Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

# HPCO—A Phosphorus-Containing Analogue of Isocyanic Acid

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Supporting Information

# 1. Experimental section

*General synthetic methods.* All reactions and product manipulations were carried out under an inert atmosphere of argon or dinitrogen using standard Schlenk-line or glovebox techniques (MBraun UNIlab glovebox maintained at < 0.1 ppm $H_2O$ and < 0.1 ppm $O_2$).

[Na(dioxane)]PCO was prepared according to a literature procedure, but dried at 60 °C for 8 hours to reduce the dioxane content.[1] Hexane (hex; Sigma-Aldrich, HPLC grade) was purified using an MBraun SPS-800 solvent system. Tetrahydrofuran (THF; Sigma-Aldrich, HPLC grade) was distilled over sodium metal/benzophenone. $D_2O$ (Acros, 99.8%) and $C_6D_6$ (Sigma-Aldrich, 99.5%) were used as received. Stearic acid (Sigma-Aldrich, 95%) and $Me_3SiCl$ (Sigma-Aldrich, 99.5%) were used as received. $NEt_3$ (Sigma-Aldrich, 99.5%) was distilled from $CaH_2$ and degassed prior to use. [$D_8$]-toluene (Sigma-Aldrich, 99.5%), $CD_2Cl_2$ (Sigma-Aldrich, 99.5%), [$D_8$]-THF (Sigma-Aldrich, 99.5%) were dried over $CaH_2$ and stored under argon in gas-tight ampoules over activated 3 Å molecular sieves.

**Characterization techniques:** $^{1}H$, $^{1}H\{^{31}P\}$, $^{2}H$, $^{13}C$, $^{13}C\{^{1}H\}$, $^{13}C$-DEPT135, $^{31}P$, and $^{31}P\{^{1}H\}$ NMR spectra were acquired at 223 K at 400.2 ($^{1}H$), 100.6 ($^{13}C$) and 162.0 ($^{31}P$) MHz, respectively, on a Bruker Avance 300 HD Ascend NMR spectrometer if not stated otherwise. $^{1}H$ and $^{13}C$ NMR spectra were referenced to the most downfield solvent resonance.[2] $^{31}P$ spectra were externally referenced to an 85% solution of $H_3PO_4$ in $H_2O$ ($\delta$ = 0 ppm). Gas-phase IR spectra were recorded at ambient conditions in cells with 10 cm path length and NaCl windows.

## 1.1 HPCO

Representative setup: A mixture of stearic acid or [$D_1$]-stearic acid (120 mg, 0.420 mmol) and [Na(dioxane)]PCO (45 mg, 0.265 mmol) was heated with an oil bath in vacuo in a Schlenk tube connected to an NMR tube with 0.5 ml of an NMR solvent ([$D_8$]-toluene, $CD_2Cl_2$, [$D_8$]-THF) frozen in a liquid nitrogen cooling trap. At 60 °C, gas evolution commenced in. The temperature was increased stepwise (5 K every 15 min) until 120 °C were reached. In the NMR tube, a yellow condensate formed. The nitrogen cooling bath was removed and quickly replaced by a dry ice/isopropanol cooling bath (–78 °C). Upon thawing, the solvent dissolved most of the yellow condensate, forming a yellow solution which was subjected to NMR experiments.

**$^{1}$HP$^{12}$CO**

**$^{1}$H NMR** ([$D_8$]-toluene, 223 K): 0.25 ($^{1}J_{HP}$ = 188 Hz). **$^{31}$P NMR** ([$D_8$]-toluene, 223 K): –316.7 ($^{1}J_{PH}$ = 188 Hz). **$^{13}$C NMR** ([$D_8$]-toluene, 223 K): 201.4 ($^{1}J_{CP}$ = 102, $^{2}J_{CH}$ = 10.5 Hz). **$^{1}$H NMR** ($CD_2Cl_2$, 223 K): 1.09 ($^{1}J_{HP}$ = 189 Hz). **$^{31}$P NMR** ($CD_2Cl_2$, 223 K): –312.8 ($^{1}J_{PH}$ = 189 Hz). **$^{13}$C NMR** ($CD_2Cl_2$, 223 K): 201.5 ($^{1}J_{CP}$ = 98 Hz). **$^{1}$H NMR** ([$D_8$]-THF, 193 K): 1.32 ($^{1}J_{HP}$ = 192 Hz). **$^{31}$P NMR** ([$D_8$]-THF, 193 K): –316.7 ($^{1}J_{PH}$ = 192 Hz). **$^{13}$C NMR** ([$D_8$]-THF, 193 K): 202.2 ($^{1}J_{CP}$ = 101 Hz). **IR** (gas, cm$^{-1}$): 2707, 2306, 2011 (vs), 1394, 1241, 1066, 873, 697, 473, 389.

**$^{1}$HP$^{13}$CO**

**$^{31}$P NMR** ([$D_8$]-toluene, 223 K): –316.7 ($^{1}J_{PH}$ = 188, $^{1}J_{PC}$ = 102 Hz). **$^{31}$P NMR** ($CD_2Cl_2$, 223 K): –312.8 ($^{1}J_{PH}$ = 189, $^{1}J_{PC}$ = 98 Hz). **IR** (gas, cm$^{-1}$): 1963.

**$^{2}$HP$^{12}$CO**

**$^{2}$H NMR** ([$D_8$]-toluene, 223 K): 0.29 ($^{1}J_{DP}$ = 29.6 Hz). **$^{31}$P NMR** ([$D_8$]-toluene, 223 K): –317.7 ($^{1}J_{PD}$ = 29.5 Hz). **$^{13}$C NMR** ([$D_8$]-toluene, 223 K): 202.05 ($^{1}J_{CP}$ = 101, $^{2}J_{CD}$ = 1.55 Hz). **$^{2}$H NMR** ($CD_2Cl_2$, 223 K): 1.15 ($^{1}J_{DP}$ = 29.8 Hz). **$^{31}$P NMR** ($CD_2Cl_2$, 223 K): –314.3 ($^{1}J_{PD}$ = 29.9 Hz). **$^{13}$C NMR** ($CD_2Cl_2$, 223 K): 201.5 ($^{1}J_{CP}$ = 101, $^{2}J_{CD}$ = 1.55 Hz). **$^{31}$P NMR** ([$D_8$]-THF, 193 K): –317.8 ($^{1}J_{PD}$ = 29.9 Hz). **IR** (gas, cm$^{-1}$): 3488/3454, 2596/2553/2522, 2012 (vs), 1620, 1423, 1193, 1065, 852, 724, 341.

**$^{2}$HP$^{13}$CO**

**$^{31}$P NMR** ([$D_8$]-toluene, 223 K): –317.9 ($^{1}J_{PD}$ = 29.5, $^{1}J_{PC}$ = 101 Hz). **$^{31}$P NMR** ($CD_2Cl_2$, 223 K): –314.6 ($^{1}J_{PD}$ = 29.5, $^{1}J_{PC}$ = 100 Hz). **IR** (gas, cm$^{-1}$): 1964.

