17410400
H	-1.32780900	-1.66592300	3.34462600
H	-0.39204300	-0.17648400	3.07182100
C	1.06173500	0.53113500	-0.12239500
O	0.26391200	0.01242800	0.87538600
O	2.43269700	0.25628500	0.13718500
C	2.72688800	-1.13554600	0.12412000
H	2.35575400	-1.62154000	1.03646100
H	2.19228900	-1.60098600	-0.72494700
H	0.82104500	0.06384800	-1.11252600
C	4.20621400	-1.33200000	-0.01907500
C	4.94634500	-0.54265800	-0.90648400
C	4.86231200	-2.32973400	0.70625200
C	6.31393100	-0.75000200	-1.06565600
H	4.44141400	0.24260000	-1.46298100
C	6.23054700	-2.54453200	0.54264600
H	4.29643000	-2.94030000	1.40741600
C	6.96026600	-1.75393700	-0.34346600
H	6.87836200	-0.12711400	-1.75451500
H	6.72764400	-3.32316000	1.11470700
H	8.02756600	-1.91476900	-0.46715900
C	0.93573100	2.03275900	-0.25186300
C	0.79910600	2.62561900	-1.50910000
C	0.90388300	2.83803500	0.89121200
C	0.62621100	4.00573100	-1.62723800
H	0.81938500	1.99784500	-2.39956000
C	0.73887000	4.21536300	0.77624500
H	1.00049100	2.36907400	1.86808600
C	0.59551700	4.80153100	-0.48373500
H	0.51356900	4.45674800	-2.60912400
H	0.71785600	4.83517400	1.66837500
H	0.45955400	5.87568500	-0.57147700
N	-2.24836500	-0.24944000	2.09599500

III (b)

First vibrational frequency: 6.54 cm⁻¹

1 2			
Co	1.58501000	-0.62825700	0.35803800
P	0.91474800	-1.32703400	-1.64262700
N	2.99838800	0.36351100	-0.62948600
C	1.37373500	-3.05728700	-1.98384200
H	0.76485300	-3.72283100	-1.36758400
C	-0.77121800	-1.16944700	-2.28726600
H	-1.44026600	-1.81135600	-1.70856500
C	2.00199500	-0.31892000	-2.73240800
H	2.15417200	-0.78889000	-3.70829200
H	1.50060500	0.64093400	-2.90274700

C	3.31153900	-0.10453100	-1.99674500
H	3.87831000	-1.03793000	-1.90582300
H	3.95325900	0.62138100	-2.50984100
C	4.16456400	0.57276500	0.25093400
H	4.79699400	1.39020600	-0.11296800
H	4.76947200	-0.33959800	0.23825300
C	3.61760200	0.87921500	1.62290000
H	3.03538100	1.80538900	1.58481900
H	4.41592600	1.00097400	2.36638100
C	1.85427400	0.28808800	3.16512100
H	1.15600800	-0.49494100	3.46861100
C	3.40485100	-1.41462000	2.43965800
H	2.68939400	-2.16344400	2.78362200
H	2.47736800	1.24599100	-0.69077400
H	-1.11814000	-0.14189600	-2.16948000
H	-0.79857500	-1.46593000	-3.33962300
H	1.21271300	-3.30269300	-3.03765100
H	2.42348900	-3.22607400	-1.73268200
H	1.29409600	1.16498300	2.83748100
H	2.48578300	0.55179300	4.02337900
H	3.95228700	-1.82578700	1.58791800
H	4.11358500	-1.19981000	3.24997700
H	0.14316600	-1.10446800	1.00816500
H	0.68137500	-1.69396600	1.23515100
C	-0.53778200	1.41583900	0.81918200
O	0.71313600	1.25578900	0.37051100
O	-1.31440400	0.23154900	0.40635300
C	-2.55339200	0.07453400	1.08812200
H	-2.37566400	0.07246100	2.17836000
H	-3.22623000	0.91774400	0.86559200
H	-0.62957500	1.42961700	1.93717100
C	-3.15060400	-1.21926000	0.62810100
C	-2.68131500	-2.43462300	1.13972300
C	-4.12354700	-1.24025600	-0.37496300
C	-3.16764000	-3.64618800	0.65364800
H	-1.93174600	-2.42656000	1.92954300
C	-4.61709100	-2.45030000	-0.86109200
H	-4.49055400	-0.29892800	-0.77972600
C	-4.13669300	-3.65581200	-0.35077000
H	-2.79698700	-4.58262700	1.06163200
H	-5.37538400	-2.45243200	-1.63945400
H	-4.52016900	-4.59923600	-0.72883900
C	-1.22110900	2.65343300	0.27423700
C	-1.98337300	3.47459200	1.10542500
C	-1.11987700	2.96904800	-1.08439400
C	-2.63583100	4.59739000	0.59310800
H	-2.06267000	3.23040800	2.16466100
C	-1.77122700	4.08434800	-1.60159200
H	-0.51379900	2.33171400	-1.72472100
C	-2.53192300	4.90283000	-0.76221900
H	-3.22436000	5.23143500	1.25085000