## NMR spectra of HPCO

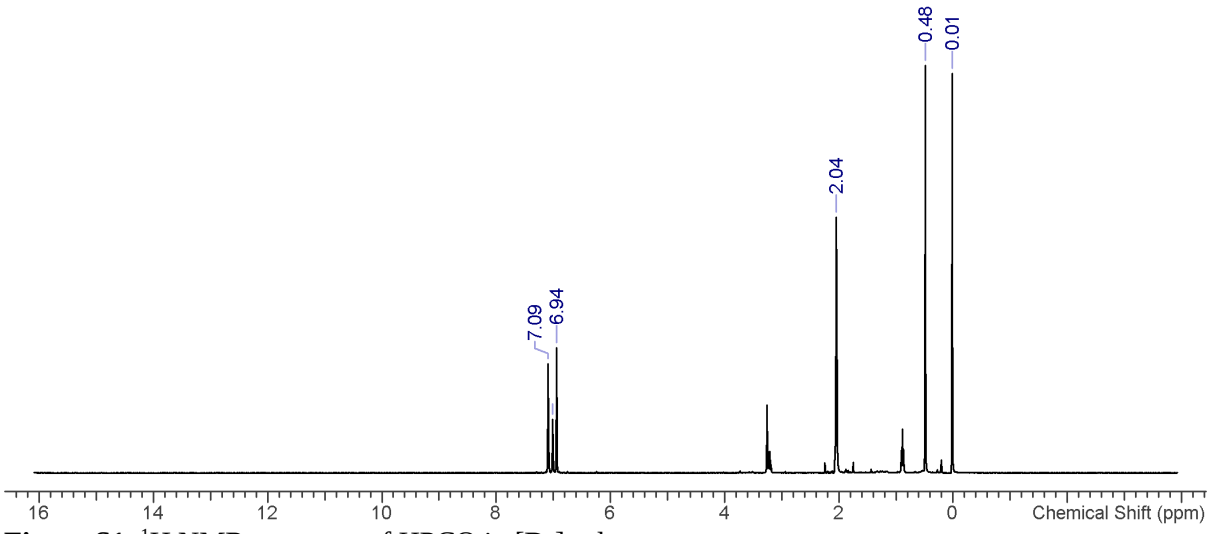


**Figure S1.** $^{1}$H NMR spectrum of HPCO in [$D_8$]-toluene.

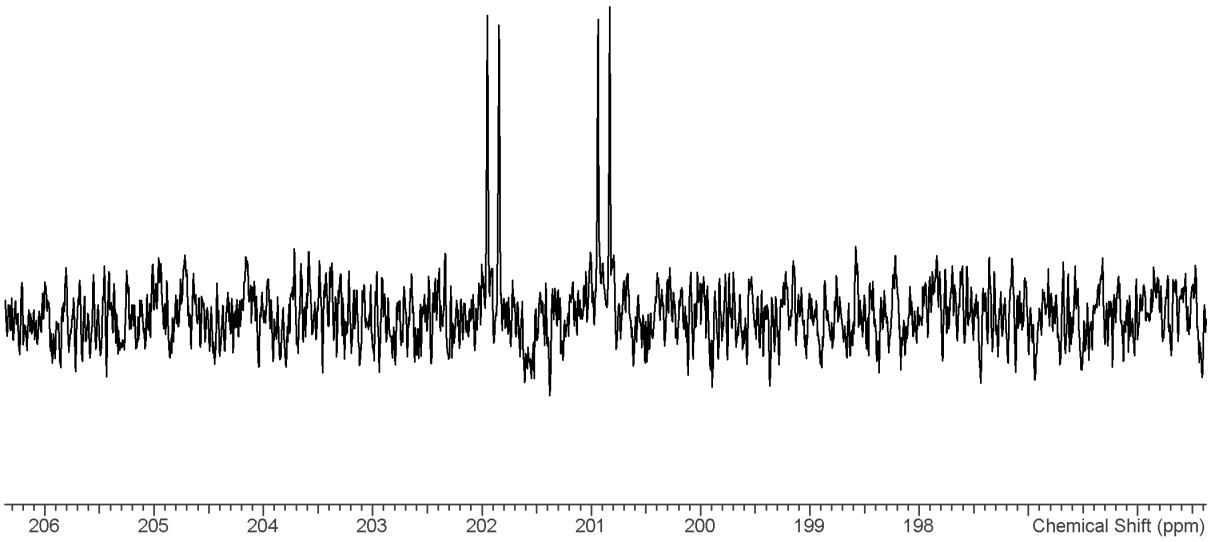


**Figure S2.** $^{13}$C NMR spectrum of HPCO in [$D_8$]-toluene.

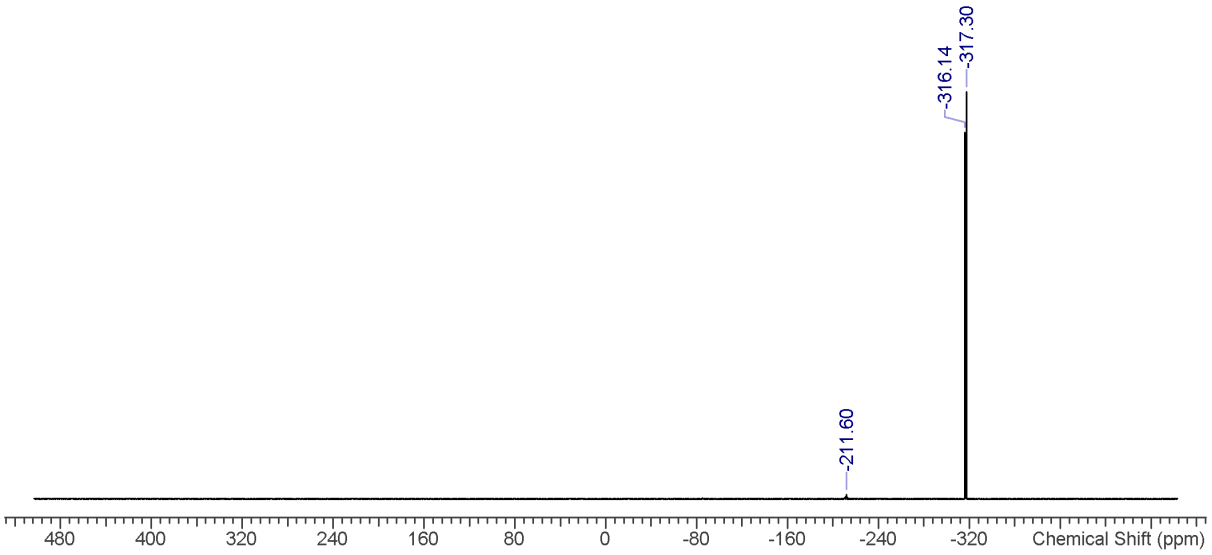


**Figure S3.** $^{31}P$ NMR spectrum of HPCO in $[D_8]$-toluene.

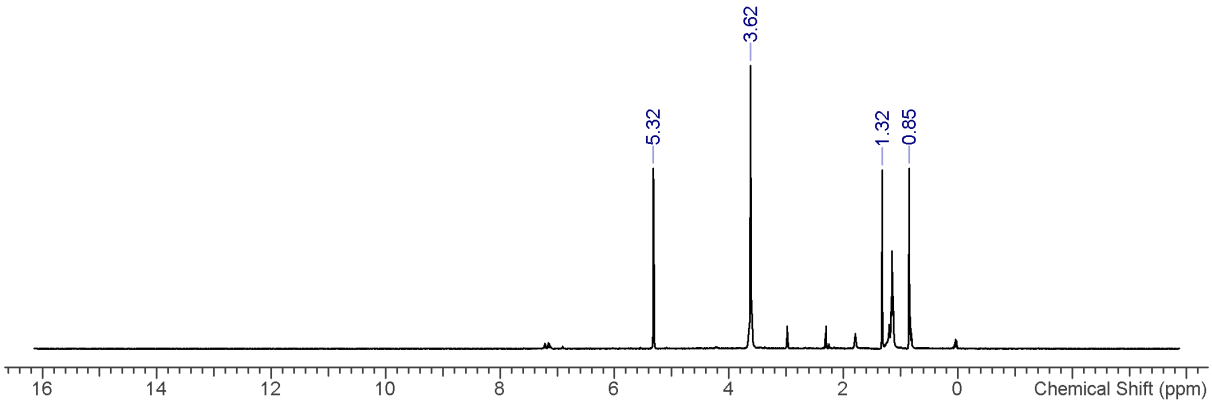


**Figure S4.** $^{1}H$ NMR spectrum of HPCO in $CD_2Cl_2$.

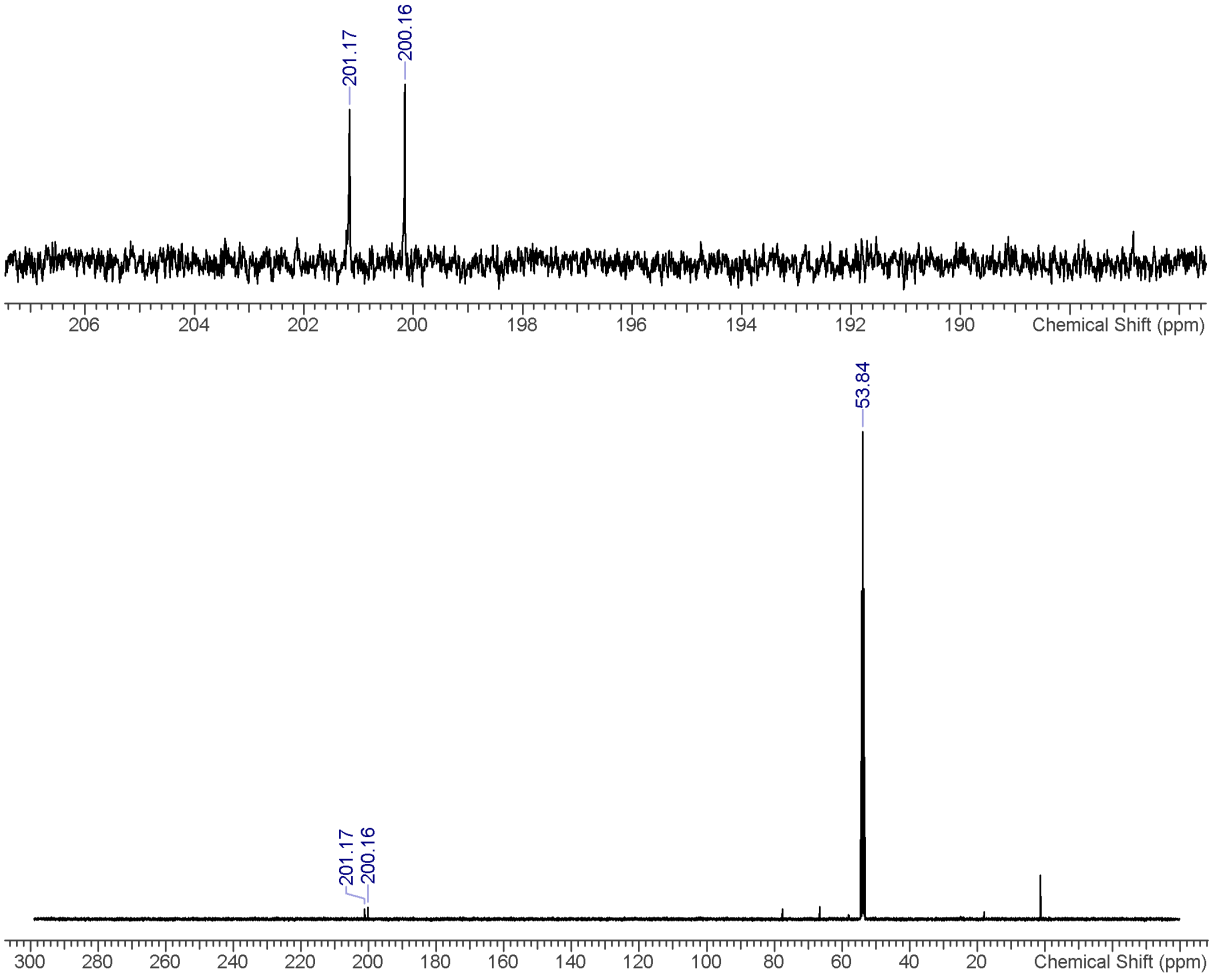


**Figure S5.** $^{13}C$ NMR spectrum of HPCO in $CD_2Cl_2$.

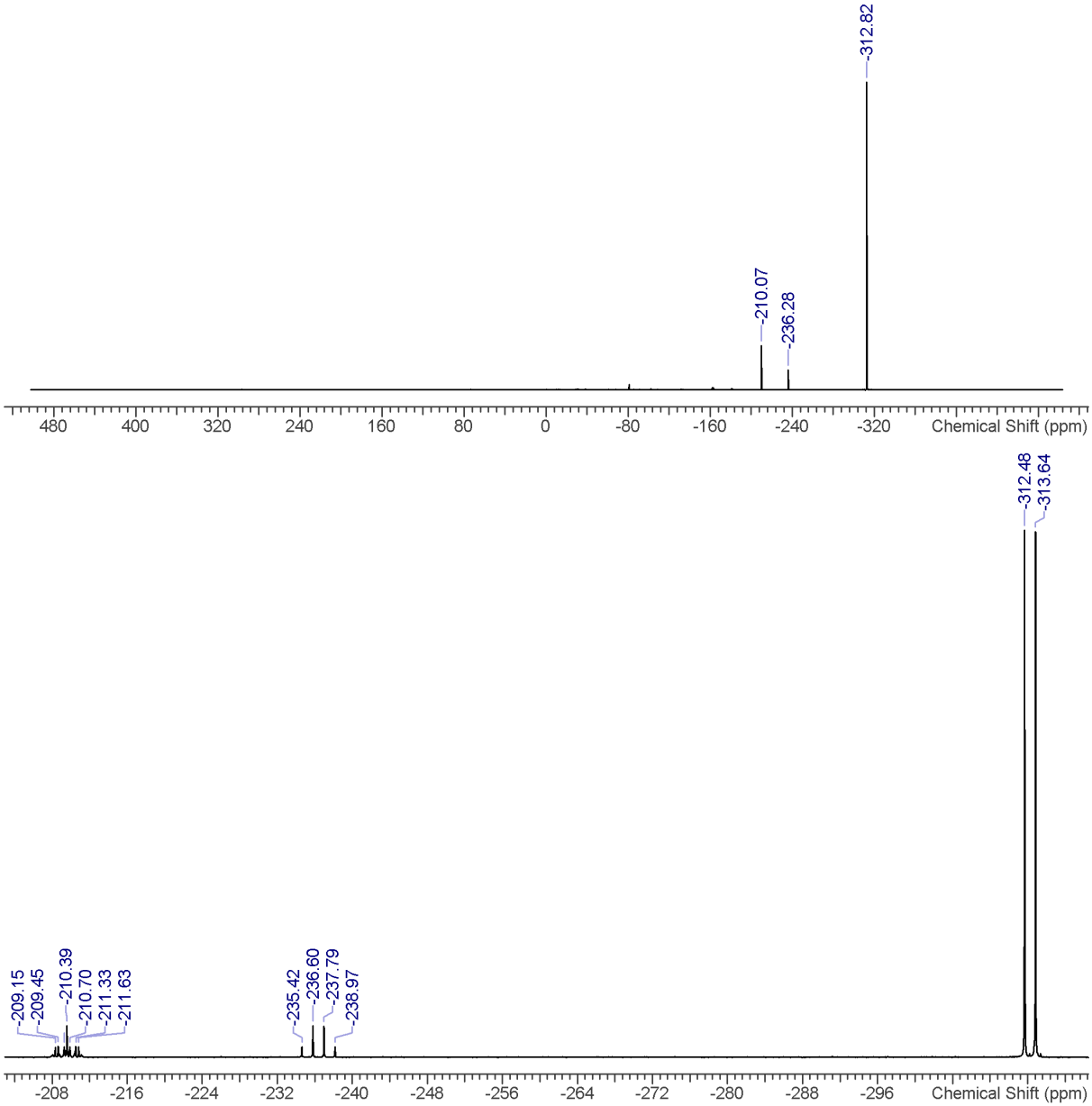


**Figure S6.** $^{1}H$ NMR spectrum of HPCO in $CD_2Cl_2$.

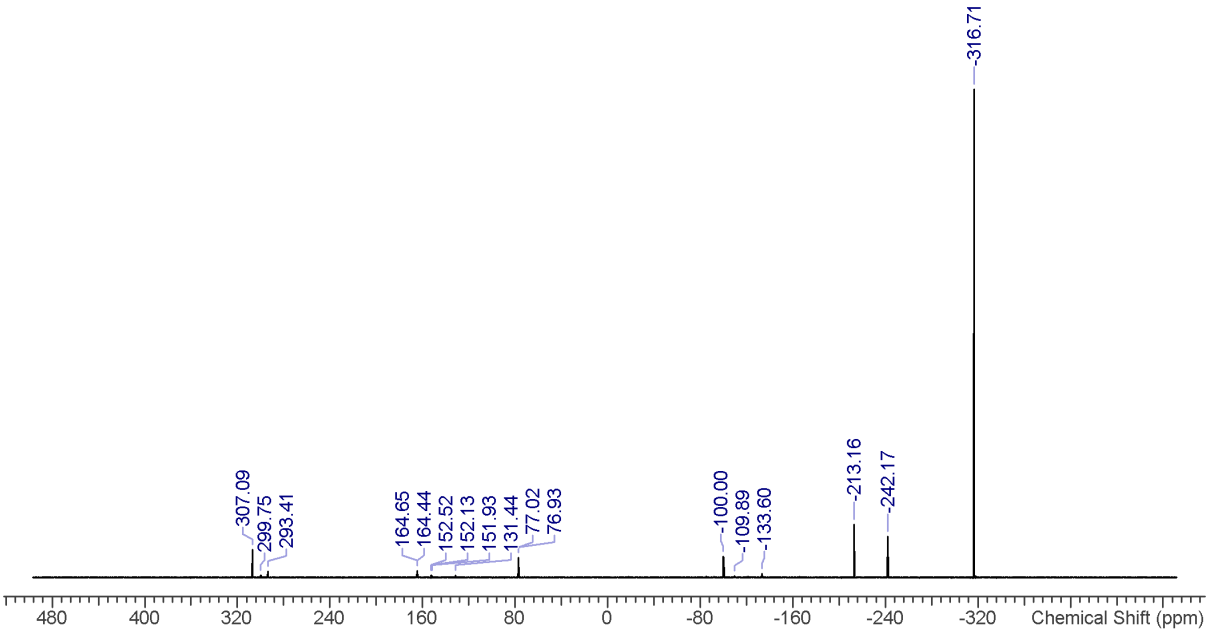


**Figure S7.** $^{31}$P NMR spectrum of HPCO in [$D_8$]-THF of the purest sample of HPCO in THF that could be obtained.

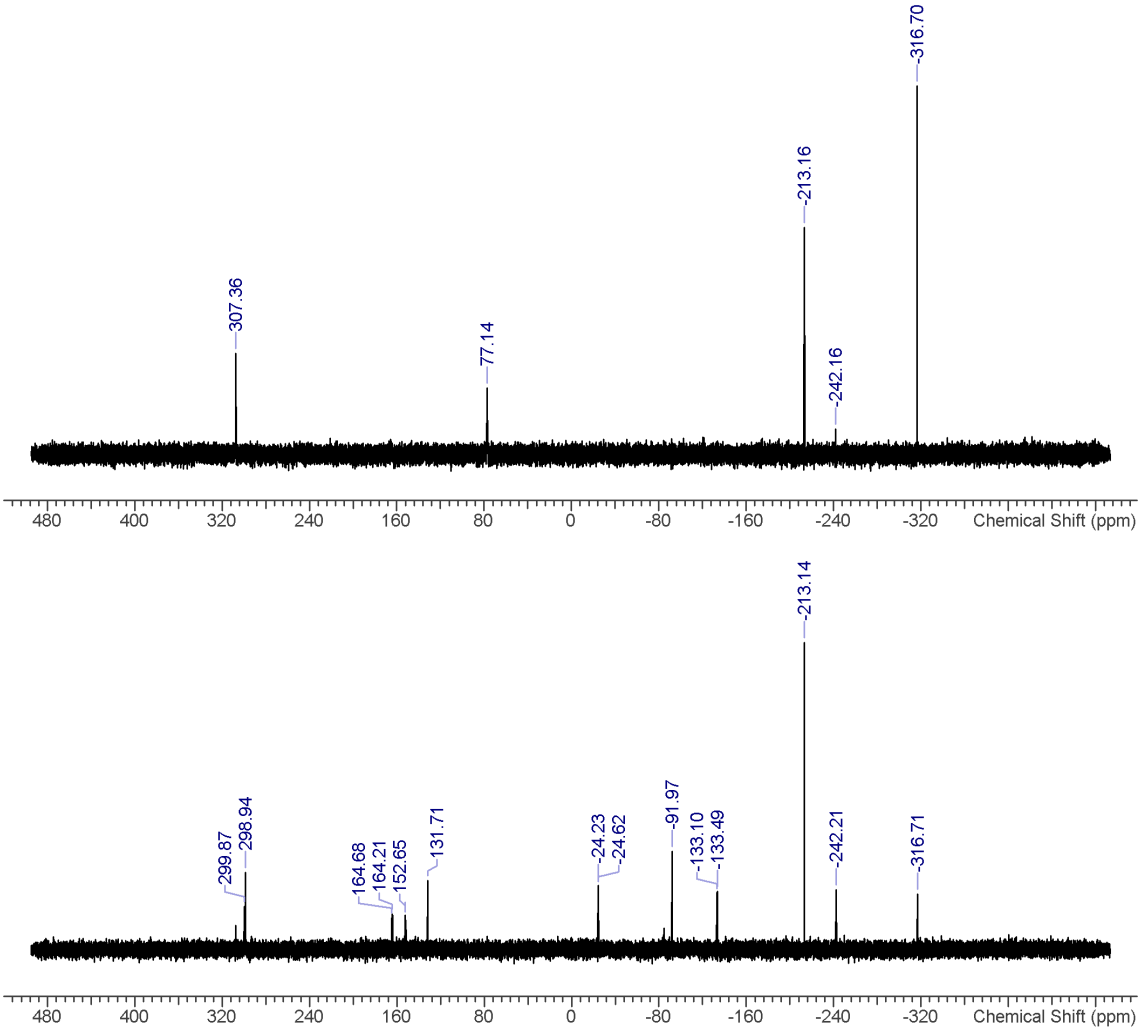


**Figure S8.** $^{31}$P NMR spectrum of a dilute solution of HPCO in [$D_8$]-THF (500 MHz spectrometer). Top: only HPCO and $(HPCO)_2$ present in solution. Bottom: tetramer and other decomposition products present in solution.

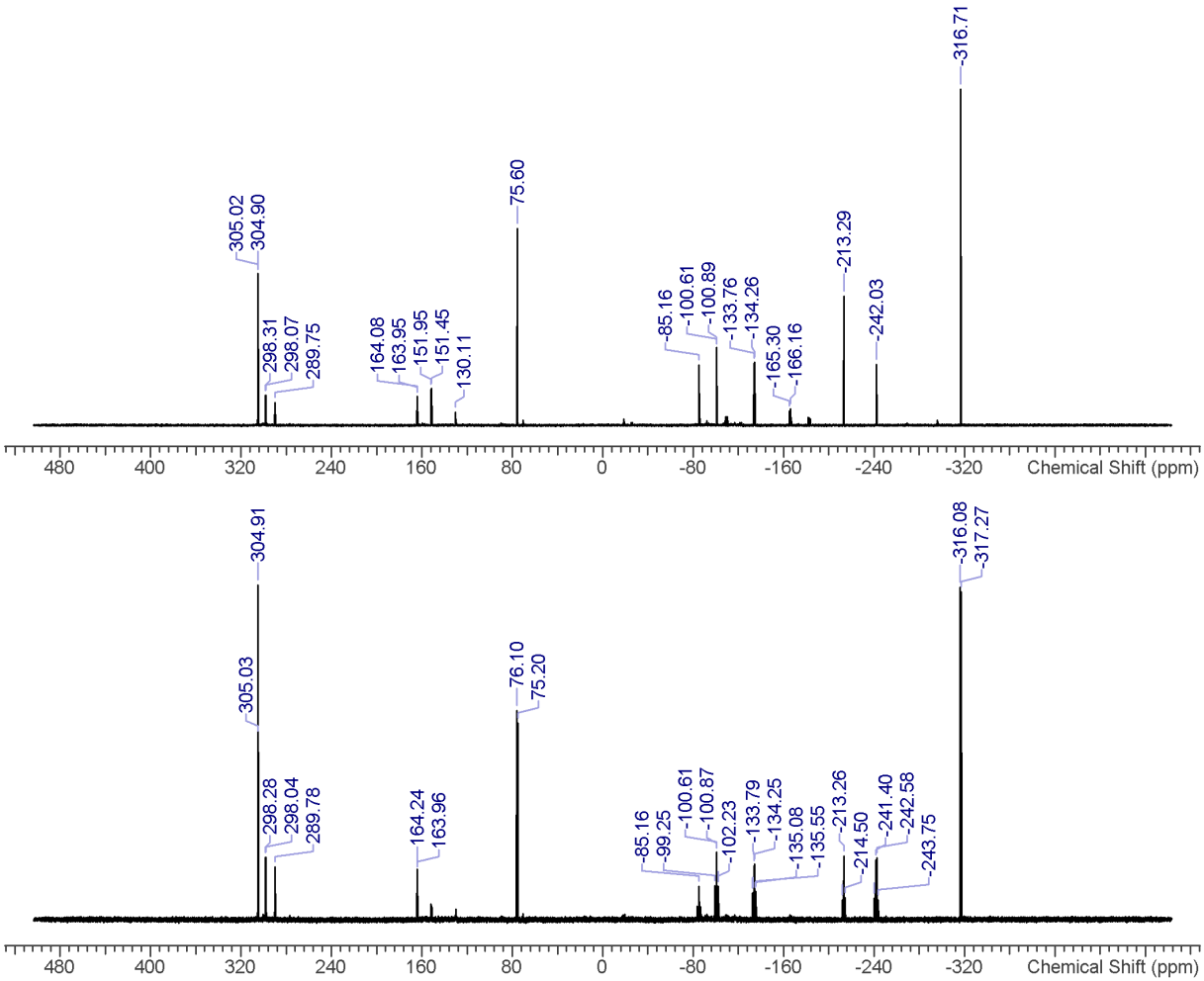


**Figure S9.** $^{31}$P NMR spectrum of a concentrated solution of HPCO in [$D_8$]-THF.

## NMR spectra of DPCO

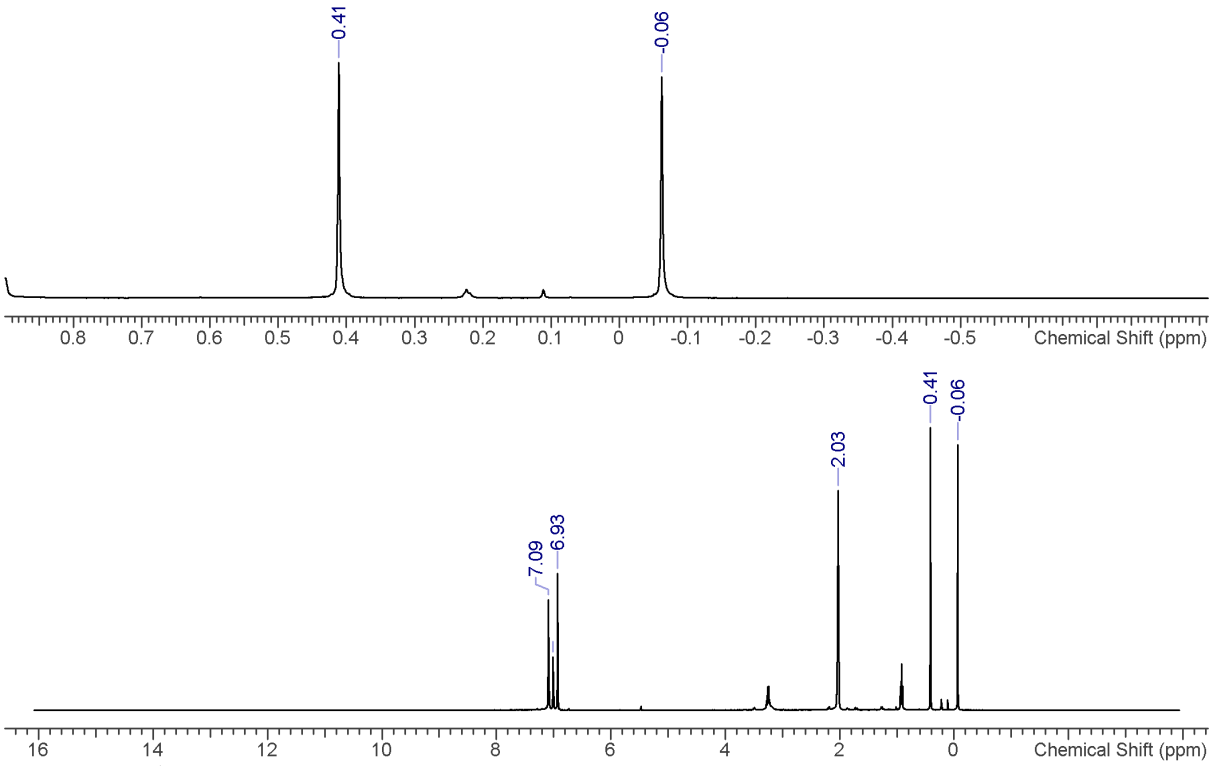


**Figure S10.** $^{1}$H NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-toluene at 223 K.

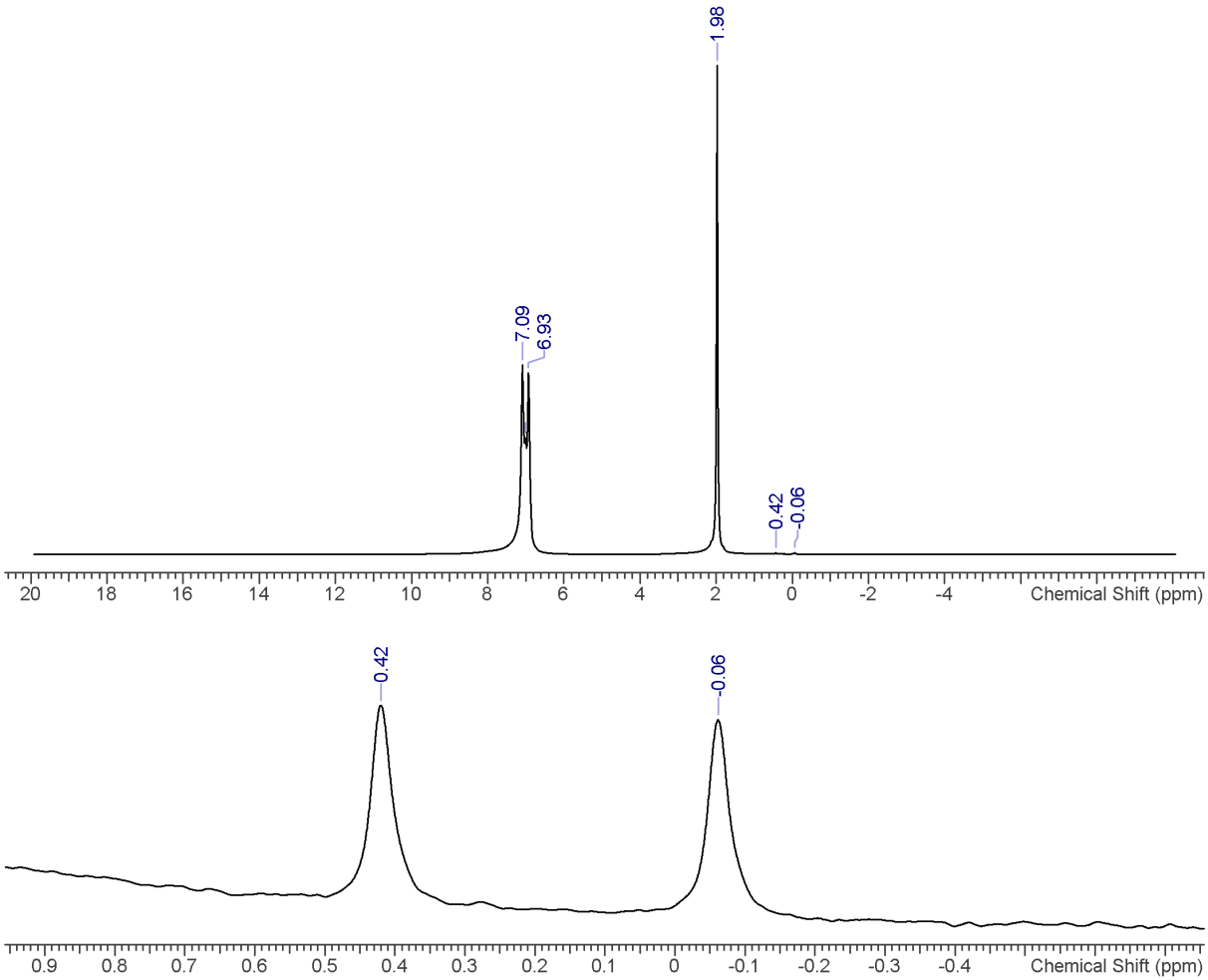


**Figure S11.** $^{2}$H NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-toluene at 223 K.

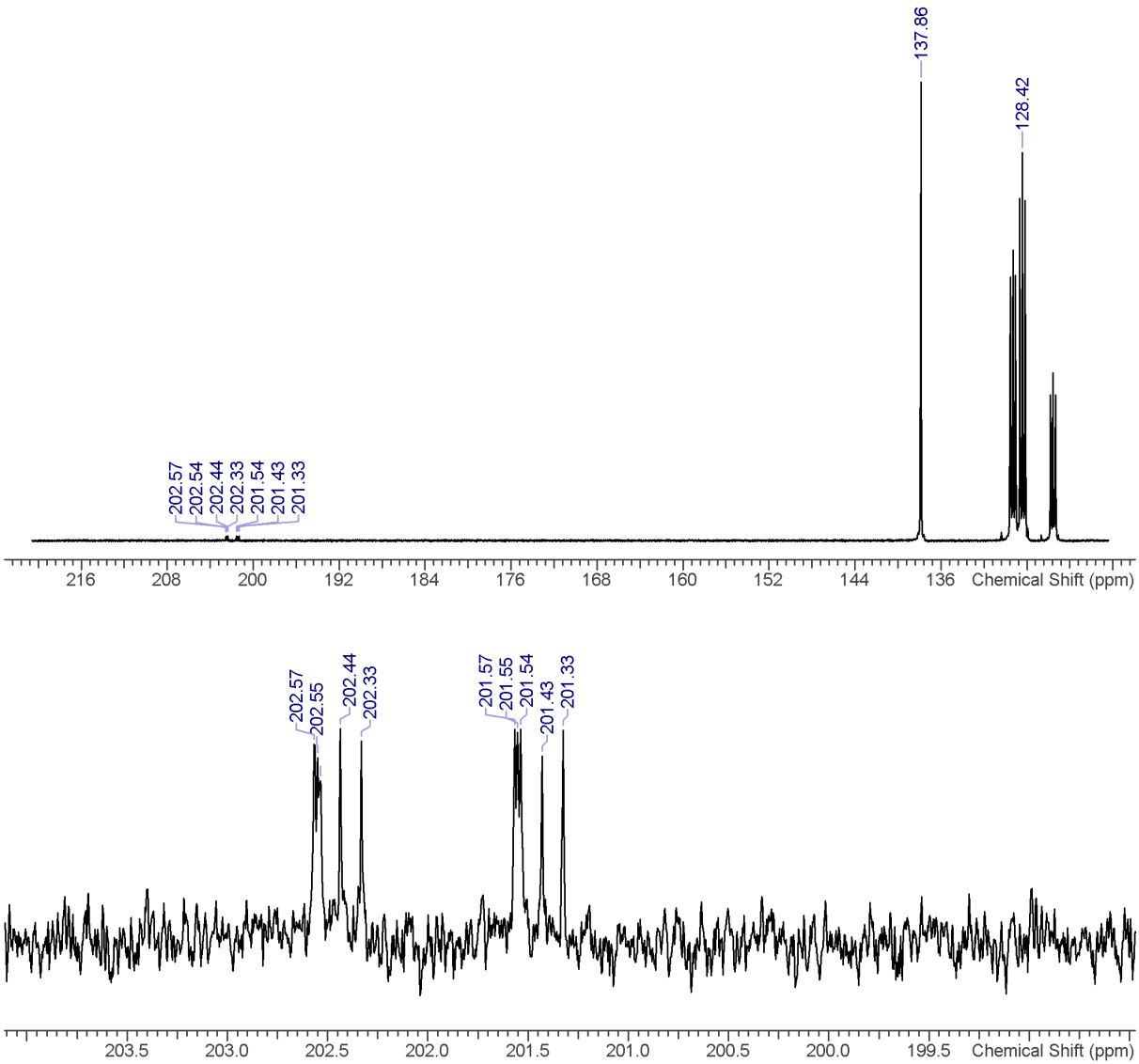


**Figure S12.** $^{13}C$ NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-toluene.

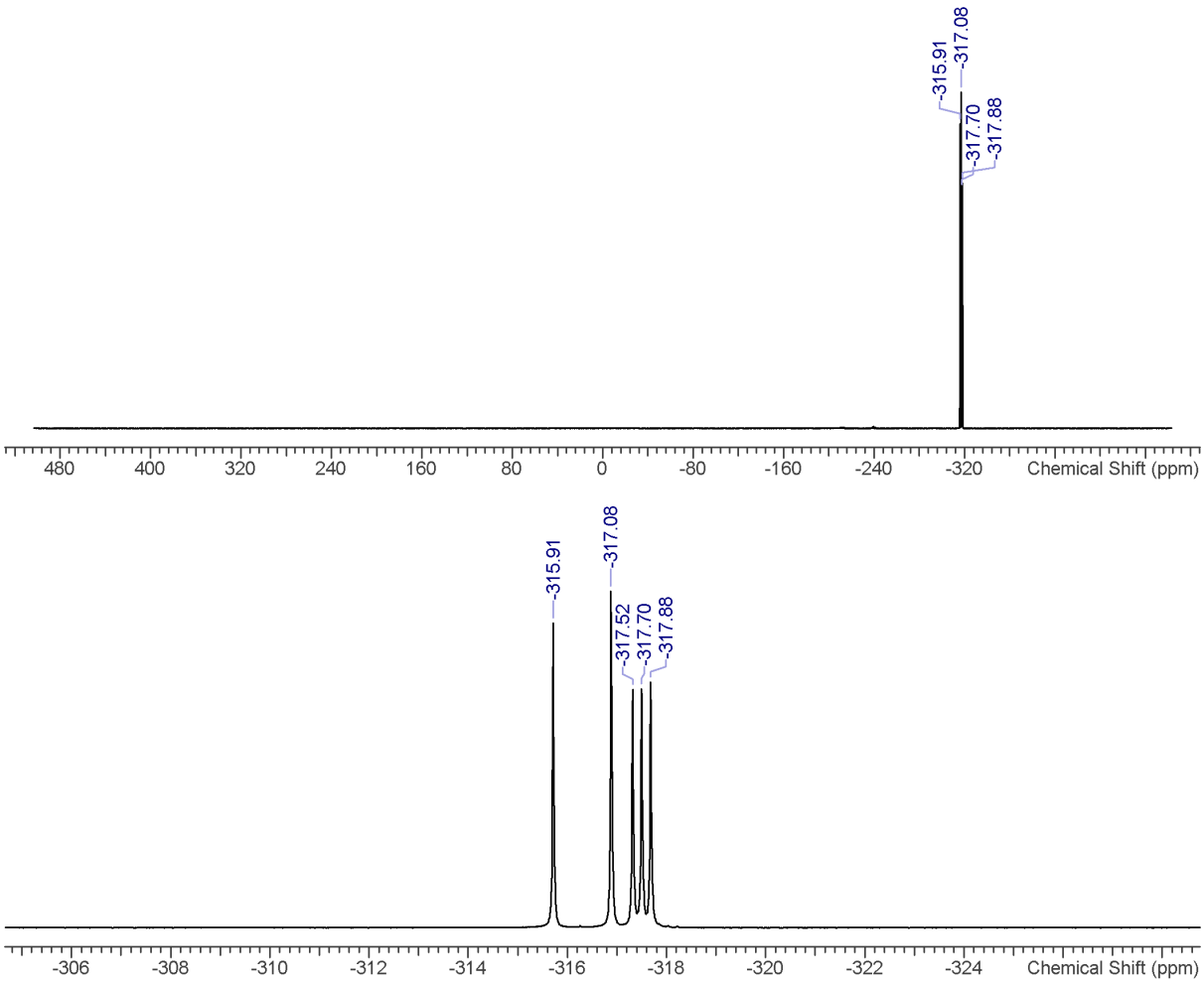


**Figure S13.** $^{31}P$ NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-toluene.

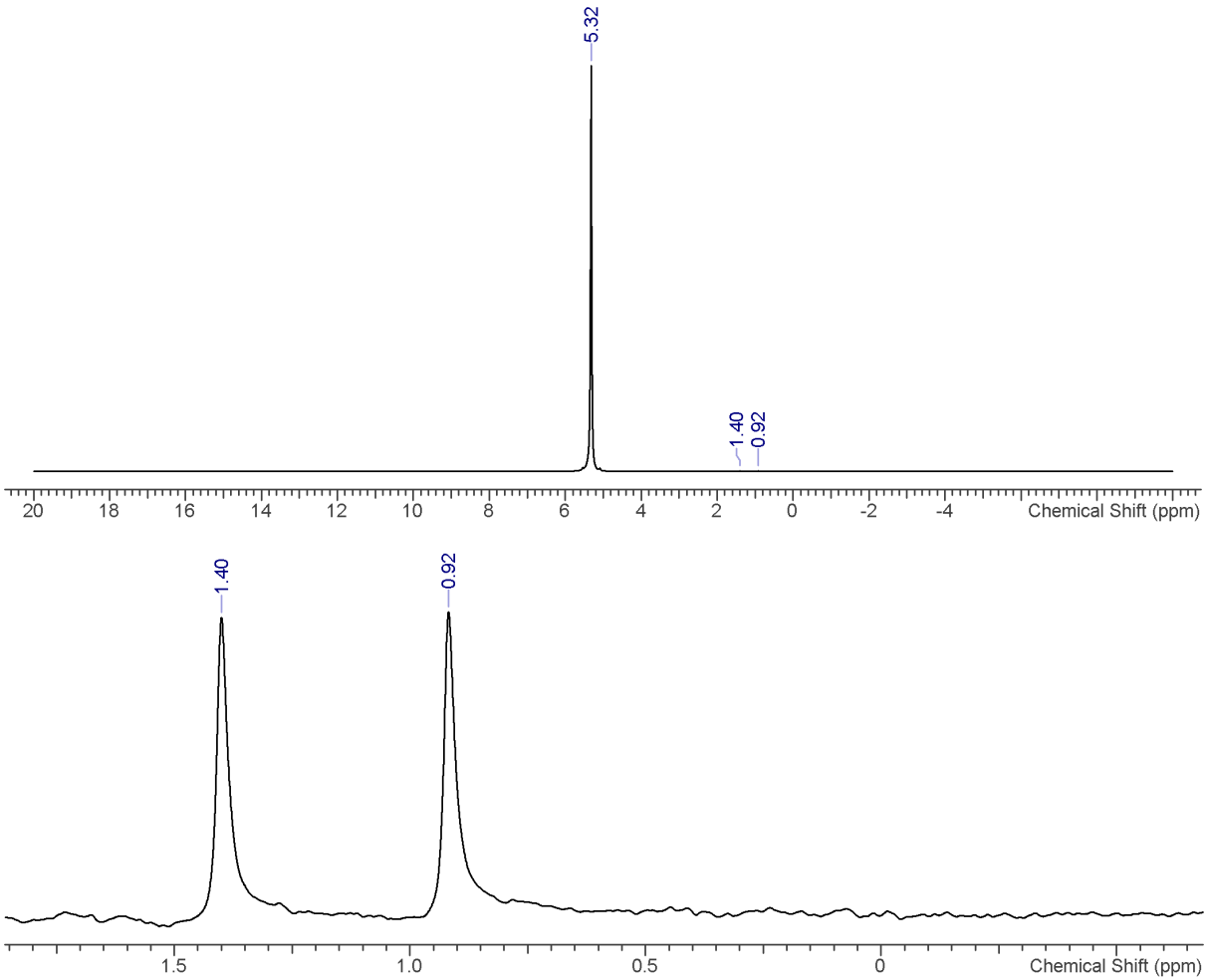


**Figure S14.** $^{2}H$ NMR spectrum of a mixture of HPCO and DPCO in $CD_2Cl_2$.

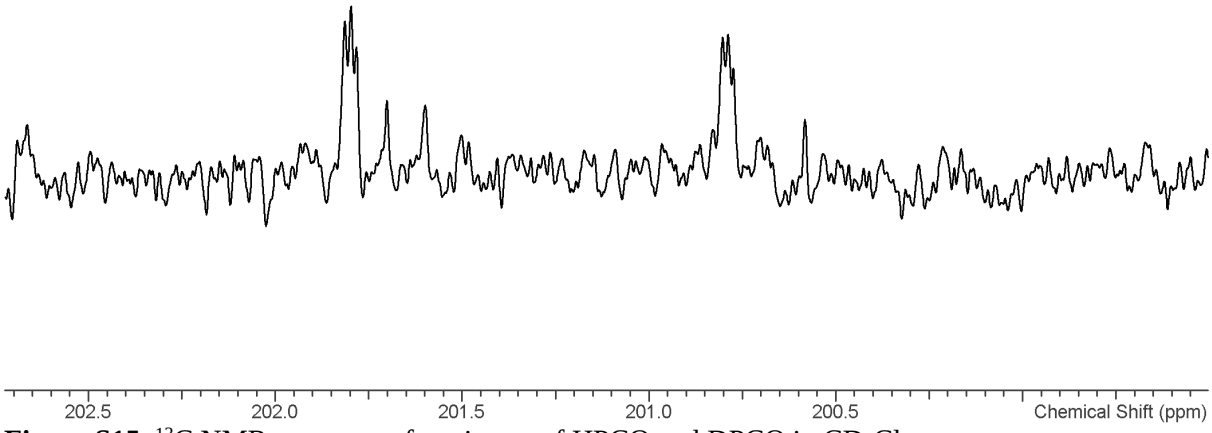


**Figure S15.** $^{13}C$ NMR spectrum of a mixture of HPCO and DPCO in $CD_2Cl_2$.

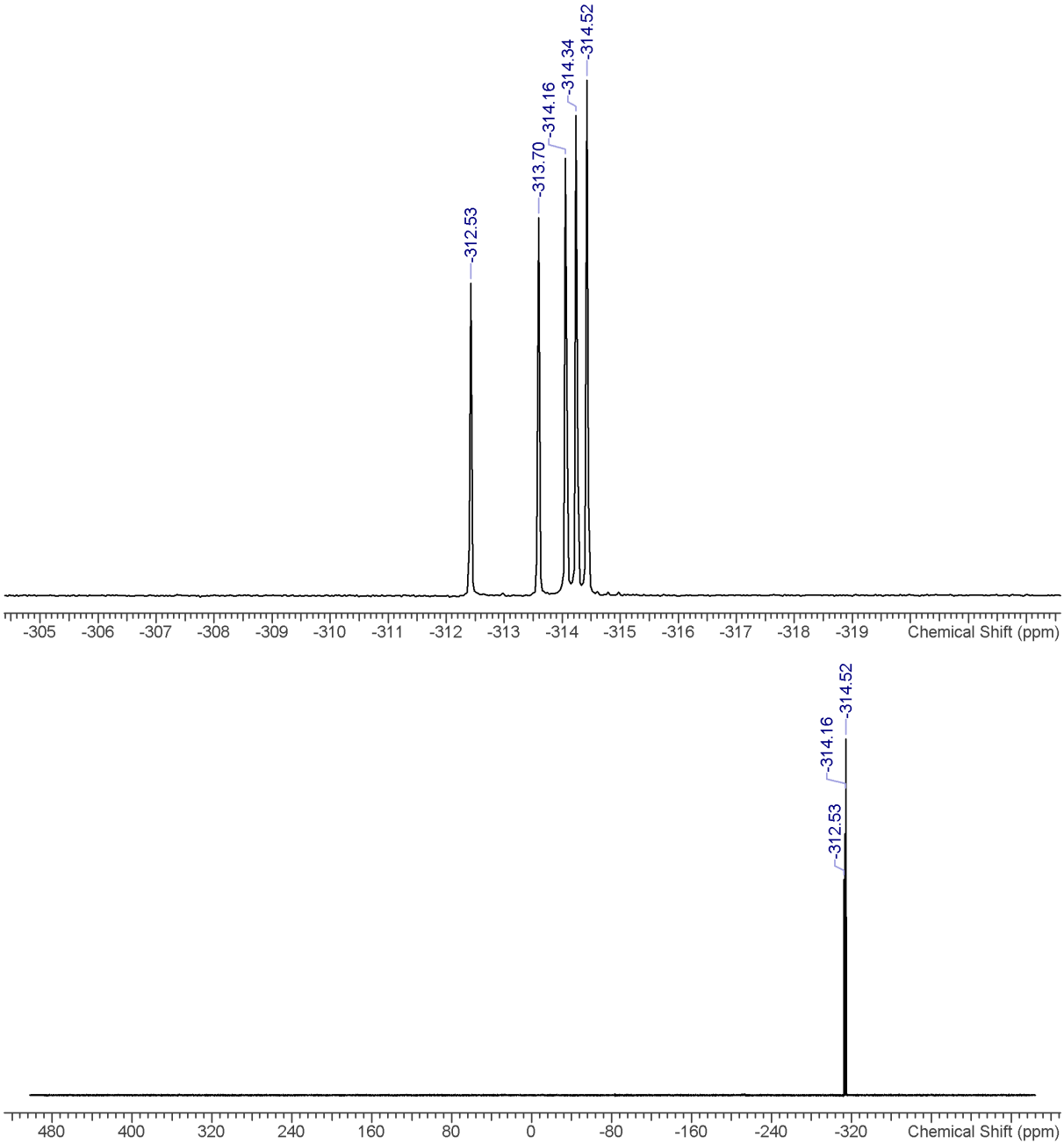


**Figure S16.** $^{31}P$ NMR spectrum of a mixture of HPCO and DPCO in $CD_2Cl_2$.

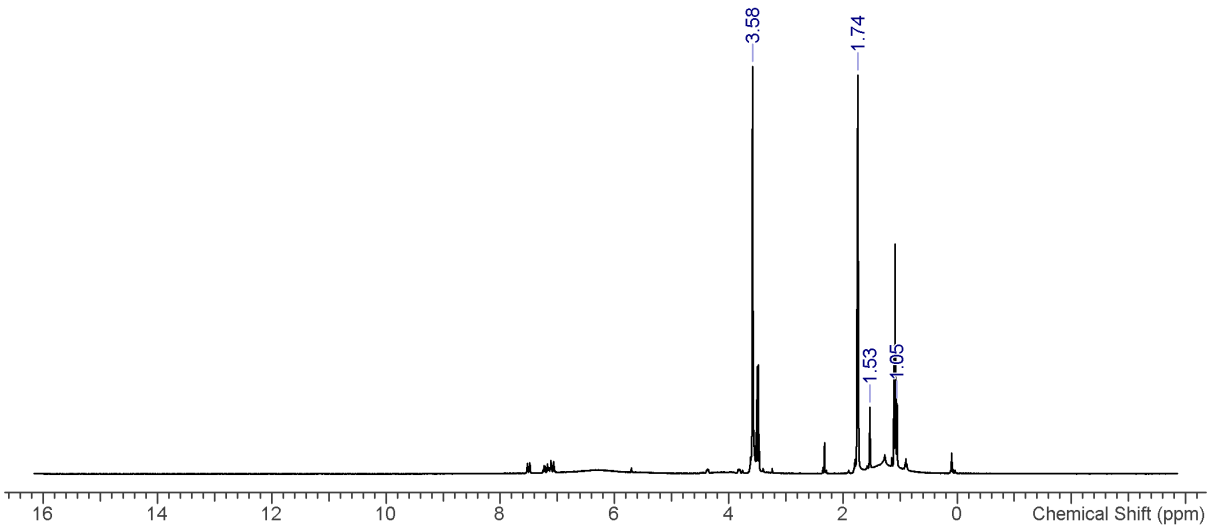


**Figure S17.** $^{1}$H NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-THF at 193 K.

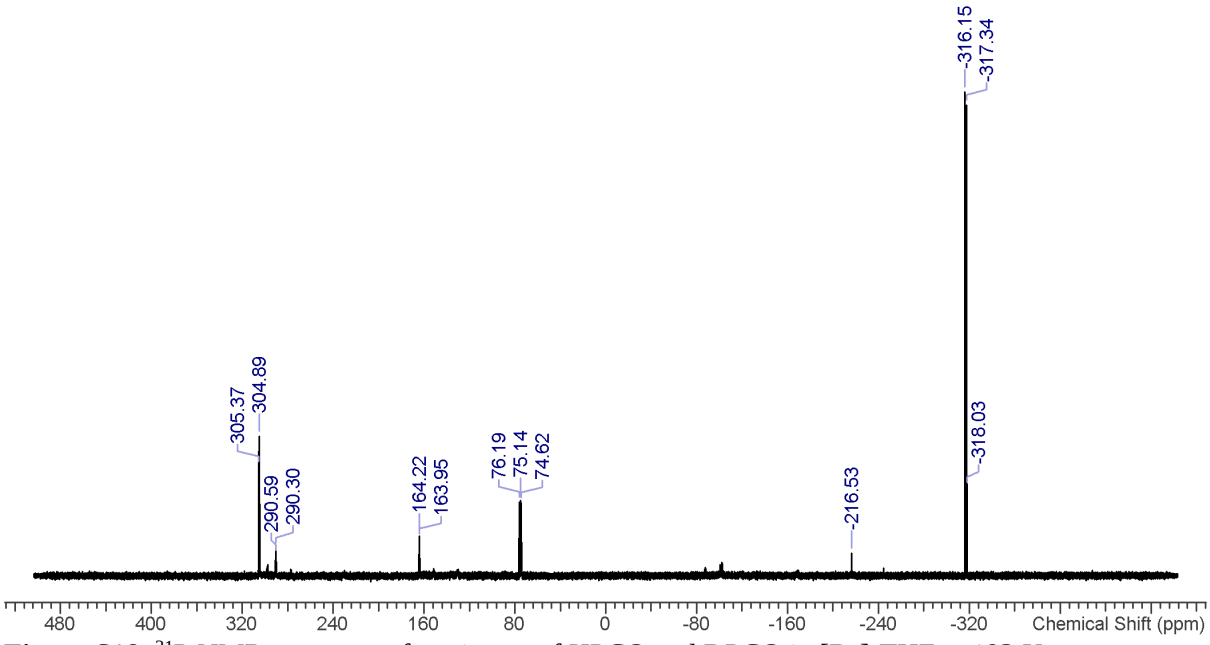


**Figure S18.** $^{31}$P NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-THF at 193 K.

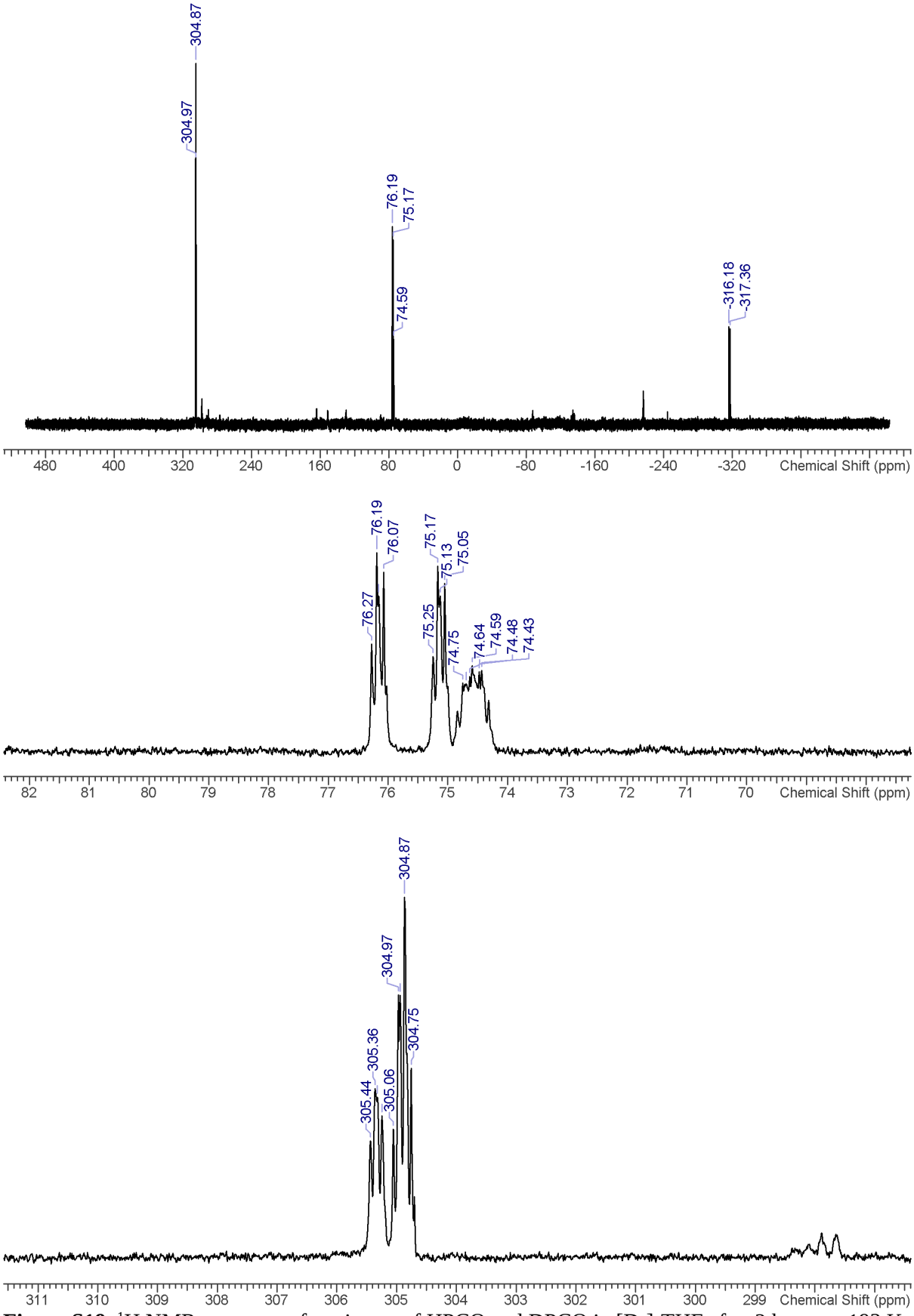


**Figure S19.** $^{1}$H NMR spectrum of a mixture of HPCO and DPCO in [$D_8$]-THF after 2 hours at 193 K.

## Gas-phase IR spectra

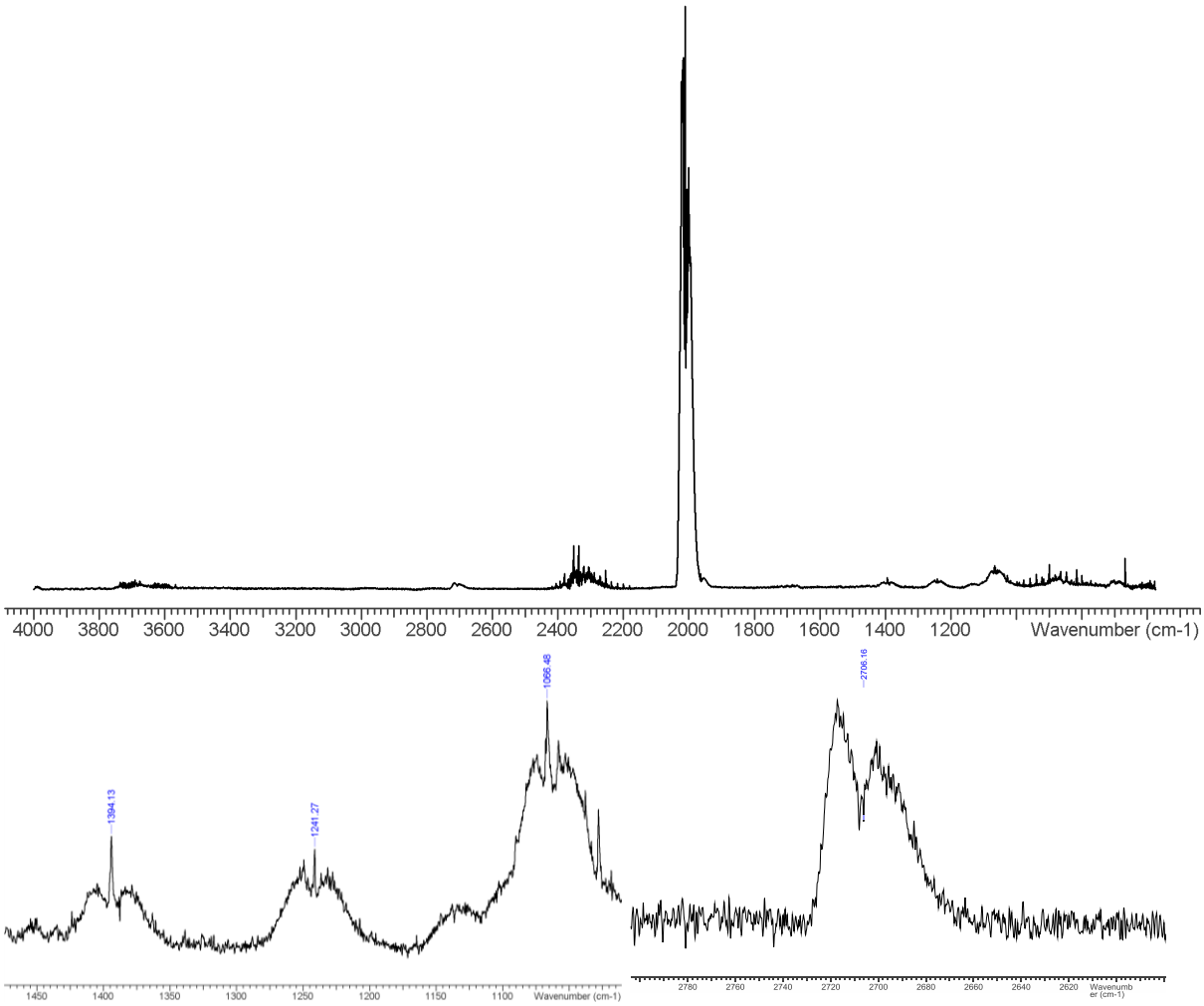


**Figure S20.** Processed gas-phase IR spectrum of HPCO (top) and magnified details (bottom).

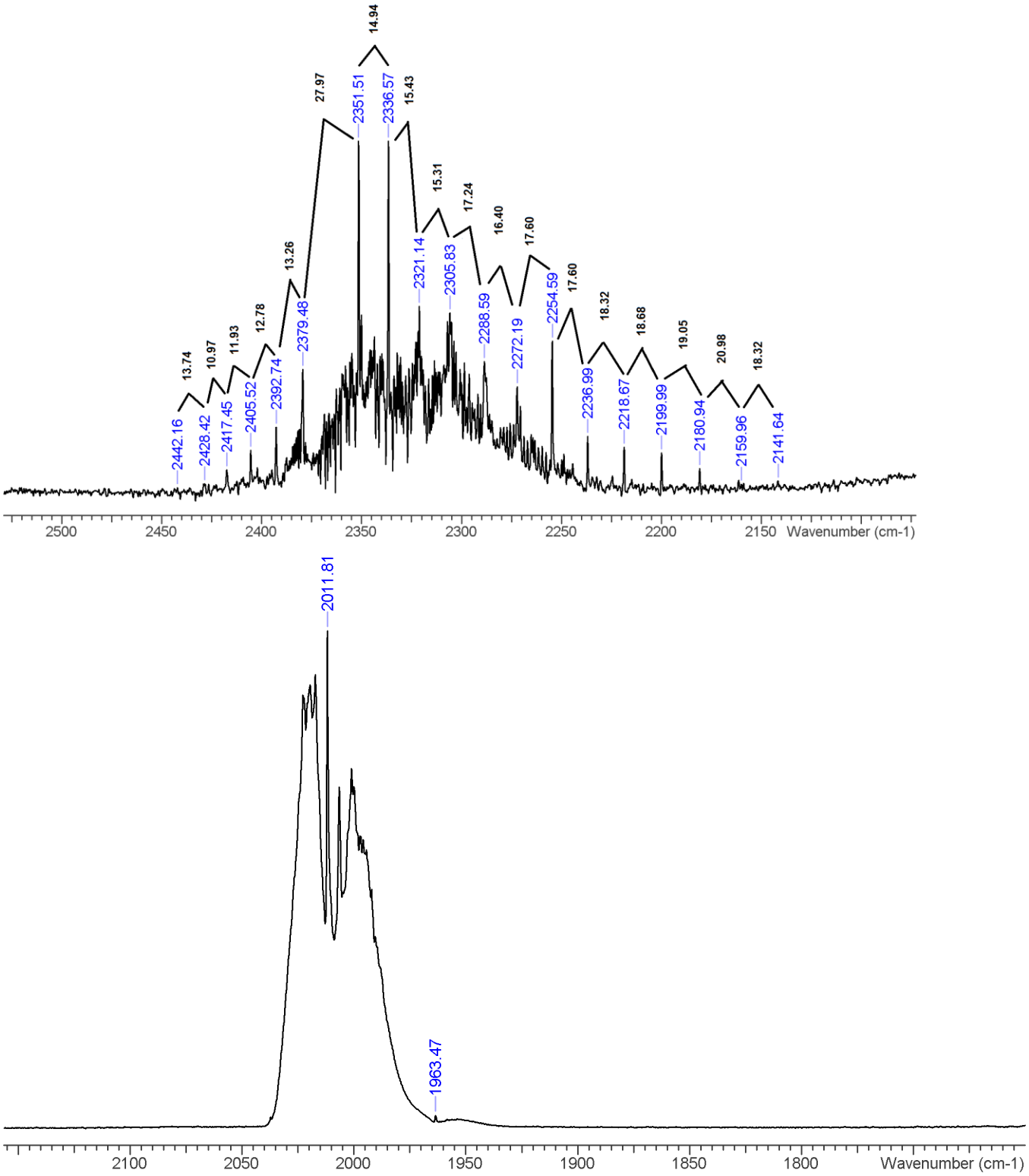


**Figure S21.** Processed gas-phase IR spectrum of HPCO, $\nu_{PH}$ (top) and $\nu_{PH}$ (bottom) range.

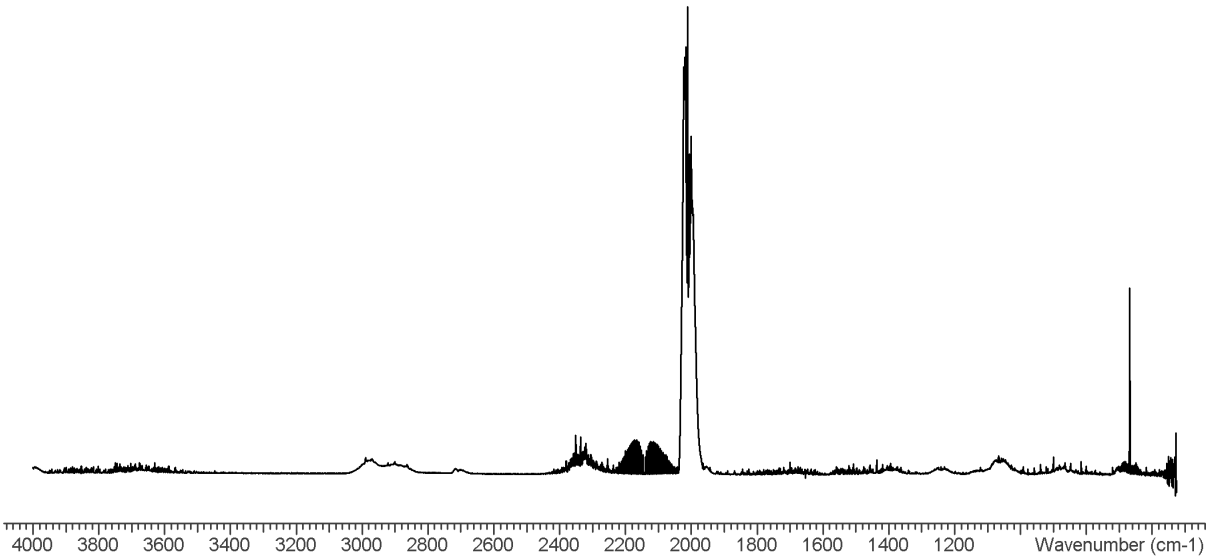


**Figure S22.** Raw gas-phase IR spectrum of HPCO.

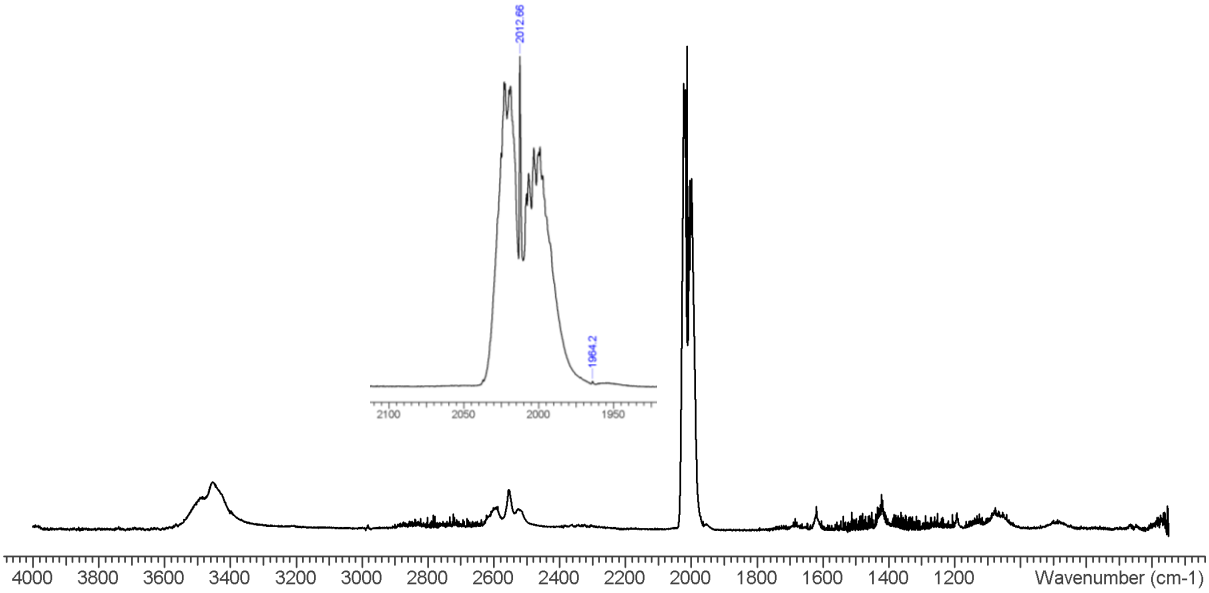


**Figure S23.** Processed gas-phase IR spectrum of DPCO.

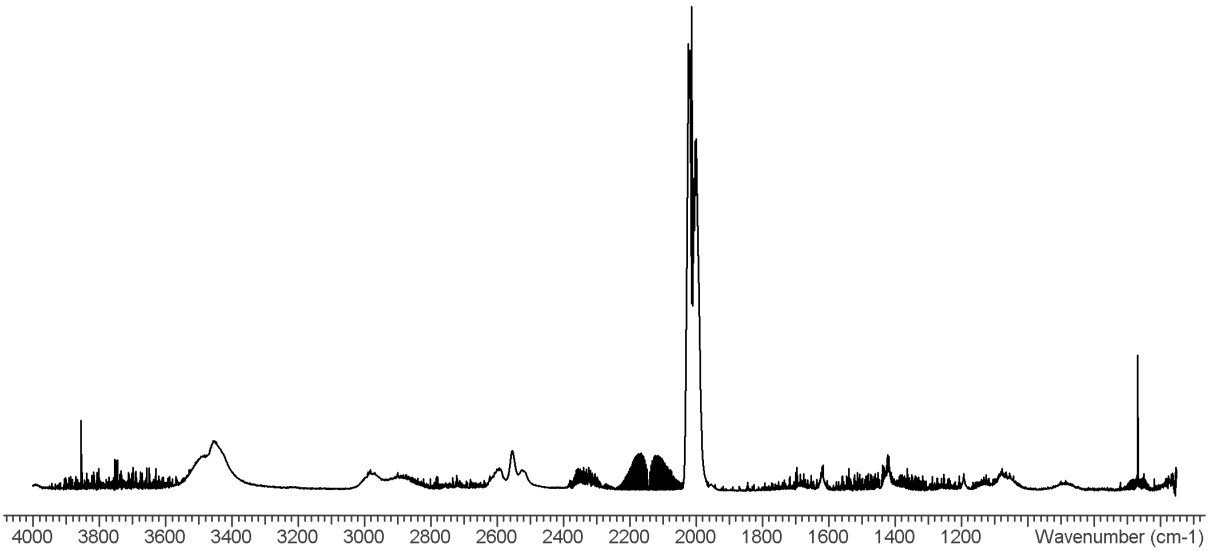


**Figure S24.** Raw gas-phase IR spectrum of DPCO.

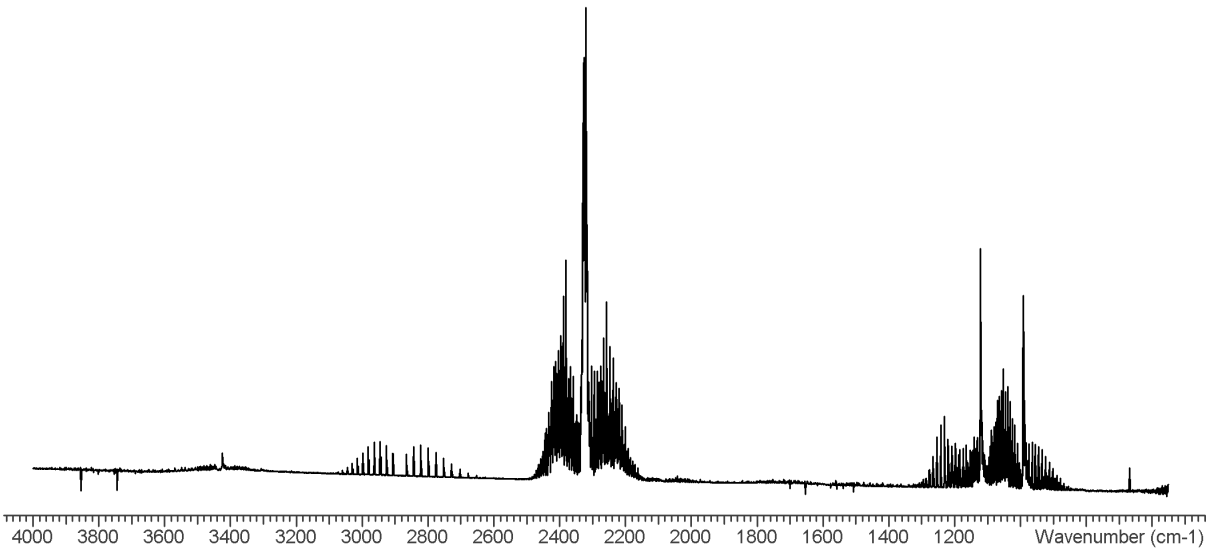


**Figure S25.** Raw gas-phase IR spectrum of $PH_3$.

## 1.2 [$D_1$]-stearic acid

Stearic acid (2100 mg, 7.34 mmol) was dissolved in THF (40 ml). To the colourless solution, $Me_3SiCl$ (900 mg, 8.28 mmol) were added via syringe at ambient temperature. after 5 minutes of stirring, $NEt_3$ (1200 mg, 11.88 mmol) was added via syringe, immediately forming a colourless precipitate. After stirring overnight, all volatiles were removed in vacuo, leaving behind a colourless precipitate. To the residue 50 ml *n*-hexane were added and the mixture was filtered. The colourless solution was evaporated in vacuo, affording a colourless solid ($CH_3$-$(CH_2)_{16}$-C(O)OSi$Me_3$, mp. 40-45 °C) in quantitative yield.

$CH_3$-$(CH_2)_{16}$-C(O)OSi$Me_3$ (2610 mg, 7.32 mmol) was dissolved in THF and 1 ml of $D_2O$ was added via syringe at ambient temperature. The mixture was stirred for three hours, then all volatiles were removed in vacuo, affording colourless [$D_1$]-stearic acid ($CH_3$-$(CH_2)_{16}$-C(O)OD) in quantitative yield.

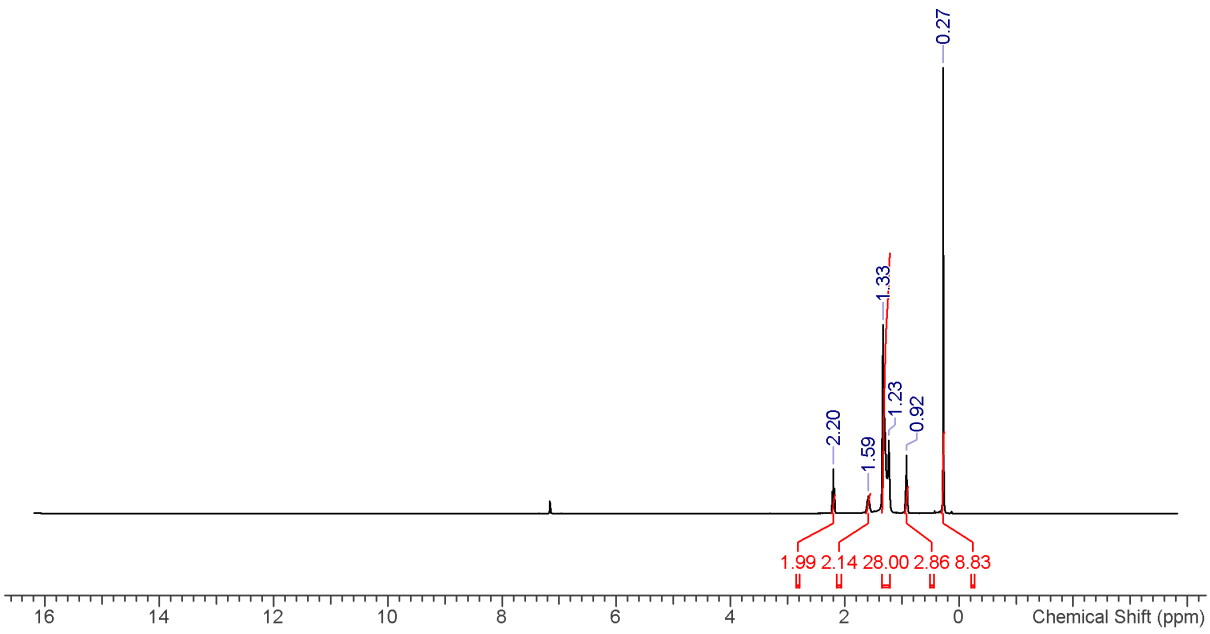


**Figure S26.** $^1$H NMR spectrum of $CH_3$-$(CH_2)_{16}$-C(O)OSi$Me_3$ in $C_6D_6$ at 298 K.

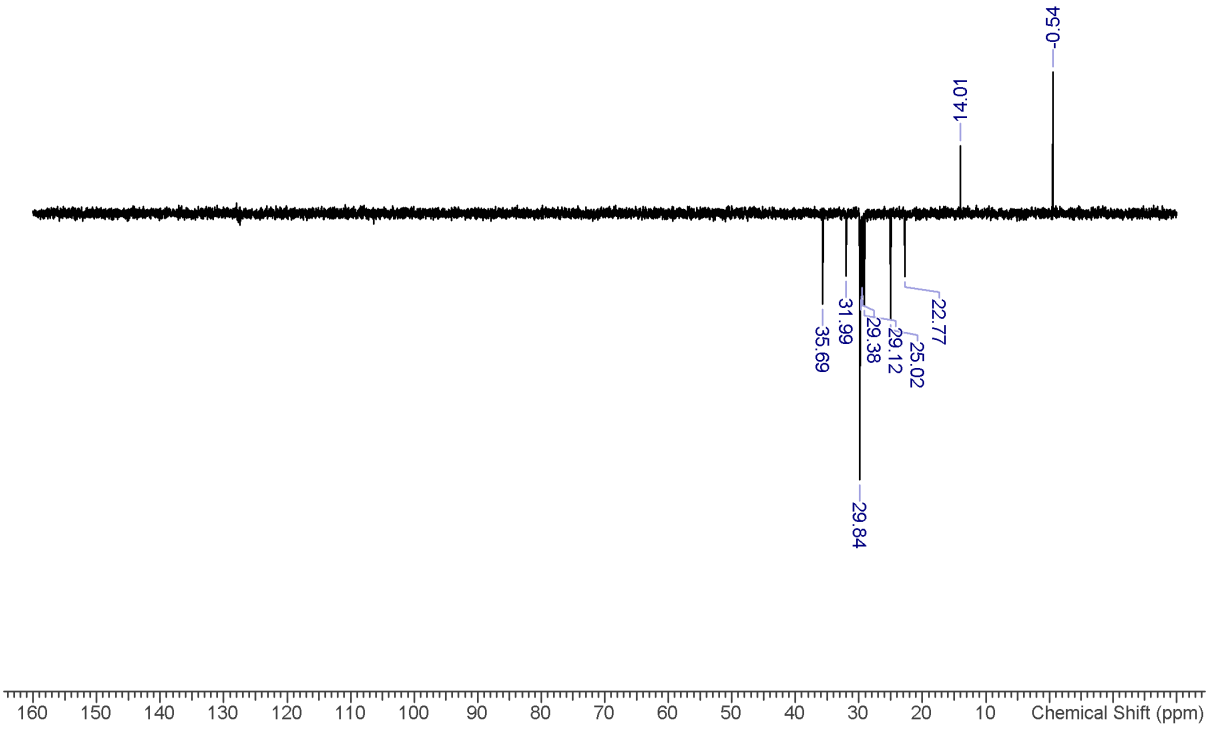