H	-1.68729100	4.32196500	-2.65910100
H	-3.03830500	5.77574300	-1.16537700
N	2.67473400	-0.19400500	2.04066300

III (b) -TS

First vibrational frequency: -1121.13 cm⁻¹

1 2

Co	-1.51955000	-0.45107700	-0.14700800
P	-1.16415600	-0.72406200	2.01219800
N	-3.13845300	0.60639200	0.38471000
C	-1.55282700	-2.35711700	2.72470700
H	-0.84485300	-3.09961100	2.35022300
C	0.40549200	-0.25568800	2.79746700
H	1.17082100	-0.99140400	2.54040800
C	-2.44678500	0.40503500	2.70514400
H	-2.73361800	0.13117400	3.72500700
H	-2.01622700	1.41313000	2.74330000
C	-3.63423700	0.37516900	1.75923700
H	-4.12284500	-0.60597500	1.76885200
H	-4.39039500	1.12240400	2.02841100
C	-4.15716000	0.49240000	-0.67665500
H	-4.91536000	1.27971600	-0.59769900
H	-4.66860500	-0.46746300	-0.55004800
C	-3.42878300	0.57388100	-1.99681100
H	-2.96162000	1.55931800	-2.09627800
H	-4.11050800	0.43680400	-2.84693500
C	-1.39757400	-0.09443700	-3.12391700
H	-0.57132800	-0.80880800	-3.12568900
C	-2.86532900	-1.78883400	-2.25349300
H	-2.03203800	-2.49097400	-2.31503900
H	-2.72854000	1.54326300	0.34093600
H	0.72913200	0.71461700	2.41482800
H	0.29985300	-0.21199700	3.88498800
H	-1.49594500	-2.33041800	3.81673200
H	-2.55804000	-2.66624000	2.42874800
H	-1.00453900	0.91069100	-2.96291500
H	-1.90240700	-0.12918800	-4.09885900
H	-3.50411200	-2.08423300	-1.41693500
H	-3.44866500	-1.83849200	-3.18283400
H	0.37294100	-0.66347200	-0.43065800
H	-0.29703500	-1.37251600	-0.60184400
C	0.58423600	1.57776300	-0.73198600
O	-0.60475200	1.48890600	-0.23604400
O	1.36335600	0.14761300	-0.29013600
C	2.44230500	-0.24981100	-1.14698600
H	2.14055700	-0.13842100	-2.20060600
H	3.28168800	0.43237900	-0.96105600
H	0.70083500	1.45763700	-1.83292700
C	2.81180400	-1.66963200	-0.84174500
C	2.40517900	-2.71123400	-1.68073400

C	3.53364400	-1.97387200	0.31787900
C	2.71591100	-4.03431200	-1.36969900
H	1.84245000	-2.48115200	-2.58407400
C	3.84329900	-3.29424800	0.63247100
H	3.85108200	-1.16597000	0.97451700
C	3.43483100	-4.32762100	-0.21208300
H	2.39845200	-4.83509100	-2.03178800
H	4.40854300	-3.51866200	1.53271600
H	3.68023300	-5.35759700	0.03024900
C	1.49332900	2.65021000	-0.21150900
C	2.57504500	3.08287000	-0.98278700
C	1.27050100	3.22772100	1.04144400
C	3.43875600	4.06510200	-0.50185300
H	2.73333600	2.65241600	-1.97066600
C	2.12939300	4.21177800	1.52296800
H	0.40774900	2.90494700	1.61954600
C	3.21856700	4.62797000	0.75470600
H	4.27780600	4.39521700	-1.10783800
H	1.95037700	4.65950600	2.49692300
H	3.88796900	5.39608300	1.13184000
N	-2.33080700	-0.42893100	-2.03580500