**Figure S27.** $^{13}$C-DEPT135 NMR spectrum of $CH_3$-$(CH_2)_{16}$-C(O)OSiMe$_3$ in $C_6D_6$ at 298 K.

# 2. Computational data

**Computational details.** All computations wer performed using Gaussian09[3] utilizing the PBE1PBE level of theory and 6-311G(d,p) basis sets. No solvent corrections were applied. Natural Bond Orbital and Natural Resonance Theory were applied to study the electronic states.[4–6]

## 3.1 HPCO and DPCO

Natural Population

| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| C | 1 | 0.34387 | 1.99962 | 3.60027 | 0.05625 | 5.65613 |
| P | 2 | 0.02542 | 9.99822 | 4.94077 | 0.03560 | 14.97458 |
| H | 3 | 0.03328 | 0.00000 | 0.96122 | 0.00550 | 0.96672 |
| O | 4 | -0.40257 | 1.99971 | 6.38248 | 0.02038 | 8.40257 |

(Occupancy) Bond orbital/ Coefficients

1. (1.99461) BD ( 1) C 1 - P 2
   ( 65.63%) 0.8101* C 1 s( 61.58%)p 0.62( 38.36%)d 0.00( 0.06%)
   ( 34.37%) 0.5863* P 2 s( 16.31%)p 5.08( 82.88%)d 0.05( 0.81%)
2. (1.99436) BD ( 2) C 1 - P 2
   ( 34.49%) 0.5873* C 1 s( 0.00%)p 1.00( 99.81%)d 0.00( 0.19%)
   ( 65.51%) 0.8094* P 2 s( 0.00%)p 1.00( 99.58%)d 0.00( 0.42%)
3. (1.99987) BD ( 1) C 1 - O 4
   ( 32.68%) 0.5717* C 1 s( 38.58%)p 1.59( 61.27%)d 0.00( 0.15%)
   ( 67.32%) 0.8205* O 4 s( 45.88%)p 1.18( 54.00%)d 0.00( 0.12%)
4. (1.99698) BD ( 2) C 1 - O 4
   ( 29.91%) 0.5469* C 1 s( 0.28%)p99.99( 99.19%)d 1.87( 0.53%)
   ( 70.09%) 0.8372* O 4 s( 0.83%)p99.99( 99.01%)d 0.19( 0.16%)
5. (1.89638) BD ( 1) P 2 - H 3
   ( 49.27%) 0.7019* P 2 s( 12.17%)p 7.16( 87.16%)d 0.06( 0.67%)
   ( 50.73%) 0.7122* H 3 s( 99.74%)p 0.00( 0.26%)
13. (1.91245) LP ( 1) P 2 s( 72.30%)p 0.38( 27.64%)d 0.00( 0.06%)

GETTING A SIMPLE ANSWER FROM A PROFESSOR IS LIKE
GETTING A THIMBLE OF WATER FROM A FIRE HYDRANT.
-- PROF. LEN SHAPIRO, NDSU

### 3.1.1 HPCO – displacement vectors for the vibrations


**Figure S28.** Displacement vectors for ν1 (left) and ν2 (right) of HPCO.

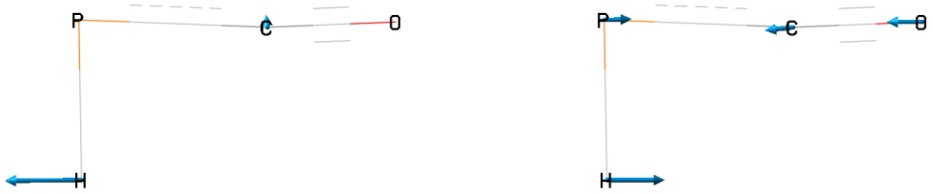


**Figure S29.** Displacement vectors for ν3 (left) and ν4 (right) of HPCO.


**Figure S30.** Displacement vectors for ν6 (left) and ν5 (right) of HPCO.

### 3.1.2 DPCO – displacement vectors for the vibrations


**Figure S31.** Displacement vectors for ν1 (left) and ν2 (right) of DPCO.

**Figure S32.** Displacement vectors for ν3 (left) and ν4 (right) of DPCO.

**Figure S33.** Displacement vectors for ν5 (left) and ν6 (right) of DPCO.

### 3.1.3 HPCO – vibrational analysis

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Derivatives of the Inertia Moments w.r.t
Normal modes (in amu^1/2.Ang)

==========

| | Ixx | Ixy | Iyy | Ixz | Iyz | Izz |
|---|---|---|---|---|---|---|
| Q( 1) | 0.09565 | 0.04900 | -2.81527 | 0.00000 | 0.00000 | -2.71962 |
| Q( 2) | -4.46827 | 0.25060 | -0.07077 | 0.00000 | 0.00000 | -4.53904 |
| Q( 3) | 2.42924 | 2.38620 | 0.15503 | 0.00000 | 0.00000 | 2.58427 |
| Q( 4) | -18.32119 | 0.42555 | 0.01517 | 0.00000 | 0.00000 | -18.30602 |
| Q( 5) | 0.67572 | 1.37596 | -0.19553 | 0.00000 | 0.00000 | 0.48019 |
| Q( 6) | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |

==========

Vibro-rotational Alpha Matrix

Vibro-Rot alpha Matrix (in cm^-1)

| | a(z) | b(x) | c(y) |
|---|---|---|---|
| Q( 1) | 0.24157 | 0.00001 | 0.00011 |
| Q( 2) | 0.00399 | 0.00099 | 0.00094 |
| Q( 3) | -0.26752 | -0.00020 | 0.00000 |
| Q( 4) | -0.00191 | 0.00073 | 0.00079 |
| Q( 5) | 2.43152 | -0.00059 | -0.00029 |
| Q( 6) | -2.32447 | -0.00019 | -0.00037 |

Vibro-Rot alpha Matrix (in MHz)

| | a | b | c |
|---|---|---|---|
| Q( 1) | 7242.04901 | 0.16560 | 3.15202 |
| Q( 2) | 119.66048 | 29.53050 | 28.24947 |
| Q( 3) | -8020.16981 | -6.08416 | -0.13669 |
| Q( 4) | -57.12735 | 21.81956 | 23.66464 |
| Q( 5) | 72895.05345 | -17.66941 | -8.63623 |
| Q( 6) | -69685.82397 | -5.67142 | -11.03286 |

Quartic Centrifugal Distortion Constants

NOTE: Values in Cartesian coords. refer to the structure in Input orientation

Quartic Centrifugal Distortion Constants Tau Prime

| | cm^-1 | MHz |
|---|---|---|
| TauP aaaa | -0.2003721854D-02 | -0.6007006998D+02 |
| TauP bbaa | -0.2343076287D-04 | -0.7024365993D+00 |
| TauP bbbb | -0.1839227044D-06 | -0.5513863964D-02 |
| TauP ccaa | -0.4376089400D-06 | -0.1311918598D-01 |
| TauP ccbb | -0.1758204046D-06 | -0.5270963125D-02 |
| TauP cccc | -0.1685109370D-06 | -0.5051830800D-02 |

Asymmetric Top Reduction
Asymmetric Top Parameter Kappa : -0.9990251599
Asymmetric Top Parameter Sigma : 4102.2369680796

Constants in the Asymmetrically reduced Hamiltonian

| | cm^-1 | MHz |
|---|---|---|
| DELTA J : | 0.4405420518D-07 | 0.1320711846D-02 |
| DELTA K : | 0.4950075239D-03 | 0.1483995223D+02 |
| DELTA JK : | 0.5878885437D-05 | 0.1762445516D+00 |
| delta J : | 0.9632354654D-09 | 0.2887707278D-04 |
| delta K : | 0.3076455124D-05 | 0.9222980435D-01 |

Effective Rotational Constants
(Include Terms due to Quartic Centrifugal Distortion Constants)

| | Be in cm^-1 | B(A) in cm^-1 | B(A) in MHz |
|---|---|---|---|
| a | 8.436553794 | 8.436553793 | 252921.51988 |
| b | 0.186258790 | 0.186259197 | 5583.91025 |
| c | 0.182235470 | 0.182235064 | 5463.26977 |

Nielsen Centrifugal Distortion Constants

| | cm^-1 | MHz |
|---|---|---|
| DJ | 0.4402942917D-07 | 0.1319969079D-02 |
| DJK | 0.5879034093D-05 | 0.1762490082D+00 |
| DK | 0.4950074000D-03 | 0.1483994852D+02 |
| dJ | 0.9632354654D-09 | 0.2887707278D-04 |

R5 -0.1436590503D-05 -0.4306789979D-01
R6 -0.1238800440D-10 -0.3713830288D-06

Constants in the Symmetrically Reduced Hamiltonian
---
| | cm^-1 | MHz |
|---|---|---|
| D J : | 0.4367923231D-07 | 0.1309470442D-02 |
| D JK : | 0.5881135275D-05 | 0.1763120000D+00 |
| D K : | 0.4950056490D-03 | 0.1483989602D+02 |
| d 1 : | -0.9632354654D-09 | -0.2887707278D-04 |
| d 2 : | -0.1874864341D-09 | -0.5620701892D-05 |

Effective Rotational Constants
(Include Terms due to Quartic Centrifugal Distortion Constants)
---
| | Be in cm^-1 | B(S) in cm^-1 | B(S) in MHz |
|---|---|---|---|
| a | 8.436553794 | 8.436553795 | 252921.51993 |
| b | 0.186258790 | 0.186253043 | 5583.72577 |
| c | 0.182235470 | 0.182241216 | 5463.45421 |

Wilson Centrifugal Distortion Constants
---
| | cm^-1 | MHz |
|---|---|---|
| DJ | 0.4598067611D-07 | 0.1378465991D-02 |
| DJK | 0.1162342008D-04 | 0.3484613677D+00 |
| DK | 0.4892610628D-03 | 0.1466767766D+02 |

Nielsen Centrifugal Distortion Constants
---
| | cm^-1 | MHz |
|---|---|---|
| DJ | 0.4402942917D-07 | 0.1319969079D-02 |
| DJK | 0.5879034093D-05 | 0.1762490082D+00 |
| DK | 0.4950074000D-03 | 0.1483994852D+02 |
| dJ | 0.9632354654D-09 | 0.2887707278D-04 |
| R5 | -0.1436590503D-05 | -0.4306789979D-01 |
| R6 | -0.1238800440D-10 | -0.3713830288D-06 |

Rotational Constants (in cm^-1)
---
equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)
Ae= 8.4365538 A00= 8.3949643 A0= 8.3949643
Be= 0.1862588 B00= 0.1858904 B0= 0.1858908
Ce= 0.1822355 C00= 0.1816474 C0= 0.1816470

Rotational Constants (in MHz)
---
equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)
Ae= 252921.520 A00= 251674.699 A0= 251674.699
Be= 5583.898 B00= 5572.853 B0= 5572.865
Ce= 5463.282 C00= 5445.652 C0= 5445.640

Test of Quartic Planarity Relationships
---
Asymmetric Reduction I r
4C*DELJ - (B-C)*DELJK - 2*(2A+B+C)*SDELJ+ 2*(B-C)*SDELK = 0
VALUE = 0.9595295106D-22
Symmetric Reduction I r
4C*DJ - (B-C)*DJK + 2*(2A+B+C)*D1 - 4*(4A+B-3C)*D2 = 0
Value = 0.1058791184D-21

==========
Sextic Centrifugal Distortion Constants
==========

Sextic Distortion Constants
---

| | in cm-1 | in Hz |
|---|---|---|
| Phi aaa | -0.1376284594D-05 | -0.4125997414D+05 |
| Phi aab | -0.7024130662D-07 | -0.2105781396D+04 |
| Phi aac | -0.6137600127D-08 | -0.1840006228D+03 |
| Phi abb | 0.4354676859D-11 | 0.1305499279D+00 |
| Phi abc | -0.3169929188D-11 | -0.9503208631D-01 |
| Phi acc | -0.6440618474D-11 | -0.1930848843D+00 |
| Phi bbb | -0.9018811379D-14 | -0.2703771631D-03 |
| Phi bbc | -0.1746360949D-13 | -0.5235458416D-03 |
| Phi bcc | -0.1992192022D-13 | -0.5972441432D-03 |
| Phi ccc | -0.1750173342D-13 | -0.5246887682D-03 |

Asymmetric Top Reduction
---
Asymmetric Top Parameter Kappa : -0.9990251599
Asymmetric Top Parameter Sigma : 4102.2369680796

Constants in the A reduced Hamiltonian
---
| | in cm^-1 | in Hz |
|---|---|---|
| Phi J : | -0.1326027240D-13 | -0.3975329657D-03 |
| Phi K : | -0.1299898204D-05 | -0.3896996777D+05 |
| Phi JK : | 0.1895582745D-11 | 0.5682814104D-01 |
| Phi KJ : | -0.7638827272D-07 | -0.2290062804D+04 |
| phi j : | 0.2120730511D-14 | 0.6357790127D-04 |
| phi k : | -0.2111541051D-07 | -0.6330240818D+03 |
| phi jk : | 0.2886598776D-11 | 0.8653805425D-01 |

rho : -0.1750984297D-09
mu : -0.3449127582D-11
nu : -0.1492020260D-15
lambda : 0.7430267049D-15

Constants in the S reduced Hamiltonian
---
| | in cm^-1 | in Hz |
|---|---|---|
| H J : | -0.1370388817D-13 | -0.4108322319D-03 |
| H K : | -0.1299883888D-05 | -0.3896953858D+05 |
| H JK : | 0.8033784983D-11 | 0.2408468147D+00 |
| H KJ : | -0.7640872674D-07 | -0.2290676000D+04 |
| h 1 : | 0.2214209091D-14 | 0.6638031858D-04 |
| h 2 : | 0.2218078846D-15 | 0.6649633093D-05 |
| h 3 : | -0.9347857935D-16 | -0.2802417307D-05 |

==========
Average Coordinates and Mean Square Amplitudes
==========

NOTE: Temperature is given in K between parentheses
For Cartesian and internal coords., units are given between parentheses next to each label

Mean Square Amplitudes of Normal Coordinates (in amu.bohr^2)
---
| Mode | <Q^2> (0) | <Q^2> (298.15) | <Q^2> (298.15) class. |
|---|---|---|---|
| 1 | 0.025108 | 0.025109 | 0.171345 |
| 2 | 0.028336 | 0.028338 | 0.218226 |
| 3 | 0.068851 | 0.070907 | 1.288429 |
| 4 | 0.082397 | 0.087394 | 1.845253 |
| 5 | 0.155528 | 0.212349 | 6.574400 |
| 6 | 0.127477 | 0.156563 | 4.416762 |

Average Normal Coordinates (in amu^1/2.bohr)
---
| Mode | <Q> (0) | <Q> (298.15) |
|---|---|---|
| 1 | -0.021521 | -0.018959 |
| 2 | 0.000743 | 0.005735 |
| 3 | 0.009742 | 0.009262 |

| | | |
|---|---|---|
| 4 | -0.029765 | -0.026154 |
| 5 | 0.012782 | 0.011615 |
| 6 | 0.000000 | 0.000000 |

Mean Square Amplitudes of Cartesian Coordinates

| Label | <(S-Se)^2>^1/2 (0) | <(S-Se)^2>^1/2 (298.15) |
|---|---|---|
| X(1) (Angs) | 0.048078 | 0.055155 |
| Y(1) (Angs) | 0.027270 | 0.027633 |
| Z(1) (Angs) | 0.047216 | 0.052326 |
| X(2) (Angs) | 0.007495 | 0.008163 |
| Y(2) (Angs) | 0.018928 | 0.019583 |
| Z(2) (Angs) | 0.006732 | 0.007461 |
| X(3) (Angs) | 0.082457 | 0.082523 |
| Y(3) (Angs) | 0.155550 | 0.168259 |
| Z(3) (Angs) | 0.021531 | 0.023862 |
| X(4) (Angs) | 0.023403 | 0.027219 |
| Y(4) (Angs) | 0.026667 | 0.027279 |
| Z(4) (Angs) | 0.021030 | 0.023306 |

Average Cartesian Coordinates

| Label | Se | <S> = Sz (0) | <S> = Sz (298.15) |
|---|---|---|---|
| X(1) (Angs) | 0.000000 | 0.000984 | 0.000879 |
| Y(1) (Angs) | 0.589147 | 0.591220 | 0.591590 |
| Z(1) (Angs) | 0.000000 | 0.000000 | 0.000000 |
| X(2) (Angs) | 0.065583 | 0.065875 | 0.065847 |
| Y(2) (Angs) | -1.091267 | -1.093430 | -1.093215 |
| Z(2) (Angs) | 0.000000 | 0.000000 | 0.000000 |
| X(3) (Angs) | -1.360798 | -1.372092 | -1.370689 |
| Y(3) (Angs) | -1.068099 | -1.064706 | -1.064737 |
| Z(3) (Angs) | 0.000000 | 0.000000 | 0.000000 |
| X(4) (Angs) | 0.047131 | 0.046539 | 0.046584 |
| Y(4) (Angs) | 1.737777 | 1.740198 | 1.739505 |
| Z(4) (Angs) | 0.000000 | 0.000000 | 0.000000 |

Internal coordinates for the Equilibrium structure (Se)

Interatomic distances:

| | | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | |
| 2 | P | 1.681693 | 0.000000 | | |
| 3 | H | 2.144350 | 1.426569 | 0.000000 | |
| 4 | O | 1.149597 | 2.829104 | 3.139300 | 0.000000 |

Interatomic angles:

C1-P2-H3= 86.8345 P2-C1-O4=175.4153 H3-C1-O4=142.9596
H3-P2-O4= 88.6958

Dihedral angles:

O4-C1-P2-H3= 180.

Internal coordinates for the vibrationally average structure at 0K (Sz)

Interatomic distances:

| | | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | |
| 2 | P | 1.685900 | 0.000000 | | |
| 3 | H | 2.151146 | 1.438254 | 0.000000 | |
| 4 | O | 1.149881 | 2.833694 | 3.143246 | 0.000000 |

Interatomic angles:

C1-P2-H3= 86.6497 P2-C1-O4=175.5236 H3-C1-O4=142.6053
H3-P2-O4= 88.4647

Dihedral angles:

O4-C1-P2-H3= 180.

Internal coordinates for the vibr. average structure at 298.15K (Sa)

Interatomic distances:

| | | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | |
| 2 | P | 1.686058 | 0.000000 | | |
| 3 | H | 2.150493 | 1.436818 | 0.000000 | |

```
 4  O    1.148825   2.832786   3.142044   0.000000
                Interatomic angles:
  C1-P2-H3= 86.656        P2-C1-O4=175.5117       H3-C1-O4=142.6526
  H3-P2-O4= 88.4747
                 Dihedral angles:
 O4-C1-P2-H3= 180.

 ================================================
  Vibrational Average of Electric-Field Properties
 ================================================

Electric dipole
---------------
------------------------------------------------------------------------
 Property at reference geometry, Unit: Debye
------------------------------------------------------------------------
   X=    -0.6671    Y=    -0.3867    Z=     0.0000
------------------------------------------------------------------------
 Temperature:     0K, Unit: Debye
------------------------------------------------------------------------
   X=    -0.6510    Y=    -0.4085    Z=     0.0000
------------------------------------------------------------------------
 Temperature:   298K, Unit: Debye
------------------------------------------------------------------------
   X=    -0.6504    Y=    -0.4075    Z=     0.0000

 ================================================
     Nuclear Magnetic Resonance Spectroscopy
 ================================================

Nuclear quadrupole tensors
--------------------------
------------------------------------------------------------------------
 Property at reference geometry
------------------------------------------------------------------------
          Nuclear Quadrupole in Principal Axis System
     Atom            a.u.   MegaHertz   Gauss  10(-4) cm-1        Axes
          Baa    -0.4455   -59.777   -21.330   -19.939  0.9993 -0.0367  0.0000
   1 C(13)  Bbb    -0.1044   -14.005    -4.997    -4.672  0.0000  0.0000  1.0000
          Bcc     0.5498    73.782    26.327    24.611  0.0367  0.9993  0.0000

          Baa    -1.2466  -269.488   -96.160   -89.891  0.4565  0.8897  0.0000
   2 P(31)  Bbb     0.1676    36.228    12.927    12.084  0.8897 -0.4565  0.0000
          Bcc     1.0790   233.259    83.233    77.807  0.0000  0.0000  1.0000

          Baa    -0.1838   -98.052   -34.987   -32.707  0.9999  0.0139  0.0000
   3 H(1)   Bbb     0.0784    41.811    14.919    13.946 -0.0139  0.9999  0.0000
          Bcc     0.1054    56.242    20.068    18.760  0.0000  0.0000  1.0000

          Baa    -0.5889    42.613    15.205    14.214  0.9999  0.0110  0.0000
   4 O(17)  Bbb    -0.0412     2.980     1.063     0.994 -0.0110  0.9999  0.0000
          Bcc     0.6301   -45.592   -16.268   -15.208  0.0000  0.0000  1.0000

------------------------------------------------------------------------
 Temperature:     0K
------------------------------------------------------------------------
          Nuclear Quadrupole in Principal Axis System
     Atom            a.u.   MegaHertz   Gauss  10(-4) cm-1        Axes
          Baa    -0.4408   -59.146   -21.105   -19.729  0.9994 -0.0336 -0.0001
   1 C(13)  Bbb    -0.1020   -13.682    -4.882    -4.564  0.0001  0.0000  1.0000
          Bcc     0.5427    72.828    25.987    24.293  0.0336  0.9994  0.0000

          Baa    -1.2129  -262.217   -93.566   -87.466  0.4641  0.8858  0.0000
   2 P(31)  Bbb     0.1167    25.224     9.001     8.414  0.8858 -0.4641  0.0000
          Bcc     1.0963   236.993    84.565    79.052  0.0000  0.0000  1.0000

          Baa    -0.1771   -94.516   -33.726   -31.527  0.9999  0.0113  0.0000
   3 H(1)   Bbb     0.0741    39.527    14.104    13.185 -0.0113  0.9999  0.0000
```

```
          Bcc     0.1031    54.989    19.621    18.342  0.0000  0.0000  1.0000

          Baa    -0.5810    42.039    15.000    14.023  0.9999  0.0134 -0.0001
    4 O(17)  Bbb    -0.0455     3.293     1.175     1.098 -0.0134  0.9999  0.0000
          Bcc     0.6265   -45.331   -16.175   -15.121  0.0001  0.0000  1.0000

-----------------------------------------------------------------------
 Temperature:   298K
-----------------------------------------------------------------------
          Nuclear Quadrupole in Principal Axis System
       Atom            a.u.   MegaHertz   Gauss  10(-4) cm-1        Axes
          Baa    -0.4399   -59.027   -21.062   -19.689  0.9994 -0.0336 -0.0001
    1 C(13)  Bbb    -0.1018   -13.665    -4.876    -4.558  0.0001  0.0000  1.0000
          Bcc     0.5417    72.692    25.938    24.247  0.0336  0.9994  0.0000

          Baa    -1.2081  -261.177   -93.194   -87.119  0.4632  0.8862  0.0000
    2 P(31)  Bbb     0.1135    24.541     8.757     8.186  0.8862 -0.4632  0.0000
          Bcc     1.0946   236.636    84.438    78.933  0.0000  0.0000  1.0000

          Baa    -0.1765   -94.181   -33.606   -31.415  0.9999  0.0117  0.0000
    3 H(1)   Bbb     0.0735    39.222    13.995    13.083 -0.0117  0.9999  0.0000
          Bcc     0.1030    54.959    19.611    18.332  0.0000  0.0000  1.0000

          Baa    -0.5823    42.135    15.035    14.055  0.9999  0.0121 -0.0001
    4 O(17)  Bbb    -0.0414     2.999     1.070     1.000 -0.0121  0.9999  0.0000
          Bcc     0.6237   -45.134   -16.105   -15.055  0.0001  0.0000  1.0000


    ==================================================
                Resonance Analysis
    ==================================================

 Thresholds
 ----------
 Maximum Difference PT2 vs. Variational (cm-1) :      1.000
 Minimum value for Darling-Dennison term (cm-1):     10.000

 Fermi resonances
 ----------------
  No Fermi resonance found

 Darling-Dennison resonances
 ---------------------------
  No Darling-Dennison resonance found

    ==================================================
                Anharmonic X Matrix
    ==================================================

 PT2 model: Deperturbed VPT2 (DVPT2)
 Ref.: V. Barone, J. Chem. Phys. 122, 1, 014108 (2005)

 Coriolis contributions to X Matrix (in cm^-1)
 ---------------------------------------------
            1           2           3           4           5
    1  0.000000D+00
    2  0.124897D-04  0.000000D+00
    3  0.397471D+00  0.114554D+00  0.000000D+00
    4  0.115801D-01  0.110884D-02  0.213853D-01  0.000000D+00
    5  0.301412D+00  0.745306D+00  0.468391D-03  0.749382D-02  0.000000D+00
    6  0.346380D+00  0.863986D+00  0.489361D+01  0.558797D-01  0.128551D+02
            6
    6  0.000000D+00

 3rd Deriv. contributions to X Matrix (in cm^-1)
 -----------------------------------------------
            1           2           3           4           5
    1 -0.905858D+02
```

```
    2 -0.123109D+01 -0.232407D+02
    3  0.470393D+02  0.164388D+01 -0.585000D+01
    4 -0.319201D+00 -0.474270D+01 -0.387102D+00 -0.600270D+01
    5  0.548201D+02  0.304157D+02 -0.302015D+02 -0.122967D+02 -0.122119D+02
    6  0.683705D+00  0.295755D+02 -0.301145D+00 -0.147659D+01 -0.111515D+02
           6
    6 -0.816466D+01

4th Deriv. contributions to X Matrix (in cm^-1)
-----------------------------------------------
           1           2           3           4           5
    1  0.717822D+02
    2  0.813928D-01  0.120578D+02
    3 -0.606904D+02 -0.496199D+01 -0.308535D+00
    4 -0.120983D+01  0.374971D+01 -0.262897D+01  0.194679D+01
    5 -0.507975D+02 -0.350812D+02  0.192249D+02 -0.295369D+01  0.154440D+02
    6 -0.122383D+01 -0.360091D+02 -0.226817D+01 -0.368478D+01  0.122043D+02
           6
    6  0.894709D+01

Total Anharmonic X Matrix (in cm^-1)
------------------------------------
           1           2           3           4           5
    1 -0.188036D+02
    2 -0.114968D+01 -0.111830D+02
    3 -0.132536D+02 -0.320356D+01 -0.615854D+01
    4 -0.151745D+01 -0.991885D+00 -0.299468D+01 -0.405591D+01
    5  0.432407D+01 -0.392021D+01 -0.109761D+02 -0.152429D+02  0.323207D+01
    6 -0.193744D+00 -0.556957D+01  0.232429D+01 -0.510550D+01  0.139080D+02
           6
    6  0.782427D+00

   ================================================
           Anharmonic Zero Point Energy
   ================================================

Anharmonic Zero Point Energy
----------------------------
Harmonic       : cm-1 =  3493.18738 ; Kcal/mol =   9.988 ; KJ/mol =  41.788
Anharm.Pot.    : cm-1 =   -17.70850 ; Kcal/mol =  -0.051 ; KJ/mol =  -0.212
Watson+Coriolis: cm-1 =    -1.54097 ; Kcal/mol =  -0.004 ; KJ/mol =  -0.018
X0F (Im. Freq.): cm-1 =     0.00000 ; Kcal/mol =   0.000 ; KJ/mol =   0.000
Total Anharm   : cm-1 =  3473.93791 ; Kcal/mol =   9.932 ; KJ/mol =  41.558

   ================================================
      Vibrational Energies at Anharmonic Level
   ================================================

Vibrational Energies and Rotational Constants (in cm^-1)
--------------------------------------------------------
Mode(Quanta)     E(harm)    E(anharm)     Aa(z)      Ba(x)      Ca(y)
Equilibrium Geometry                    8.436554   0.186259   0.182235
Ground State      3493.187   3473.938     8.394964   0.185891   0.181647
Fundamental Bands (DE w.r.t. Ground State)
  1(1) active     2397.602   2354.100     8.153396   0.185885   0.181542
  2(1) active     2124.515   2094.732     8.390973   0.184906   0.180705
  3(1) active      874.345    847.976     8.662488   0.186094   0.181652
  4(1) active      730.609    709.571     8.396870   0.185163   0.180858
  5(1) active      387.066    387.576     5.963447   0.186480   0.181935
  6(1) active      472.238    476.485    10.719433   0.186080   0.182015
Overtones (DE w.r.t. Ground State)
  1(2)            4795.204   4670.592     7.911827   0.185880   0.181437
  2(2)            4249.031   4167.098     8.386981   0.183921   0.179762
  3(2)            1748.689   1683.634     8.930012   0.186297   0.181656
  4(2)            1461.218   1411.030     8.398775   0.184435   0.180068
  5(2)             774.132    781.617     3.531930   0.187070   0.182223
  6(2)             944.476    954.534    13.043902   0.186269   0.182383
Combination Bands (DE w.r.t. Ground State)
```

| | | | | | | |
|---|---|---|---|---|---|---|
| 2(1) | 1(1) | 4522.117 | 4447.682 | 8.149404 | 0.184900 | 0.180600 |
| 3(1) | 1(1) | 3271.947 | 3188.822 | 8.420920 | 0.186088 | 0.181546 |
| 3(1) | 2(1) | 2998.860 | 2939.504 | 8.658497 | 0.185109 | 0.180709 |
| 4(1) | 1(1) | 3128.211 | 3062.153 | 8.155301 | 0.185157 | 0.180752 |
| 4(1) | 2(1) | 2855.124 | 2803.311 | 8.392878 | 0.184178 | 0.179915 |
| 4(1) | 3(1) | 1604.953 | 1554.552 | 8.664394 | 0.185366 | 0.180862 |
| 5(1) | 1(1) | 2784.668 | 2746.000 | 5.721878 | 0.186475 | 0.181830 |
| 5(1) | 2(1) | 2511.581 | 2478.388 | 5.959456 | 0.185495 | 0.180993 |
| 5(1) | 3(1) | 1261.410 | 1224.576 | 6.230971 | 0.186683 | 0.181940 |
| 5(1) | 4(1) | 1117.675 | 1081.904 | 5.965353 | 0.185752 | 0.181146 |
| 6(1) | 1(1) | 2869.840 | 2830.390 | 10.477864 | 0.186074 | 0.181910 |
| 6(1) | 2(1) | 2596.753 | 2565.647 | 10.715442 | 0.185095 | 0.181073 |
| 6(1) | 3(1) | 1346.583 | 1326.785 | 10.986957 | 0.186283 | 0.182020 |
| 6(1) | 4(1) | 1202.847 | 1180.950 | 10.721339 | 0.185352 | 0.181226 |
| 6(1) | 5(1) | 859.304 | 877.969 | 8.287916 | 0.186669 | 0.182303 |