IV (c) -TS

First vibrational frequency: 28.18 cm⁻¹

1 2			
Co	-0.81988300	-0.34662200	-0.35042900
P	-2.84763600	-1.14921500	-0.19399800
N	-1.06048600	0.30094400	1.62237000
H	-0.36991100	-0.20739600	2.17068600
C	-2.98519200	-1.24096400	1.64491700
H	-4.01777900	-1.39049200	1.97925100
H	-2.40321300	-2.10801500	1.97796900
C	-2.40316300	0.04156100	2.20834000
H	-2.34410600	0.01820300	3.30243400
H	-3.04593700	0.88973000	1.94895500
C	-1.34900900	2.43105000	0.45921500
H	-1.13497200	3.51056400	0.47769700
H	-2.43885200	2.32371300	0.51873800
C	-0.69301400	1.73591400	1.63383600
H	-0.98140000	2.21780900	2.57680300
H	0.39704700	1.79340300	1.55561400
C	-4.35722700	-0.24127200	-0.68779700
H	-4.38316800	-0.11065800	-1.77197300
H	-5.24840900	-0.79486400	-0.37702300
H	-4.38271500	0.74736300	-0.22058500
C	-1.86308800	2.12232700	-1.88736700
H	-1.92252000	3.20503800	-2.07785200
H	-1.54278200	1.62077700	-2.80293700
H	-2.85673300	1.75898500	-1.62105000
C	0.40625600	2.32693000	-1.20723900

H	0.75781000	1.77454900	-2.08243900
H	0.35354900	3.39671100	-1.45842700
H	1.13093000	2.19008100	-0.40286900
C	-3.19210300	-2.84135600	-0.77352800
H	-4.14988200	-3.20084500	-0.38689200
H	-3.22189800	-2.85551000	-1.86499300
H	-2.39771900	-3.51460400	-0.44493300
C	2.07458200	-0.63602400	-0.69612200
O	1.11931000	-0.25358900	0.00544100
H	1.87872500	-1.05965400	-1.69548700
H	-0.66794400	-0.84172500	-1.76970100
C	3.45208100	-0.53594000	-0.27160200
C	3.79489200	0.02732200	0.97207100
C	4.46173000	-0.99611400	-1.13346100
C	5.12709300	0.12162700	1.34128600
H	3.00388800	0.38319600	1.62684700
C	5.79549600	-0.89875700	-0.75734600
H	4.18772500	-1.42637300	-2.09404900
C	6.12695100	-0.34126900	0.47832300
H	5.39731200	0.55514400	2.29935900
H	6.57656400	-1.25460500	-1.42167800
H	7.16951300	-0.26536600	0.77305000
N	-0.91436200	1.81625200	-0.81203400

IV(c) -TS

First vibrational frequency: -363.25 cm⁻¹

1	2		
Co	0.36054600	-0.48715200	0.01964800
P	0.52764700	1.59854200	-0.63779600
N	1.48224800	0.01547300	1.63367500
H	0.88070100	-0.13462200	2.44175500
C	0.92547000	2.33441100	1.00470000
H	1.28836200	3.36437100	0.92686700
H	-0.00240100	2.35204600	1.58897200
C	1.95180700	1.43104900	1.66095500
H	2.16872000	1.73306700	2.69092600
H	2.89907700	1.47424500	1.11263400
C	3.17247800	-1.13807600	0.30265100
H	4.02435900	-1.83350300	0.32136400
H	3.55425600	-0.17825600	-0.06602700
C	2.59384000	-0.96637800	1.69098200
H	3.36839000	-0.64377900	2.39658900
H	2.18028600	-1.90854700	2.06111400
C	1.80371800	2.25873400	-1.76163300
H	1.65377400	1.86785900	-2.77030300
H	1.75137100	3.35085000	-1.79318600
H	2.80110900	1.96603000	-1.42284700
C	2.54207400	-1.31874500	-2.02577700
H	3.45729900	-1.86945100	-2.28879000
H	1.74313500	-1.62067600	-2.70632300