==========
Thermodynamic properties and Partition Functions
==========

ZPE(harm) = 0.41788D+02 kJ/mol ZPE(anh)= 0.41558D+02 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

| | Harmonic value | SPT anharmonic value | |
|---|---|---|---|
| Qvib | 0.65813D-07 | 0.72402D-07 | |
| QZvib | 0.13779D+01 | 0.13813D+01 | |
| Energy | 0.51137D+02 | 0.50934D+02 | kJ/mol |
| Enthalpy | 0.53616D+02 | 0.53413D+02 | kJ/mol |
| Entropy | 0.25784D+03 | 0.25795D+03 | J/(mol K) |
| Sp.Heat(V) | 0.42211D+02 | 0.42500D+02 | J/(mol K) |
| Sp.Heat(P) | 0.50526D+02 | 0.50814D+02 | J/(mol K) |

T = 298.15 K; P = 1.00 atm

| | Harmonic value | SPT anharmonic value | |
|---|---|---|---|
| Qvib | 0.65813D-07 | 0.72402D-07 | |
| QZvib | 0.13779D+01 | 0.13813D+01 | |
| Energy | 0.51137D+02 | 0.50934D+02 | kJ/mol |
| Enthalpy | 0.53616D+02 | 0.53413D+02 | kJ/mol |
| Entropy | 0.25784D+03 | 0.25795D+03 | J/(mol K) |
| Sp.Heat(V) | 0.42211D+02 | 0.42500D+02 | J/(mol K) |
| Sp.Heat(P) | 0.50526D+02 | 0.50814D+02 | J/(mol K) |

T = 500.00 K; P = 1.00 atm

| | Harmonic value | SPT anharmonic value | |
|---|---|---|---|
| Qvib | 0.10738D-03 | 0.11476D-03 | |
| QZvib | 0.24910D+01 | 0.25188D+01 | |
| Energy | 0.60697D+02 | 0.60557D+02 | kJ/mol |
| Enthalpy | 0.64854D+02 | 0.64714D+02 | kJ/mol |
| Entropy | 0.28641D+03 | 0.28669D+03 | J/(mol K) |
| Sp.Heat(V) | 0.51543D+02 | 0.51861D+02 | J/(mol K) |
| Sp.Heat(P) | 0.59857D+02 | 0.60175D+02 | J/(mol K) |

T = 1000.00 K; P = 1.00 atm

| | Harmonic value | SPT anharmonic value | |
|---|---|---|---|
| Qvib | 0.72582D-01 | 0.76830D-01 | |
| QZvib | 0.11055D+02 | 0.11382D+02 | |
| Energy | 0.89797D+02 | 0.89808D+02 | kJ/mol |
| Enthalpy | 0.98111D+02 | 0.98122D+02 | kJ/mol |
| Entropy | 0.33205D+03 | 0.33253D+03 | J/(mol K) |
| Sp.Heat(V) | 0.63313D+02 | 0.63582D+02 | J/(mol K) |
| Sp.Heat(P) | 0.71628D+02 | 0.71896D+02 | J/(mol K) |

T = 1500.00 K; P = 1.00 atm

| | Harmonic value | SPT anharmonic value | |
|---|---|---|---|
| Qvib | 0.13868D+01 | 0.14717D+01 | |
| QZvib | 0.39553D+02 | 0.41205D+02 | |
| Energy | 0.12294D+03 | 0.12306D+03 | kJ/mol |
| Enthalpy | 0.13541D+03 | 0.13553D+03 | kJ/mol |

| | | | |
|---|---|---|---|
| Entropy | 0.36222D+03 | 0.36280D+03 | J/(mol K) |
| Sp.Heat(V) | 0.68560D+02 | 0.68737D+02 | J/(mol K) |
| Sp.Heat(P) | 0.76874D+02 | 0.77051D+02 | J/(mol K) |

T = 2000.00 K;  P =  1.00 atm

| | Harmonic value | SPT anharmonic value | |
|---|---|---|---|
| Qvib | 0.94238D+01 | 0.10032D+02 | |
| QZvib | 0.11630D+03 | 0.12211D+03 | |
| Energy | 0.15790D+03 | 0.15810D+03 | kJ/mol |
| Enthalpy | 0.17453D+03 | 0.17472D+03 | kJ/mol |
| Entropy | 0.38471D+03 | 0.38533D+03 | J/(mol K) |
| Sp.Heat(V) | 0.71007D+02 | 0.71123D+02 | J/(mol K) |
| Sp.Heat(P) | 0.79321D+02 | 0.79438D+02 | J/(mol K) |

==========

Anharmonic Transition Moments

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Electric dipole : Fundamental Bands

| Mode(Quanta) | X | Y | Z |
|---|---|---|---|
| 1(1) | -0.202030E-01 | -0.521957E-02 | 0.121075E-05 |
| 2(1) | 0.506949E-02 | 0.141696 | -0.875508E-06 |
| 3(1) | 0.254319E-01 | -0.147616E-01 | -0.987147E-06 |
| 4(1) | 0.230256E-02 | -0.203568E-01 | 0.705510E-13 |
| 5(1) | 0.330765E-01 | 0.128453E-01 | -0.292233E-05 |
| 6(1) | 0.154851E-12 | -0.131370E-05 | 0.316247E-02 |

Electric dipole : Overtones

| Mode(Quanta) | X | Y | Z |
|---|---|---|---|
| 1(2) | -0.194582E-03 | 0.310704E-03 | 0.169556E-13 |
| 2(2) | 0.150599E-03 | 0.934808E-02 | -0.447082E-14 |
| 3(2) | -0.304696E-02 | -0.431908E-02 | 0.176215E-13 |
| 4(2) | -0.305587E-03 | 0.423701E-02 | -0.187956E-14 |
| 5(2) | -0.573122E-03 | 0.116518E-01 | -0.259840E-13 |
| 6(2) | 0.861630E-03 | 0.650419E-02 | -0.115270E-13 |

Electric dipole : Combination Bands

| Mode(Quanta) | | X | Y | Z |
|---|---|---|---|---|
| 2(1) | 1(1) | -0.237073E-02 | -0.670918E-04 | 0.675588E-15 |
| 3(1) | 1(1) | 0.238137E-03 | -0.657890E-03 | -0.504806E-14 |
| 3(1) | 2(1) | 0.389841E-03 | -0.256330E-02 | 0.316042E-15 |
| 4(1) | 1(1) | 0.175716E-02 | -0.873543E-03 | -0.562337E-15 |
| 4(1) | 2(1) | 0.788197E-03 | 0.102210E-01 | -0.735385E-14 |
| 4(1) | 3(1) | -0.180804E-03 | -0.291041E-02 | 0.278977E-14 |
| 5(1) | 1(1) | 0.103888E-02 | 0.141674E-02 | -0.625682E-14 |
| 5(1) | 2(1) | 0.838431E-03 | 0.804261E-05 | -0.338008E-15 |
| 5(1) | 3(1) | -0.333575E-02 | -0.119550E-01 | 0.242904E-13 |
| 5(1) | 4(1) | -0.109541E-02 | -0.131268E-02 | 0.294296E-14 |
| 6(1) | 1(1) | 0.786269E-17 | -0.110649E-15 | -0.539258E-03 |
| 6(1) | 2(1) | -0.228913E-14 | 0.322140E-13 | 0.242393E-03 |
| 6(1) | 3(1) | 0.754280E-16 | -0.106147E-14 | -0.154994E-02 |
| 6(1) | 4(1) | -0.232129E-14 | 0.326666E-13 | -0.390013E-03 |
| 6(1) | 5(1) | -0.670123E-15 | 0.943038E-14 | 0.131145E-04 |

ERROR: Missing derivatives of the polarizability tensor moment.

==========

Anharmonic Infrared Spectroscopy

==========

Units: Energies (E) in cm^-1

Integrated intensity (I) in km.mol^-1

Fundamental Bands

| Mode(Quanta) | E(harm) | E(anharm) | I(harm) | I(anharm) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1(1) | 2397.602 | 2354.100 | 15.64554092 | 16.59877824 |
| 2(1) | 2124.515 | 2094.732 | 706.83958695 | 681.95255009 |
| 3(1) | 874.345 | 847.976 | 12.43306229 | 11.87406086 |
| 4(1) | 730.609 | 709.571 | 6.20967207 | 4.82271436 |
| 5(1) | 387.066 | 387.576 | 8.20547358 | 7.90239049 |
| 6(1) | 472.238 | 476.485 | 0.08407113 | 0.07717163 |

Overtones

| Mode(Quanta) | E(harm) | E(anharm) | I(anharm) |
|---|---|---|---|
| 1(2) | 4795.204 | 4670.592 | 0.01016545 |
| 2(2) | 4249.031 | 4167.098 | 5.89859610 |
| 3(2) | 1748.689 | 1683.634 | 0.76174120 |
| 4(2) | 1461.218 | 1411.030 | 0.41234971 |
| 5(2) | 774.132 | 781.617 | 1.72259843 |
| 6(2) | 944.476 | 954.534 | 0.66541041 |

Combination Bands

| Mode(Quanta) | | E(harm) | E(anharm) | I(anharm) |
|---|---|---|---|---|
| 2(1) | 1(1) | 4522.117 | 4447.682 | 0.40513905 |
| 3(1) | 1(1) | 3271.947 | 3188.822 | 0.02527932 |
| 3(1) | 2(1) | 2998.860 | 2939.504 | 0.32000899 |
| 4(1) | 1(1) | 3128.211 | 3062.153 | 0.19095180 |
| 4(1) | 2(1) | 2855.124 | 2803.311 | 4.77077948 |
| 4(1) | 3(1) | 1604.953 | 1554.552 | 0.21406353 |
| 5(1) | 1(1) | 2784.668 | 2746.000 | 0.13724955 |
| 5(1) | 2(1) | 2511.581 | 2478.388 | 0.02821639 |
| 5(1) | 3(1) | 1261.410 | 1224.576 | 3.05494818 |
| 5(1) | 4(1) | 1117.675 | 1081.904 | 0.05121325 |
| 6(1) | 1(1) | 2869.840 | 2830.390 | 0.01332897 |
| 6(1) | 2(1) | 2596.753 | 2565.647 | 0.00244115 |
| 6(1) | 3(1) | 1346.583 | 1326.785 | 0.05161650 |
| 6(1) | 4(1) | 1202.847 | 1180.950 | 0.00290902 |
| 6(1) | 5(1) | 859.304 | 877.969 | 0.00000245 |

### 3.1.4 DPCO – vibrational analysis

==========
Derivatives of the Inertia Moments w.r.t
Normal modes (in amu^1/2.Ang)
==========

| | Ixx | Ixy | Iyy | Ixz | Iyz | Izz |
|---|---|---|---|---|---|---|
| Q( 1) | -4.46959 | 0.25011 | 0.04059 | 0.00000 | 0.00000 | -4.42900 |
| Q( 2) | -0.06016 | 0.06569 | -3.92373 | 0.00000 | 0.00000 | -3.98389 |
| Q( 3) | 14.37964 | 1.58234 | 0.05935 | 0.00000 | 0.00000 | 14.43899 |
| Q( 4) | -11.78577 | 2.30525 | 0.07161 | 0.00000 | 0.00000 | -11.71416 |
| Q( 5) | -0.83425 | 2.65938 | -0.12836 | 0.00000 | 0.00000 | -0.96261 |
| Q( 6) | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |

==========
Vibro-rotational Alpha Matrix
==========

Vibro-Rot alpha Matrix (in cm^-1)

| | a(z) | b(x) | c(y) |
|---|---|---|---|
| Q( 1) | 0.00157 | 0.00097 | 0.00090 |
| Q( 2) | 0.09114 | -0.00003 | 0.00010 |
| Q( 3) | -0.05573 | 0.00054 | 0.00045 |
| Q( 4) | -0.12253 | -0.00003 | 0.00030 |
| Q( 5) | 0.27478 | -0.00064 | -0.00022 |
| Q( 6) | -0.15894 | -0.00019 | -0.00035 |

Vibro-Rot alpha Matrix (in MHz)

---

| | a | b | c |
|---|---|---|---|
| Q( 1) | 47.12532 | 29.15029 | 26.87539 |
| Q( 2) | 2732.16628 | -0.90877 | 3.05857 |
| Q( 3) | -1670.79146 | 16.07469 | 13.60570 |
| Q( 4) | -3673.30256 | -0.78327 | 9.13977 |
| Q( 5) | 8237.76049 | -19.31603 | -6.57153 |
| Q( 6) | -4764.99421 | -5.78791 | -10.58410 |

==========
Quartic Centrifugal Distortion Constants
==========

NOTE: Values in Cartesian coords. refer to the structure in Input orientation

Quartic Centrifugal Distortion Constants Tau Prime
---

| | cm^-1 | MHz |
|---|---|---|
| TauP aaaa | -0.4661373702D-03 | -0.1397444680D+02 |
| TauP bbaa | -0.2322547432D-04 | -0.6962822036D+00 |
| TauP bbbb | -0.1815874715D-06 | -0.5443855443D-02 |
| TauP ccaa | -0.8390622327D-06 | -0.2515445292D-01 |
| TauP ccbb | -0.1673826811D-06 | -0.5018006538D-02 |
| TauP cccc | -0.1555209815D-06 | -0.4662401732D-02 |

Asymmetric Top Reduction
Asymmetric Top Parameter Kappa : -0.9964695461
Asymmetric Top Parameter Sigma : 1131.9987773354

Constants in the Asymmetrically reduced Hamiltonian
---

| | cm^-1 | MHz |
|---|---|---|
| DELTA J : | 0.4213855663D-07 | 0.1263282147D-02 |
| DELTA K : | 0.1105606399D-03 | 0.3314524598D+01 |
| DELTA JK : | 0.5931564140D-05 | 0.1778238193D+00 |
| delta J : | 0.1629155625D-08 | 0.4884085693D-04 |
| delta K : | 0.2962445860D-05 | 0.8881189262D-01 |

Effective Rotational Constants
(Include Terms due to Quartic Centrifugal Distortion Constants)
---

| | Be in cm^-1 | B(A) in cm^-1 | B(A) in MHz |
|---|---|---|---|
| a | 4.376534287 | 4.376534287 | 131205.19713 |
| b | 0.183878356 | 0.183878688 | 5512.54438 |
| c | 0.176464279 | 0.176463948 | 5290.25607 |

Nielsen Centrifugal Distortion Constants
---

| | cm^-1 | MHz |
|---|---|---|
| DJ | 0.4206533504D-07 | 0.1261087019D-02 |
| DJK | 0.5932003469D-05 | 0.1778369901D+00 |
| DK | 0.1105602738D-03 | 0.3314513622D+01 |
| dJ | 0.1629155625D-08 | 0.4884085693D-04 |
| R5 | -0.1398336178D-05 | -0.4192106399D-01 |
| R6 | -0.3661079588D-10 | -0.1097564049D-05 |

Constants in the Symmetrically Reduced Hamiltonian
---

| | cm^-1 | MHz |
|---|---|---|
| D J : | 0.4083005440D-07 | 0.1224054237D-02 |
| D JK : | 0.5939415153D-05 | 0.1780591868D+00 |
| D K : | 0.1105540973D-03 | 0.3314328459D+01 |
| d 1 : | -0.1629155625D-08 | -0.4884085693D-04 |
| d 2 : | -0.6542511175D-09 | -0.1961395507D-04 |

Effective Rotational Constants

(Include Terms due to Quartic Centrifugal Distortion Constants)

| | Be in cm^-1 | B(S) in cm^-1 | B(S) in MHz |
|---|---|---|---|
| a | 4.376534287 | 4.376534293 | 131205.19733 |
| b | 0.183878356 | 0.183872760 | 5512.36668 |
| c | 0.176464279 | 0.176469870 | 5290.43362 |

Wilson Centrifugal Distortion Constants

| | cm^-1 | MHz |
|---|---|---|
| DJ | 0.4539686788D-07 | 0.1360963861D-02 |
| DJK | 0.1152194343D-04 | 0.3454191741D+00 |
| DK | 0.1049670023D-03 | 0.3146831562D+01 |

Nielsen Centrifugal Distortion Constants

| | cm^-1 | MHz |
|---|---|---|
| DJ | 0.4206533504D-07 | 0.1261087019D-02 |
| DJK | 0.5932003469D-05 | 0.1778369901D+00 |
| DK | 0.1105602738D-03 | 0.3314513622D+01 |
| dJ | 0.1629155625D-08 | 0.4884085693D-04 |
| R5 | -0.1398336178D-05 | -0.4192106399D-01 |
| R6 | -0.3661079588D-10 | -0.1097564049D-05 |

Rotational Constants (in cm^-1)

equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)

| | | | | | |
|---|---|---|---|---|---|
| Ae= | 4.3765343 | A00= | 4.3613911 | A0= | 4.3613911 |
| Be= | 0.1838784 | B00= | 0.1835710 | B0= | 0.1835713 |
| Ce= | 0.1764643 | C00= | 0.1758718 | C0= | 0.1758715 |

Rotational Constants (in MHz)

equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)

| | | | | | |
|---|---|---|---|---|---|
| Ae= | 131205.197 | A00= | 130751.215 | A0= | 130751.215 |
| Be= | 5512.534 | B00= | 5503.320 | B0= | 5503.330 |
| Ce= | 5290.266 | C00= | 5272.504 | C0= | 5272.494 |

Test of Quartic Planarity Relationships

Asymmetric Reduction I r

4C*DELJ - (B-C)*DELJK - 2*(2A+B+C)*SDELJ+ 2*(B-C)*SDELK = 0

VALUE = -0.5293955920D-22

Symmetric Reduction I r

4C*DJ - (B-C)*DJK + 2*(2A+B+C)*D1 - 4*(4A+B-3C)*D2 = 0

Value = -0.5293955920D-22

## Sextic Centrifugal Distortion Constants

Sextic Distortion Constants

| | in cm-1 | in Hz |
|---|---|---|
| Phi aaa | -0.6273608711D-08 | -0.1880780576D+03 |
| Phi aab | -0.1511046531D-07 | -0.4530003536D+03 |
| Phi aac | -0.3094483438D-08 | -0.9277027961D+02 |
| Phi abb | 0.2027863845D-10 | 0.6079382866D+00 |
| Phi abc | 0.1397119605D-10 | 0.4188459204D+00 |
| Phi acc | -0.2082873282D-11 | -0.6244297010D-01 |
| Phi bbb | -0.8035701647D-14 | -0.2409042749D-03 |
| Phi bbc | -0.2293178358D-13 | -0.6874775767D-03 |
| Phi bcc | -0.1679987751D-13 | -0.5036476573D-03 |
| Phi ccc | -0.1403052349D-13 | -0.4206245123D-03 |

Asymmetric Top Reduction

Asymmetric Top Parameter Kappa : -0.9964695461
Asymmetric Top Parameter Sigma : 1131.9987773354

Constants in the A reduced Hamiltonian

| | in cm^-1 | in Hz |
|---|---|---|
| Phi J : | -0.1103311257D-13 | -0.3307643936D-03 |
| Phi K : | 0.1196404184D-07 | 0.3586729510D+03 |
| Phi JK : | 0.2383465618D-10 | 0.7145450161D+00 |
| Phi KJ : | -0.1826147417D-07 | -0.5474652228D+03 |
| phi j : | 0.1498705460D-14 | 0.4493005936D-04 |
| phi k : | -0.1238561333D-08 | -0.3713113463D+02 |
| phi jk : | 0.1314104718D-10 | 0.3939586834D+00 |

rho : -0.6176403217D-09
mu : -0.1791811881D-11
nu : -0.2141235974D-15
lambda : 0.4274539604D-14

Constants in the S reduced Hamiltonian

| | in cm^-1 | in Hz |
|---|---|---|
| H J : | -0.1613669259D-13 | -0.4837658737D-03 |
| H K : | 0.1196103420D-07 | 0.3585827844D+03 |
| H JK : | 0.2257629223D-10 | 0.6768202140D+00 |
| H KJ : | -0.1825720307D-07 | -0.5473371785D+03 |
| h 1 : | 0.1427537901D-14 | 0.4279650963D-04 |
| h 2 : | 0.2551790014D-14 | 0.7650074006D-04 |
| h 3 : | 0.7116755858D-16 | 0.2133549732D-05 |

## Average Coordinates and Mean Square Amplitudes

NOTE: Temperature is given in K between parentheses
For Cartesian and internal coords., units are given between parentheses next to each label

Mean Square Amplitudes of Normal Coordinates (in amu.bohr^2)

| Mode | <Q^2> (0) | <Q^2> (298.15) | <Q^2> (298.15) class. |
|---|---|---|---|
| 1 | 0.028333 | 0.028335 | 0.218191 |
| 2 | 0.034982 | 0.034999 | 0.332599 |
| 3 | 0.079078 | 0.083197 | 1.699610 |
| 4 | 0.088817 | 0.095829 | 2.144020 |
| 5 | 0.174435 | 0.255798 | 8.269954 |
| 6 | 0.127896 | 0.157320 | 4.445781 |

Average Normal Coordinates (in amu^1/2.bohr)

| Mode | <Q> (0) | <Q> (298.15) |
|---|---|---|
| 1 | 0.002011 | 0.007234 |
| 2 | -0.021884 | -0.017129 |
| 3 | 0.026563 | 0.023376 |
| 4 | -0.018183 | -0.015622 |
| 5 | 0.008896 | 0.007599 |
| 6 | 0.000000 | 0.000000 |

Mean Square Amplitudes of Cartesian Coordinates

| Label | <(S-Se)^2>^1/2 (0) | <(S-Se)^2>^1/2 (298.15) |
|---|---|---|
| X(1) (Angs) | 0.047429 | 0.054619 |
| Y(1) (Angs) | 0.027523 | 0.027981 |
| Z(1) (Angs) | 0.047449 | 0.052625 |
| X(2) (Angs) | 0.008256 | 0.008606 |
| Y(2) (Angs) | 0.019254 | 0.020064 |
| Z(2) (Angs) | 0.006765 | 0.007503 |
| X(3) (Angs) | 0.067890 | 0.067950 |

| | | |
|---|---|---|
| Y(3) (Angs) | 0.128577 | 0.148095 |
| Z(3) (Angs) | 0.010827 | 0.012008 |
| X(4) (Angs) | 0.024740 | 0.029553 |
| Y(4) (Angs) | 0.026864 | 0.027504 |
| Z(4) (Angs) | 0.021134 | 0.023439 |

Average Cartesian Coordinates

| Label | Se | <S> = Sz (0) | <S> = Sz (298.15) |
|---|---|---|---|
| X(1) (Angs) | 0.000000 | 0.000772 | 0.000648 |
| Y(1) (Angs) | 0.589147 | 0.591327 | 0.591718 |
| Z(1) (Angs) | 0.000000 | 0.000000 | 0.000000 |
| X(2) (Angs) | 0.065583 | 0.066046 | 0.065953 |
| Y(2) (Angs) | -1.091267 | -1.093446 | -1.093202 |
| Z(2) (Angs) | 0.000000 | 0.000000 | 0.000000 |
| X(3) (Angs) | -1.360798 | -1.368797 | -1.367085 |
| Y(3) (Angs) | -1.068099 | -1.066842 | -1.066961 |
| Z(3) (Angs) | 0.000000 | 0.000000 | 0.000000 |
| X(4) (Angs) | 0.047131 | 0.046661 | 0.046721 |
| Y(4) (Angs) | 1.737777 | 1.740202 | 1.739452 |
| Z(4) (Angs) | 0.000000 | 0.000000 | 0.000000 |

Internal coordinates for the Equilibrium structure (Se)

Interatomic distances:

| | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 1 C | 0.000000 | | | |
| 2 P | 1.681693 | 0.000000 | | |
| 3 H | 2.144350 | 1.426569 | 0.000000 | |
| 4 O | 1.149597 | 2.829104 | 3.139300 | 0.000000 |

Interatomic angles:

C1-P2-H3= 86.8345 P2-C1-O4=175.4153 H3-C1-O4=142.9596
H3-P2-O4= 88.6958

Dihedral angles:

O4-C1-P2-H3= 180.