H	2.72730300	-0.25095900	-2.15469700
C	1.90306900	-3.04032000	-0.50385600
H	1.08801000	-3.34080800	-1.16572500
H	2.80863300	-3.60267800	-0.77414900
H	1.61140600	-3.28608300	0.51672000
C	-1.00665100	2.40713300	-1.18498300
H	-0.88984800	3.49394100	-1.21580500
H	-1.27591500	2.04846000	-2.18130800
H	-1.81879500	2.14898400	-0.49933200
C	-1.30764500	-1.67225300	-0.17445900
O	-0.55543800	-1.99863100	0.84518700
H	-1.43232600	-2.41428600	-0.98168200
H	-0.43530600	-0.82312100	-1.23086800
C	-2.47873700	-0.76658400	0.02944800
C	-2.68475000	-0.14579700	1.26752200
C	-3.35712800	-0.50323700	-1.02753100
C	-3.74764500	0.73602100	1.44030200
H	-2.00348000	-0.36728900	2.08614000
C	-4.41886700	0.37904700	-0.85404300
H	-3.19571600	-0.98401200	-1.99089700
C	-4.61406700	1.00376500	0.37921300
H	-3.90384100	1.21276500	2.40384700
H	-5.09550800	0.58171300	-1.67937500
H	-5.44181300	1.69417500	0.51342000
N	2.13018900	-1.59243000	-0.64367200

v(b)

First vibrational frequency: 32.70 cm⁻¹

1 2			
Co	0.96478700	-0.62873300	-0.12626300
P	0.55068200	1.46466900	-0.74221000
N	1.71105000	0.06122000	1.73959800
C	1.68041800	2.62843000	-1.58571400
H	1.82536800	2.33118700	-2.62683900
C	-1.07800100	1.89672200	-1.43104500
H	-1.15101600	1.57891600	-2.47332900
C	0.47253800	2.08068900	0.99319900
H	0.45356800	3.17528600	1.03366400
H	-0.47135400	1.70705600	1.40611600
C	1.65214600	1.54322800	1.79120100
H	2.58983400	1.91926900	1.36486300
H	1.61794400	1.89889300	2.82761100
C	3.06793400	-0.50639300	1.93410000
H	3.18581100	-0.94252700	2.92961100
H	3.80126200	0.30182200	1.86113200
C	3.32603800	-1.56395300	0.87710100
H	2.72778500	-2.45891400	1.08341800
H	4.38136300	-1.87029100	0.86812500
C	2.95502900	-2.18984000	-1.43620300
H	2.62614900	-1.82927600	-2.41260400

C	3.81720000	-0.00890700	-0.94076100
H	3.48820700	0.33017800	-1.92421200
H	-1.46177800	-0.88964700	-1.45680100
H	1.07355700	-0.31517900	2.43645300
C	-3.39910200	-0.00124600	1.00119000
C	-4.70949400	0.38921800	1.28284900
C	-5.75471100	-0.00861100	0.45234400
C	-5.48176900	-0.80257300	-0.66385700
C	-4.17496100	-1.19396800	-0.94020400
C	-3.11889000	-0.79677000	-0.11139400
C	-1.70757300	-1.23274100	-0.43032600
H	-2.57583800	0.30355000	1.64162100
H	-4.91337900	1.00550900	2.15487100
H	-6.77478000	0.29499200	0.67062300
H	-6.29047300	-1.11714300	-1.31845200
H	-3.96771700	-1.81532800	-1.81041500
H	-1.85892000	1.39590900	-0.85390600
H	-1.23507700	2.97800800	-1.38102400
H	1.26069700	3.63848900	-1.56341000
H	2.65790200	2.65005200	-1.09889000
H	2.28720100	-2.98805400	-1.10395900
H	3.97084200	-2.59559300	-1.52874800
H	3.79884200	0.83870500	-0.25352000
H	4.84856100	-0.37779100	-1.01395200
O	-0.77185000	-0.76432500	0.49314700
H	-1.69331000	-2.33711600	-0.49531400
N	2.91512800	-1.07412600	-0.47110500

VI (a)

First vibrational frequency: 21.52 cm⁻¹

1 2			
Co	1.35557900	-0.04592100	-0.55084700
P	0.61086000	2.03806100	-0.54120300
N	1.56341400	0.19839600	1.42331000
C	1.65112100	3.30207000	-1.33811600
H	1.67066600	3.13853800	-2.41762800
C	-1.08176200	2.40339200	-1.08133300
H	-1.17644200	2.24473100	-2.15757200
C	0.65036300	2.42707900	1.26062800
H	0.80007700	3.49562600	1.43833000
H	-0.32951100	2.15957700	1.67275700
C	1.73600700	1.58412400	1.90261900
H	2.73669200	1.91792700	1.60658800
H	1.68439400	1.62203800	2.99738400
C	2.51951100	-0.79407700	1.94591500
H	2.40953600	-0.92703300	3.02805500
H	3.53328400	-0.42449300	1.76078600
C	2.23495700	-2.07978400	1.20829800
H	1.21257800	-2.40528200	1.42752900
H	2.92528300	-2.88343000	1.49442600