Internal coordinates for the vibrationally average structure at 0K (Sz)

Interatomic distances:

| | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 1 C | 0.000000 | | | |
| 2 P | 1.686037 | 0.000000 | | |
| 3 H | 2.150638 | 1.435090 | 0.000000 | |
| 4 O | 1.149791 | 2.833715 | 3.143727 | 0.000000 |

Interatomic angles:

C1-P2-H3= 86.7191 P2-C1-O4=175.494 H3-C1-O4=142.7322
H3-P2-O4= 88.5458

Dihedral angles:

O4-C1-P2-H3= 180.

Internal coordinates for the vibr. average structure at 298.15K (Sa)

Interatomic distances:

| | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 1 C | 0.000000 | | | |
| 2 P | 1.686185 | 0.000000 | | |
| 3 H | 2.149863 | 1.433278 | 0.000000 | |
| 4 O | 1.148659 | 2.832719 | 3.142420 | 0.000000 |

Interatomic angles:

C1-P2-H3= 86.7314 P2-C1-O4=175.4817 H3-C1-O4=142.79
H3-P2-O4= 88.562

Dihedral angles:

O4-C1-P2-H3= 180.

==========

Vibrational Average of Electric-Field Properties

==========

Electric dipole

---

---

Property at reference geometry, Unit: Debye

---

X= -0.6671 Y= -0.3867 Z= 0.0000

---

Temperature: 0K, Unit: Debye

---

X= -0.6548 Y= -0.4050 Z= 0.0000

---

Temperature: 298K, Unit: Debye

---

X= -0.6546 Y= -0.4050 Z= 0.0000

==========

Nuclear Magnetic Resonance Spectroscopy

==========

Nuclear quadrupole tensors

---

---

Property at reference geometry

---

Nuclear Quadrupole in Principal Axis System

| Atom | | a.u. | MegaHertz | Gauss | 10(-4) cm-1 | Axes | | |
|---|---|---|---|---|---|---|---|---|
| | Baa | -0.4455 | -59.777 | -21.330 | -19.939 | 0.9993 | -0.0367 | 0.0000 |
| 1 C(13) | Bbb | -0.1044 | -14.005 | -4.997 | -4.672 | 0.0000 | 0.0000 | 1.0000 |
| | Bcc | 0.5498 | 73.782 | 26.327 | 24.611 | 0.0367 | 0.9993 | 0.0000 |
| | Baa | -1.2466 | -269.488 | -96.160 | -89.891 | 0.4565 | 0.8897 | 0.0000 |
| 2 P(31) | Bbb | 0.1676 | 36.228 | 12.927 | 12.084 | 0.8897 | -0.4565 | 0.0000 |
| | Bcc | 1.0790 | 233.259 | 83.233 | 77.807 | 0.0000 | 0.0000 | 1.0000 |
| | Baa | -0.1838 | -15.052 | -5.371 | -5.021 | 0.9999 | 0.0139 | 0.0000 |
| 3 H(2) | Bbb | 0.0784 | 6.418 | 2.290 | 2.141 | -0.0139 | 0.9999 | 0.0000 |
| | Bcc | 0.1054 | 8.633 | 3.081 | 2.880 | 0.0000 | 0.0000 | 1.0000 |
| | Baa | -0.5889 | 42.613 | 15.205 | 14.214 | 0.9999 | 0.0110 | 0.0000 |
| 4 O(17) | Bbb | -0.0412 | 2.980 | 1.063 | 0.994 | -0.0110 | 0.9999 | 0.0000 |
| | Bcc | 0.6301 | -45.592 | -16.268 | -15.208 | 0.0000 | 0.0000 | 1.0000 |

---

Temperature: 0K

---

Nuclear Quadrupole in Principal Axis System

| Atom | | a.u. | MegaHertz | Gauss | 10(-4) cm-1 | Axes | | |
|---|---|---|---|---|---|---|---|---|
| | Baa | -0.4414 | -59.232 | -21.135 | -19.758 | 0.9994 | -0.0345 | -0.0001 |
| 1 C(13) | Bbb | -0.1018 | -13.667 | -4.877 | -4.559 | 0.0001 | 0.0000 | 1.0000 |
| | Bcc | 0.5432 | 72.899 | 26.012 | 24.316 | 0.0345 | 0.9994 | 0.0000 |
| | Baa | -1.2237 | -264.534 | -94.392 | -88.239 | 0.4605 | 0.8877 | 0.0000 |
| 2 P(31) | Bbb | 0.1341 | 28.996 | 10.347 | 9.672 | 0.8877 | -0.4605 | 0.0000 |
| | Bcc | 1.0895 | 235.538 | 84.046 | 78.567 | 0.0000 | 0.0000 | 1.0000 |
| | Baa | -0.1790 | -14.662 | -5.232 | -4.891 | 0.9999 | 0.0123 | 0.0000 |
| 3 H(2) | Bbb | 0.0753 | 6.167 | 2.201 | 2.057 | -0.0123 | 0.9999 | 0.0000 |
| | Bcc | 0.1037 | 8.495 | 3.031 | 2.834 | 0.0000 | 0.0000 | 1.0000 |
| | Baa | -0.5843 | 42.278 | 15.086 | 14.102 | 0.9999 | 0.0123 | -0.0001 |
| 4 O(17) | Bbb | -0.0439 | 3.176 | 1.133 | 1.059 | -0.0123 | 0.9999 | 0.0000 |
| | Bcc | 0.6282 | -45.454 | -16.219 | -15.162 | 0.0001 | 0.0000 | 1.0000 |

---

Temperature: 298K

---

Nuclear Quadrupole in Principal Axis System

| Atom | | a.u. | MegaHertz | Gauss | 10(-4) cm-1 | Axes | | |
|---|---|---|---|---|---|---|---|---|
| | Baa | -0.4403 | -59.080 | -21.081 | -19.707 | 0.9994 | -0.0344 | -0.0001 |
| 1 C(13) | Bbb | -0.1017 | -13.650 | -4.871 | -4.553 | 0.0001 | 0.0000 | 1.0000 |
| | Bcc | 0.5420 | 72.730 | 25.952 | 24.260 | 0.0344 | 0.9994 | 0.0000 |

```
        Baa    -1.2180  -263.313   -93.957   -87.832  0.4594  0.8882  0.0000
  2 P(31)  Bbb     0.1296    28.010     9.995     9.343  0.8882 -0.4594  0.0001
        Bcc     1.0884   235.303    83.962    78.489  0.0000  0.0000  1.0000

        Baa    -0.1782   -14.591    -5.206    -4.867  0.9999  0.0129  0.0000
  3 H(2)   Bbb     0.0745     6.104     2.178     2.036 -0.0129  0.9999  0.0000
        Bcc     0.1036     8.488     3.029     2.831  0.0000  0.0000  1.0000

        Baa    -0.5850    42.327    15.103    14.119  0.9999  0.0105 -0.0001
  4 O(17)  Bbb    -0.0402     2.906     1.037     0.969 -0.0105  0.9999  0.0000
        Bcc     0.6251   -45.232   -16.140   -15.088  0.0001  0.0000  1.0000


  ================================================
            Resonance Analysis
  ================================================

Thresholds
----------
Maximum Difference PT2 vs. Variational (cm-1) :      1.000
Minimum value for Darling-Dennison term (cm-1):     10.000

Fermi resonances
----------------
 I   J + K   Freq.Diff.  Reduced Cubic Const.  PT2-Variat.Diff.
 4   5   5     -12.431        -35.272              -3.148

  1 Active Fermi resonances over    1

Darling-Dennison resonances
---------------------------
 No Darling-Dennison resonance found

  ================================================
            Anharmonic X Matrix
  ================================================

PT2 model: Deperturbed VPT2 (DVPT2)
Ref.: V. Barone, J. Chem. Phys. 122, 1, 014108 (2005)

Coriolis contributions to X Matrix (in cm^-1)
---------------------------------------------
           1           2           3           4           5
   1  0.000000D+00
   2  0.000000D+00  0.000000D+00
   3  0.741427D-01  0.109373D+00  0.000000D+00
   4  0.159505D+00  0.148318D+00  0.324756D-01  0.000000D+00
   5  0.617226D+00  0.405093D+00  0.129903D-03  0.520670D-03  0.000000D+00
   6  0.844795D+00  0.270615D-01  0.161729D+01  0.291742D+01  0.479159D+01
           6
   6  0.000000D+00

3rd Deriv. contributions to X Matrix (in cm^-1)
-----------------------------------------------
           1           2           3           4           5
   1 -0.232485D+02
   2 -0.764224D+00 -0.469258D+02
   3 -0.834599D+00  0.796081D+01 -0.444914D+01
   4  0.313163D+01  0.364128D+01 -0.557813D+01 -0.723107D+00
   5  0.254078D+02  0.409471D+02 -0.380826D+01 -0.103212D+02 -0.143773D+02
   6  0.299406D+02 -0.589695D-01 -0.217509D+01 -0.181376D+01 -0.927582D+01
           6
   6 -0.828542D+01

4th Deriv. contributions to X Matrix (in cm^-1)
-----------------------------------------------
           1           2           3           4           5
```

```
   1  0.120649D+02
   2 -0.495610D-01  0.373357D+02
   3 -0.507890D+00 -0.873211D+01  0.647246D+00
   4 -0.646607D+01 -0.101559D+02  0.239038D+01 -0.105010D+01
   5 -0.291802D+02 -0.390929D+02  0.391662D+01  0.451613D+01  0.130077D+02
   6 -0.363710D+02 -0.923961D-01 -0.255410D+01 -0.180181D+00  0.986822D+01
          6
   6  0.914529D+01

Total Anharmonic X Matrix (in cm^-1)
------------------------------------
          1          2          3          4          5
   1 -0.111836D+02
   2 -0.813785D+00 -0.959016D+01
   3 -0.126835D+01 -0.661921D+00 -0.380190D+01
   4 -0.317493D+01 -0.636634D+01 -0.315528D+01 -0.177321D+01
   5 -0.315518D+01  0.225933D+01  0.108496D+00 -0.580453D+01 -0.136956D+01
   6 -0.558563D+01 -0.124304D+00 -0.311190D+01  0.923476D+00  0.538399D+01
          6
   6  0.859871D+00

  ==================================================
       Deperturbed terms for anharmonicity
  ==================================================

Deperturbed terms in FMat (Fermi Resonances)
--------------------------------------------

     4                   5   5
 0.66546D+03   -0.88181D+01    0.68080D+03

Vibrational Energies (cm^-1)
----------------------------
 Mode(Quanta)   E(depert.)  E(after diag.)
  4(1)          665.460     661.443
  5(2)          680.801     684.818

  ==================================================
          Anharmonic Zero Point Energy
  ==================================================

Anharmonic Zero Point Energy
----------------------------
Harmonic       : cm-1 =  3050.22227 ; Kcal/mol =   8.721 ; KJ/mol =  36.489
Anharm.Pot.    : cm-1 =   -13.22606 ; Kcal/mol =  -0.038 ; KJ/mol =  -0.158
Watson+Coriolis: cm-1 =    -0.70465 ; Kcal/mol =  -0.002 ; KJ/mol =  -0.008
X0F (Im. Freq.): cm-1 =     0.00000 ; Kcal/mol =   0.000 ; KJ/mol =   0.000
Total Anharm   : cm-1 =  3036.29156 ; Kcal/mol =   8.681 ; KJ/mol =  36.322

  ==================================================
     Vibrational Energies at Anharmonic Level
  ==================================================

Vibrational Energies and Rotational Constants (in cm^-1)
--------------------------------------------------------
Mode(Quanta)     E(harm)    E(anharm)    Aa(z)      Ba(x)      Ca(y)
Equilibrium Geometry                    4.376534   0.183879   0.176464
Ground State      3050.222   3036.292    4.361391   0.183571   0.175871
Fundamental Bands (DE w.r.t. Ground State)
  1(1) active     2124.686   2095.320    4.359819   0.182599   0.174975
  2(1) active     1720.887   1698.853    4.270256   0.183602   0.175769
  3(1) active      761.269    749.621    4.417123   0.183035   0.175418
  4(1) active      677.795    661.443    4.483919   0.183597   0.175567
  5(1) active      345.113    341.770    4.086609   0.184216   0.176091
  6(1) active      470.694    471.157    4.520334   0.183764   0.176225
Overtones (DE w.r.t. Ground State)
  1(2)           4249.372   4168.273    4.358247   0.181627   0.174079
  2(2)           3441.773   3378.525    4.179121   0.183632   0.175667
```

| | | | | | | |
|---|---|---|---|---|---|---|
| 3(2) | | 1522.539 | 1491.638 | 4.472854 | 0.182499 | 0.174964 |
| 4(2) | | 1355.590 | 1327.373 | 4.606447 | 0.183624 | 0.175262 |
| 5(2) | | 690.226 | 684.818 | 3.811827 | 0.184860 | 0.176310 |
| 6(2) | | 941.389 | 944.033 | 4.679277 | 0.183957 | 0.176578 |

Combination Bands (DE w.r.t. Ground State)

| | | | | | | |
|---|---|---|---|---|---|---|
| 2(1) | 1(1) | 3845.573 | 3793.359 | 4.268684 | 0.182629 | 0.174873 |
| 3(1) | 1(1) | 2885.955 | 2843.673 | 4.415551 | 0.182063 | 0.174521 |
| 3(1) | 2(1) | 2482.156 | 2447.812 | 4.325987 | 0.183065 | 0.175316 |
| 4(1) | 1(1) | 2802.481 | 2757.605 | 4.482347 | 0.182625 | 0.174670 |
| 4(1) | 2(1) | 2398.682 | 2357.946 | 4.392784 | 0.183628 | 0.175465 |
| 4(1) | 3(1) | 1439.064 | 1411.926 | 4.539651 | 0.183061 | 0.175113 |
| 5(1) | 1(1) | 2469.799 | 2433.935 | 4.085037 | 0.183243 | 0.175194 |
| 5(1) | 2(1) | 2066.000 | 2042.882 | 3.995474 | 0.184246 | 0.175989 |
| 5(1) | 3(1) | 1106.382 | 1091.499 | 4.142341 | 0.183679 | 0.175637 |
| 5(1) | 4(1) | 1022.908 | 1001.425 | 4.209137 | 0.184242 | 0.175786 |
| 6(1) | 1(1) | 2595.380 | 2560.891 | 4.518762 | 0.182792 | 0.175328 |
| 6(1) | 2(1) | 2191.581 | 2169.885 | 4.429199 | 0.183795 | 0.176122 |
| 6(1) | 3(1) | 1231.964 | 1217.666 | 4.576066 | 0.183228 | 0.175771 |
| 6(1) | 4(1) | 1148.489 | 1137.540 | 4.642862 | 0.183791 | 0.175920 |
| 6(1) | 5(1) | 815.807 | 818.311 | 4.245552 | 0.184409 | 0.176444 |

Fundamental Bands

| Mode(Quanta) | E(harm) | E(anharm) | I(harm) | I(anharm) |
|---|---|---|---|---|
| 1(1) | 2124.686 | 2095.320 | 707.59437296 | 683.21702311 |
| 2(1) | 1720.887 | 1698.853 | 7.72098939 | 8.08585516 |
| 3(1) | 761.269 | 749.621 | 2.06939703 | 1.87600731 |
| 4(1) | 677.795 | 661.443 | 9.51484366 | 9.25582879 |
| 5(1) | 345.113 | 341.770 | 7.05123387 | 6.75066349 |
| 6(1) | 470.694 | 471.157 | 0.21359226 | 0.19114589 |

Overtones

| Mode(Quanta) | E(harm) | E(anharm) | I(anharm) |
|---|---|---|---|
| 1(2) | 4249.372 | 4168.273 | 5.89113341 |
| 2(2) | 3441.773 | 3378.525 | 0.00753993 |
| 3(2) | 1522.539 | 1491.638 | 0.39553377 |
| 4(2) | 1355.590 | 1327.373 | 0.08960907 |
| 5(2) | 690.226 | 684.818 | 0.03201394 |
| 6(2) | 941.389 | 944.033 | 0.58339411 |

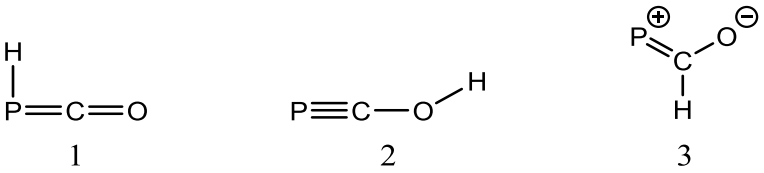
Combination Bands

| Mode(Quanta) | | E(harm) | E(anharm) | I(anharm) |
|---|---|---|---|---|
| 2(1) | 1(1) | 3845.573 | 3793.359 | 0.22451524 |
| 3(1) | 1(1) | 2885.955 | 2843.673 | 3.68530025 |
| 3(1) | 2(1) | 2482.156 | 2447.812 | 0.07897302 |
| 4(1) | 1(1) | 2802.481 | 2757.605 | 1.41992537 |
| 4(1) | 2(1) | 2398.682 | 2357.946 | 0.21123331 |
| 4(1) | 3(1) | 1439.064 | 1411.926 | 0.12877370 |
| 5(1) | 1(1) | 2469.799 | 2433.935 | 0.01784993 |
| 5(1) | 2(1) | 2066.000 | 2042.882 | 0.16755293 |
| 5(1) | 3(1) | 1106.382 | 1091.499 | 0.88171421 |
| 5(1) | 4(1) | 1022.908 | 1001.425 | 1.30351877 |
| 6(1) | 1(1) | 2595.380 | 2560.891 | 0.00125199 |
| 6(1) | 2(1) | 2191.581 | 2169.885 | 0.00140216 |
| 6(1) | 3(1) | 1231.964 | 1217.666 | 0.01310488 |
| 6(1) | 4(1) | 1148.489 | 1137.540 | 0.03173962 |
| 6(1) | 5(1) | 815.807 | 818.311 | 0.00209583 |

## 3.2 Isomers of HPCO

**Table S1.** Computed isomers of HPCO.

| monomer | a.u. E | kJ ΔE | ppm $^{31}$P | ppm $^{1}$H |
|---|---|---|---|---|
| HPCO | -455.0317333 | 0.0 | -310 | 1.8 |
| PCOH | -454.9982745 | 87.8 | -245 | 4.5 |
| PC(H)O | -454.9067496 | 328.1 | +858 | 12.4 |




1 2 3

**Figure S34.** Computed isomers of HPCO.

1_01
0 1

| | | | |
|---|---|---|---|
| C | -0.99173548 | 0.10051244 | -0.00004274 |
| P | -2.62770635 | -0.15755215 | 0.00059353 |
| H | -3.24369053 | 0.86098386 | 0.63749845 |
| O | -0.22142652 | 1.30530456 | -0.00020426 |

1_02
0 1

| | | | |
|---|---|---|---|
| C | -0.99173548 | 0.10051244 | -0.00004274 |
| P | -2.62770635 | -0.15755215 | 0.00059353 |
| O | -0.22142652 | 1.30530456 | -0.00020426 |
| H | 0.71350511 | 1.08735309 | -0.00017504 |

1_03
0 1

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.89334000 | 0.00000000 |
| O | 1.16218400 | 0.32462700 | 0.00000000 |
| P | -0.60769600 | -0.66192100 | 0.00000000 |
| H | -0.18204200 | 1.97175900 | 0.00000000 |

## 3.3 Isomers of $(HPCO)_2$

**Table S2.** Computed isomers of $(HPCO)_2$. Isomers with a suitable coupling pattern (number of multiplets due to $^1J_{P–H}$ coupling) are shown in bold.

| | energy [a.u.] | rel. E [kJ mol$^{-1}$] | | |
|---|---|---|---|---|
| dimer | -910.089692288 | | $\delta(^{31}P)$ | $\delta\ (^{31}P)$ |
| 1 | -910.079870700 | 25.8 | 172 | 172 |
| 2 | -910.079272490 | 27.4 | 155 | 155 |
| **3** | **-910.075835700** | **36.4** | **101** | **367** |
| 4 | -910.045414150 | 116.3 | 177 | 177 |
| 5 | -910.045379637 | 116.3 | 71 | 129 |
| 6 | -910.071516941 | 47.7 | 23 | 112 |
| **7** | **-910.046679684** | **112.9** | **84** | **174** |
| 8 | -910.062443388 | 71.5 | 87 | 283 |
| **9** | **-910.046917064** | **112.3** | **158** | **415** |
| 10 | -910.028743625 | 160.0 | -47 | -47 |
| 11 | -910.039732055 | 131.2 | 148 | 148 |
| 12 | -910.085548158 | 10.9 | -35 | -35 |
| 13 | -910.089692288 | 0.0 | -20 | -20 |
| **14** | **-910.071515472** | **47.7** | **-11** | **83** |
| **15** | **-910.021492230** | **179.1** | **12** | **783** |
| 16 | -909.938939441 | 395.8 | 51 | 66 |
| 17 | -909.901606526 | 493.8 | -43 | -43 |
| 18 | -909.899599633 | 499.1 | -60 | -1 |
| 19 | -909.983347118 | 279.2 | 148 | 260 |
| 20 | -909.989131436 | 264.0 | 148 | 148 |