C	1.62520200	-2.95534500	-0.95809400
H	1.68850000	-2.79868300	-2.03684000
C	3.68763500	-1.70973800	-0.72246300
H	3.69701800	-1.59980800	-1.80805600
H	0.61133700	-0.11613700	1.64719500
C	-3.00010200	-0.27257700	1.00774900
C	-4.27040000	-0.04721200	1.54202800
C	-5.40770700	-0.30871500	0.78124800
C	-5.26602000	-0.79953300	-0.51927700
C	-3.99760200	-1.02580500	-1.04641300
C	-2.84837700	-0.76533000	-0.28999600
C	-1.47248900	-0.99937200	-0.87967700
H	-2.10357900	-0.07523600	1.59070300
H	-4.37100700	0.33295300	2.55591500
H	-6.39715500	-0.13570700	1.19559500
H	-6.14723000	-1.00855000	-1.12053200
H	-3.89316600	-1.41198000	-2.06000800
H	-1.77500100	1.73474000	-0.56330500
H	-1.33719700	3.44158400	-0.85179300
H	1.26238500	4.30430700	-1.13750700
H	2.67467100	3.23474500	-0.96281100
H	0.57724000	-2.97099600	-0.65428600
H	2.10364500	-3.91169100	-0.71107000
H	4.15057800	-0.82310100	-0.28153000
H	4.27713900	-2.59430600	-0.44938700
O	-0.44563200	-0.78966000	0.01253200
H	-1.46104700	-2.02951800	-1.30350700
H	-1.39152600	-0.34388000	-1.77694900
H	1.66064600	0.00285500	-2.16545300
H	0.95950300	-0.43211900	-2.09081800
N	2.29190100	-1.84218600	-0.25963000

VI (a) -TS

First vibrational frequency: -611.58 cm⁻¹

1	2		
Co	1.05883500	-0.22407900	-0.70951500
P	0.20302900	1.80262400	-0.95249400
N	0.77692700	0.05954300	1.24585100
C	1.54776400	3.00753300	-1.22480300
H	1.93734100	2.89850600	-2.23901700
C	-1.11169700	2.36413300	-2.07276900
H	-0.82355400	2.17214200	-3.10838800
C	-0.38085900	2.14826100	0.75884100
H	-0.44837300	3.22116900	0.96287800
H	-1.38875300	1.72502300	0.86496100
C	0.58759500	1.45861200	1.70160000
H	1.57062200	1.94271000	1.68689700
H	0.22865900	1.47292600	2.73759300
C	1.77903600	-0.70549200	2.01907900
H	1.43104300	-0.89646300	3.04011300

H	2.68522600	-0.09646200	2.09268800
C	2.02523300	-1.99674200	1.27838300
H	1.11315700	-2.60376300	1.26974500
H	2.81995000	-2.58878800	1.75196500
C	2.29853400	-2.96510300	-0.91706400
H	2.56917500	-2.75885900	-1.95391400
C	3.71254400	-1.12992400	-0.26157000
H	3.93679400	-0.97096200	-1.31762800
H	-0.12589000	-0.41505700	1.34709900
C	-2.20200400	-1.27849200	0.95413600
C	-2.88950800	-0.79331200	2.06657700
C	-3.88150600	0.17470100	1.90749900
C	-4.19260100	0.63460400	0.62777100
C	-3.49766400	0.14868600	-0.47918900
C	-2.47833700	-0.79777600	-0.33098300
C	-1.70574900	-1.31387700	-1.52241000
H	-1.44309200	-2.05091700	1.06623400
H	-2.65508100	-1.17545500	3.05711600
H	-4.41509300	0.55928500	2.77201500
H	-4.97242300	1.37896800	0.49193600
H	-3.75088500	0.50914900	-1.47545400
H	-2.03670300	1.82498900	-1.86040300
H	-1.28768100	3.43569600	-1.94307700
H	1.18731100	4.03149800	-1.08917900
H	2.36786100	2.82168700	-0.52653500
H	1.27912200	-3.35001800	-0.88771400
H	2.99722900	-3.70544000	-0.50648300
H	3.76145300	-0.16491200	0.24979400
H	4.46809300	-1.79985800	0.16972600
O	-0.41573700	-1.73491100	-1.19729800
H	-2.26792800	-2.15667000	-1.96653300
H	-1.70474500	-0.52842000	-2.30447900
H	1.22054800	-0.52815000	-2.31738600
H	0.54142100	-1.09479000	-2.05090000
N	2.36012900	-1.71221200	-0.14182100