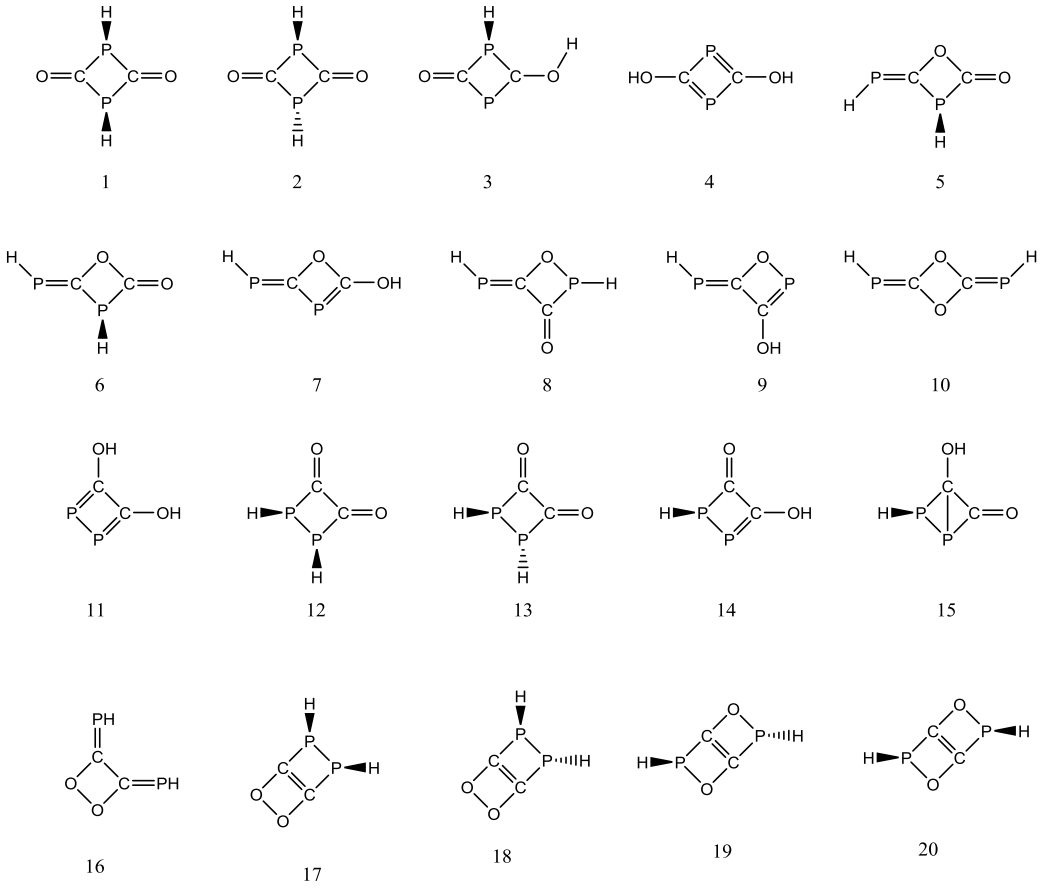



**Figure S35.** Computed isomers of $(HPCO)_2$.

2_01
0 1
C 1.07666700 0.03208700 -0.00052000
C -1.07636800 -0.03185600 -0.00002500
P -0.13679400 1.43767300 -0.00022200
P 0.13669500 -1.43740200 -0.00022900
O -2.36968500 -0.23586900 0.00047800
O 2.36972300 0.23530400 0.00058500
H -2.84600300 0.60538500 0.00056800
H 2.84538100 -0.60630600 0.00098200
2_02
0 1
C -1.25692900 -0.05486000 -0.00082200
C 1.03260700 -0.09026400 0.01664200
P -0.02520300 -1.44540800 -0.04311600
P -0.01795000 1.41995800 -0.14454500
H -0.02030400 1.80937300 1.23148300
O 2.35226700 -0.13593700 0.08445100
O -2.44165400 -0.02728100 0.09542200
H 2.72863100 0.74885600 0.04953700
2_03
0 1
C -1.20619300 0.00011400 0.03212700
C 1.20625700 -0.00012200 0.03219800
P -0.00018000 -1.45012300 -0.23497000
H -0.00037700 -1.88373700 1.11867600
P 0.00012400 1.45012500 -0.23497100
H 0.00031900 1.88381200 1.11865100
O 2.36751200 -0.00016800 0.27659400
O -2.36744800 0.00016000 0.27663600
2_04
0 1
C 1.07754400 0.03509600 0.00010200
C -1.07753000 -0.03507000 0.00007200
P -0.13513500 1.44323200 0.00025100
P 0.13509200 -1.44317200 0.00025100
O -2.37249000 -0.23387500 -0.00037700
O 2.37256300 0.23376300 -0.00038600
H 2.84841200 -0.61088000 -0.00124200
H -2.84843300 0.61071200 -0.00123700
2_05
0 1
C 1.30579100 0.22718000 -0.00003100
C -0.67529600 -0.01556100 -0.00011700
P 0.57943200 -1.35143400 -0.00001700
O 2.47349700 0.81721700 0.00017400
H 3.16850700 0.15099000 -0.00011000
P -2.34325600 0.14963500 0.00008900
H -2.30230100 1.57723200 -0.00012300
O 0.25252600 1.06141400 -0.00016900
2_06
0 1
C -1.45502200 0.35503200 -0.01108100
C 0.63921100 0.05315700 -0.00252900
O -2.54243100 0.80317800 0.02368400
P 2.31181300 0.14847200 0.00857900
H 2.34193200 1.57525700 0.04925600
O -0.27757200 1.09110800 -0.01720900
P -0.59088800 -1.32493600 -0.09706400
H -0.70092000 -1.53172700 1.30787300
2_07
0 1
O -0.26848400 1.06468800 -0.00055300
C 0.67597500 -0.00642200 -0.00055100
P 2.31803900 0.33440700 0.00029300
H 2.67293200 -1.04589200 0.00003000
O -2.48351300 0.79675300 0.00050100
H -3.16973400 0.12162700 0.00005700

| | | | |
|---|---|---|---|
| C | -1.30851300 | 0.22205300 | -0.00010500 |
| P | -0.56417200 | -1.35181000 | -0.00000900 |

2_08

0 1

| | | | |
|---|---|---|---|
| O | 0.34100500 | -1.29531400 | 0.08112100 |
| C | -0.51227600 | -0.23677400 | 0.03619600 |
| P | -2.19787400 | -0.28952100 | -0.03418200 |
| H | -2.25946100 | 1.13511100 | -0.04133700 |
| P | 1.84726800 | -0.44387100 | 0.04507700 |
| C | 0.47231800 | 0.89712000 | 0.03038000 |
| O | 0.37943300 | 2.07888300 | 0.02557900 |
| H | 1.99479200 | -0.36485000 | -1.37514600 |

2_09

0 1

| | | | |
|---|---|---|---|
| O | 0.24759400 | -1.43211700 | 0.00036100 |
| C | -0.47426500 | -0.26465200 | 0.00014900 |
| P | -2.16098300 | -0.18064400 | -0.00016300 |
| H | -2.14366400 | 1.24520900 | 0.00018700 |
| P | 1.77103700 | -0.55322700 | -0.00019600 |
| C | 0.61459800 | 0.69907100 | 0.00006000 |
| O | 0.47848600 | 2.02129400 | 0.00023300 |
| H | 1.34222200 | 2.44293000 | -0.00080200 |

2_10

0 1

| | | | |
|---|---|---|---|
| O | -0.00905400 | 0.99966500 | 0.00006800 |
| O | 0.00907700 | -0.99974100 | 0.00002100 |
| C | -0.93958600 | -0.00601200 | 0.00002900 |
| C | 0.93959800 | 0.00591900 | 0.00003700 |
| P | 2.61933000 | 0.09228700 | -0.00004100 |
| H | 2.69735600 | -1.32933400 | 0.00004400 |
| P | -2.61935900 | -0.09221400 | -0.00002200 |
| H | -2.69717400 | 1.32940800 | -0.00021700 |

2_11

0 1

| | | | |
|---|---|---|---|
| C | -0.45505600 | -0.73709500 | -0.00039000 |
| C | -0.45367600 | 0.73792700 | 0.00038800 |
| O | -1.56954700 | 1.48874100 | -0.00823700 |
| O | -1.57232500 | -1.48588600 | 0.00808800 |
| P | 1.17198500 | 1.21357000 | 0.03178500 |
| P | 1.16968000 | -1.21565800 | -0.03177200 |
| H | -2.26802200 | 1.01663300 | -0.47598200 |
| H | -2.26958700 | -1.01313800 | 0.47699000 |

2_12

0 1

| | | | |
|---|---|---|---|
| C | -0.75563800 | 0.79418100 | -0.04264200 |
| C | -0.77043900 | -0.78094400 | -0.04607100 |
| H | 1.12997100 | -1.38958400 | 1.32691100 |
| O | -1.70501100 | -1.50398100 | 0.01168400 |
| O | -1.67541400 | 1.53420300 | 0.03547100 |
| P | 1.11972600 | -1.13367100 | -0.07339000 |
| P | 1.14007400 | 1.11196900 | -0.09160300 |
| H | 1.17289000 | 1.39392400 | 1.30301300 |

2_13

0 1

| | | | |
|---|---|---|---|
| C | 0.76779000 | 0.79053800 | 0.00255800 |
| C | 0.76747600 | -0.79093700 | -0.00220100 |
| H | -1.26622500 | -1.45503300 | -1.20933700 |
| O | 1.69181800 | -1.52461400 | -0.07245400 |
| O | 1.69240700 | 1.52392600 | 0.07229500 |
| P | -1.12543700 | -1.10031000 | 0.16071500 |
| P | -1.12480000 | 1.10081600 | -0.16077600 |
| H | -1.26562300 | 1.45532600 | 1.20937100 |

2_14

0 1

| | | | |
|---|---|---|---|
| C | 0.82590600 | -0.43625300 | -0.02825200 |
| C | 0.27548500 | 0.93218900 | -0.00748600 |
| H | -1.87791600 | 0.79588000 | 1.21696200 |
| O | 0.88951900 | 1.95881200 | 0.09386900 |

O 2.12919200 -0.67365900 -0.06343600
P -1.57345700 0.52596500 -0.15158000
P -0.52353000 -1.47524100 0.07258500
H 2.57469200 0.18641000 -0.06108600
2_15
0 1
C 1.47390500 0.84946600 -0.00323200
C 1.00629200 -0.39621400 0.01991800
H -0.71647500 -2.08955900 -0.25619400
O 1.87460800 -1.46888500 -0.03293800
H 1.99950600 -1.79441200 0.86379500
O 1.83899000 1.94122300 -0.02835800
P -0.76879800 -0.68151200 -0.06965700
P -2.28940100 0.50722900 0.05516800
2_16
0 1
C -0.71706300 0.19145600 0.00008100
C 0.73045200 0.20567900 -0.00009500
O -0.73782700 1.56749100 0.00017000
O 0.71874900 1.58778800 -0.00019900
P 2.09577200 -0.78803600 0.00008000
P -1.97756700 -0.92955300 -0.00004600
H 1.27353400 -1.95196600 -0.00036500
H -2.97432300 0.09075300 0.00016900
2_17
0 1
C -0.57346200 -0.66867700 0.38003700
C -0.57255900 0.66846200 0.37901300
H 1.66388900 1.48056500 1.11874200
P 1.11861300 1.14244400 -0.15381100
O -1.87406500 0.73012800 -0.13588800
O -1.87522500 -0.72891900 -0.13480200
P 1.11752700 -1.14282900 -0.15448700
H 1.66445400 -1.48316200 1.11694600
2_18
0 1
C -0.61740900 -0.66476700 0.42715700
C -0.53418600 0.66331600 0.33011200
H 1.10720900 1.29666700 -1.34198800
P 1.23803500 1.10837500 0.06654300
O -1.81335100 0.80309600 -0.18903300
O -1.92679200 -0.65233500 -0.09875000
P 1.03561900 -1.16492600 -0.19410000
H 1.61869300 -1.64578600 1.01398100
2_19
0 1
C 0.05400300 0.65356200 0.44560000
C -0.08169300 -0.68660600 0.43686100
H -2.60887200 -0.64005700 0.76524400
H 1.41873200 0.48291300 -1.50730100
P -1.71860900 -0.36211400 -0.31885300
P 1.81216200 0.38264800 -0.13635600
O 1.16347000 -1.21013200 0.12603500
O -1.16934800 1.21605600 0.15839400
2_20
0 1
C 0.07245400 0.67313000 0.43132700
C -0.07301100 -0.67410500 0.43175900
H -2.58051100 -0.62828700 0.81999600
H 2.57857600 0.62885400 0.82126500
P -1.73106500 -0.36242000 -0.29902000
P 1.73141300 0.36279100 -0.29882700
O 1.16344400 -1.21749900 0.13405800
O -1.16343700 1.21746400 0.13443400

## 3.4 Isomers of $(HPCO)_3$

**Table S3.** Computed isomers of $(HPCO)_3$. Isomers with a suitable coupling pattern (number of multiplets due to $^1J_{P–H}$ coupling) are shown in bold.

| trimer | energy [a.u.] | rel. E [kJ mol$^{-1}$] | $\delta(^{31}P)$ ppm | $\delta(^{31}P)$ ppm | $\delta(^{31}P)$ ppm |
|---|---|---|---|---|---|
| 1 | -1365.14456616 | 23.8 | 140 | 158 | 178 |
| 2 | -1365.12504082 | 75.0 | 4 | 184 | 184 |
| 3 | -1365.12944181 | 63.5 | -32 | 182 | 182 |
| 4 | -1365.13496085 | 49.0 | 8 | 23 | 218 |
| 5 | -1365.13496080 | 49.0 | 8 | 24 | 218 |
| 6 | -1365.13710403 | 43.4 | 17 | 49 | 203 |
| 7 | -1365.10657401 | 123.5 | -81 | 13 | 69 |
| 8 | -1365.13911130 | 38.1 | -8 | 1 | 155 |
| **9** | **-1365.12601701** | **72.5** | **-92** | **71** | **176** |
| **10** | **-1365.12462676** | **76.1** | **-92** | **82** | **182** |
| **11** | **-1365.13883026** | **38.8** | **-85** | **114** | **124** |
| **12** | **-1365.13609998** | **46.0** | **-85** | **118** | **131** |
| **13** | **-1365.15361528** | **0.0** | **-80** | **82** | **173** |
| 14 | -1365.13961226 | 36.8 | -110 | 115 | 298 |
| 15 | -1365.13983020 | 36.2 | -111 | 148 | 318 |
| **16** | **-1365.13131840** | **58.5** | **-92** | **184** | **468** |
| 17 | -1365.12253762 | 81.6 | 101 | 259 | 328 |
| 18 | -1365.12467566 | 76.0 | 95 | 259 | 325 |
| 19 | -1365.12498118 | 75.2 | 46 | 243 | 339 |
| 20 | -1365.13077310 | 60.0 | 149 | 184 | 397 |
| **21** | **-1365.07164120** | **215.2** | **-75** | **223** | **246** |
| **22** | **-1365.06173429** | **241.2** | **-75** | **165** | **291** |
| **23** | **-1365.12918536** | **64.1** | **-110** | **181** | **297** |
| 24 | -1365.12841380 | 66.2 | 168 | 168 | 397 |
| 25 | -1365.13221488 | 56.2 | 157 | 166 | 367 |
| **26** | **-1365.11422561** | **103.4** | **-85** | **-49** | **9** |
| 27 | -1365.11701760 | 96.1 | -144 | 41 | 233 |
| 28 | -1365.12141031 | 84.6 | -118 | 47 | 106 |
| **29** | **-1365.10320186** | **132.4** | **-135** | **-88** | **324** |
| **30** | **-1365.11054578** | **113.1** | **-94** | **-43** | **180** |
| **31** | **-1365.07857380** | **197.0** | **-113** | **403** | **417** |
| 32 | -1365.14515367 | 22.2 | 73 | 73 | 73 |
| 33 | -1365.14092327 | 33.3 | 43 | 43 | 50 |
| 34 | -1365.13814103 | 40.6 | 5 | 69 | 69 |

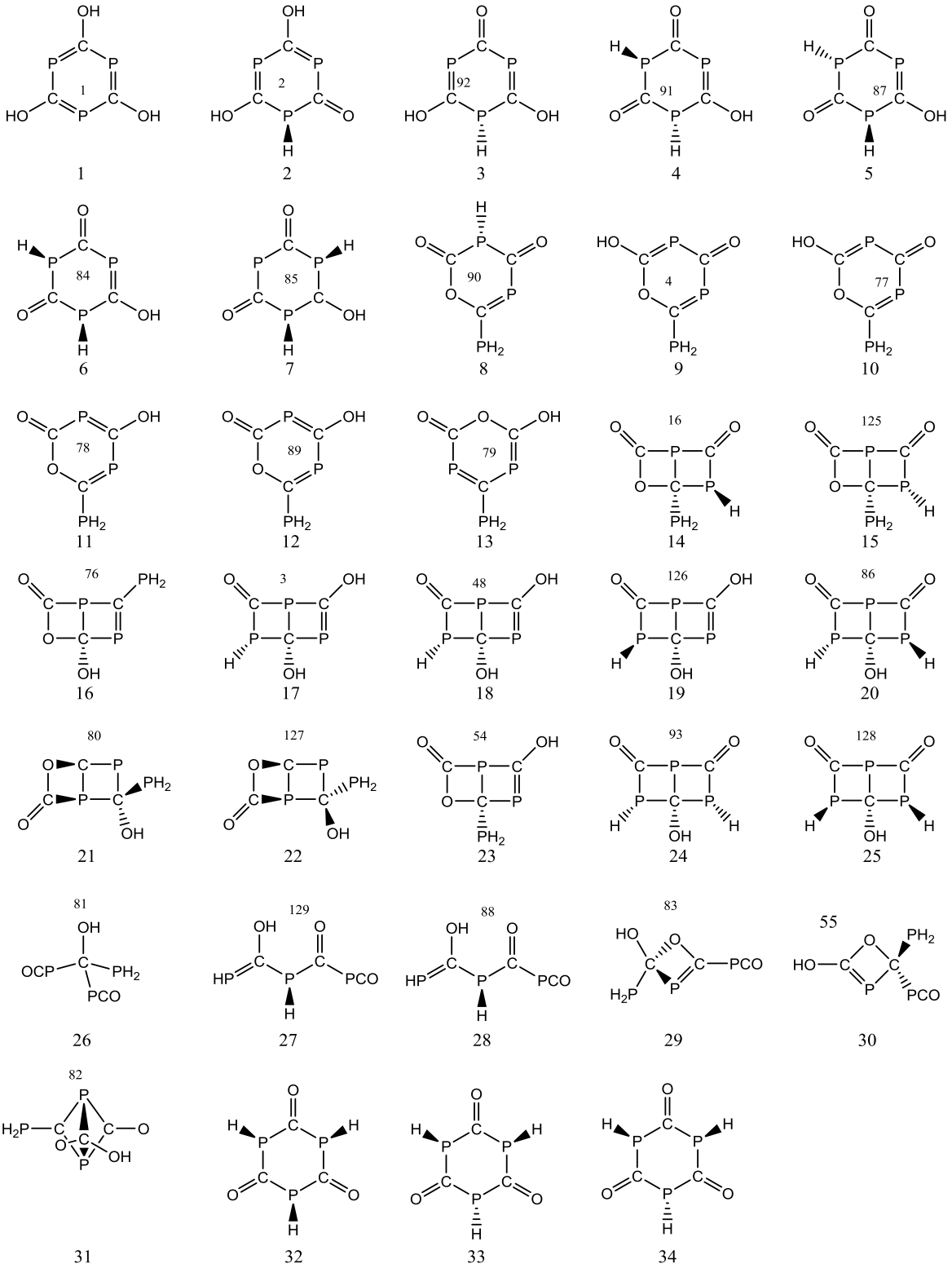


**Figure S36.** Computed isomers of $(HPCO)_3$.

3_01
0 1
C 1.49811000 -0.52984100 0.00007000
C -0.29473900 1.58434600 0.00023300
C -1.19778000 -1.06197900 -0.00017900
O -0.49416300 2.92485700 0.00037000
O 2.76045800 -1.02516900 0.00022900
O -2.19293900 -1.98259100 -0.00037000
P 0.35739900 -1.86413200 0.00016000
P 1.41492700 1.22186800 -0.00076000
P -1.74084600 0.60466200 0.00021800
H 3.39830100 -0.30118600 0.00283600
H -1.43905500 3.11762700 0.00042500
H -3.05182900 -1.54433300 -0.00011000
3_02
0 1
C 1.34608500 -0.78737200 0.06923300
C -1.44282900 -0.72132600 -0.02770900
C 0.16854200 1.70112000 -0.16753900
O -2.65813900 -1.25516700 -0.24406600
O 2.41795700 -1.59324700 0.23065300
O 0.09073200 2.81886300 -0.60454800
P 1.79906500 0.87681400 0.03796900
P -0.13464300 -1.79333500 -0.27499500
P -1.37799200 0.96196000 0.62871300
H -2.32509500 1.51344400 -0.27907200
H 2.14185500 -2.51879600 0.23144200
H -3.34839500 -0.59434700 -0.12790100
3_03
0 1
C 0.00068600 1.71429100 0.12946100
C -1.43427600 -0.69286400 -0.06591600
C 1.43369900 -0.69384400 -0.06607800
O -2.44975600 -1.56585000 -0.22369300
O 0.00067700 2.86872300 0.48359500
O 2.44886500 -1.56717200 -0.22372000
P 1.67753500 0.97970500 -0.24275900
P -1.67678500 0.98065500 -0.24317700
P -0.00054500 -1.63035800 0.55408900
H 3.26286300 -1.08655200 -0.42229400
H -0.00091200 -2.62984900 -0.45415500
H -3.26398000 -1.08474100 -0.42008700
3_04
0 1
C -0.45066100 1.60268100 0.21477500
C -1.26188300 -1.18985500 -0.04711100
C 1.53348300 -0.31392900 -0.09313900
O -2.07602700 -2.07289400 -0.06399400
O -0.79539100 2.58350800 0.81738800
O 2.72171400 -0.89060200 -0.34855200
P 1.35822200 1.38043100 -0.21006500
P -1.73379800 0.51918200 -0.62384500
P 0.43827000 -1.59395000 0.62828100
H 3.36264000 -0.22026400 -0.62071300
H -2.75697700 0.68697000 0.34256000
H 0.72593600 -2.60513500 -0.32329800
3_05
0 1
C 0.45034300 1.60285100 0.21470900
C 1.26204700 -1.18974700 -0.04703200
C -1.53346800 -0.31410300 -0.09316200
O 2.07634100 -2.07265400 -0.06374700
O 0.79486500 2.58396400 0.81704000
O -2.72163400 -0.89094700 -0.34839300
P -1.35836000 1.38021700 -0.20998400
P 1.73381500 0.51938100 -0.62367500
P -0.43803500 -1.59417500 0.62796500
H -0.72530800 -2.60510500 -0.32401300

H 2.75684900 0.68748600 0.34283700
H -3.36295100 -0.22063000 -0.61971100
3_06
0 1
C 1.16154600 -1.27397100 0.03605400
C 0.60243000 1.55933800 0.20333500
C -1.53620000 -0.35334900 -0.02239200
O 0.93203700 2.48817600 0.88696800
O 1.97927700 -2.11174700 0.32106600
O -2.87468900 -0.43465400 0.09928800
P -0.61831500 -1.79271800 0.10894000
P 1.80717500 0.38135600 -0.57783200
P -1.15995600 1.39545600 -0.41021400
H -1.78074000 1.94985600 0.73812400
H -3.13320600 -1.34783000 0.28484400
H 2.82073700 0.51026100 0.40305700
3_07
0 1
C -1.73641600 0.12623100 -0.01121800
C 0.81284400 -1.37721700 0.10858100
C 0.75203800 1.60456500 0.05599800
O 1.25549200 -2.16382900 1.07532400
O -2.91246100 -0.08552200 0.10191400
O 1.61087100 2.40462200 0.25155600
P -1.00740200 1.76032900 0.21396500
P -0.84919000 -1.59020700 -0.47959600
P 1.70910500 -0.10921200 -0.70399000
H 2.77179800 -0.04424900 0.24426200
H 2.17254700 -1.94943600 1.29157300
H -1.33405200 -2.28360900 0.65795800
3_08
0 1
C -1.13952600 -0.07239300 -0.02369000
C 0.68174800 1.55682000 -0.13962900
C 1.39566000 -1.18220300 -0.10245400
P -2.95855900 0.06234500 0.21658900
H -3.24209800 0.60899400 -1.06569600
H -3.25890500 -1.27853000 -0.13766700
P -0.41494200 -1.61452800 -0.07756900
P 1.89635700 0.43813300 0.68633300
O 2.21603900 -1.96870300 -0.49011400
O 0.95271500 2.62653300 -0.57503700
O -0.66031600 1.19191900 -0.10988500
H 2.96336000 0.76896000 -0.18200100
3_09
0 1
C 1.15045600 -0.12924300 0.01977900
C -1.42115200 -1.21925900 -0.02142500
C -0.65830000 1.44296000 0.00098900
P -2.09565400 0.48937200 0.01665500
P 0.38744600 -1.64049200 0.07973400
P 2.97848700 0.02666600 -0.13358600
H 3.20437400 0.53093500 1.17949900
H 3.24712500 -1.32394000 0.20903000
O 0.63349000 1.12855600 -0.02933600
O -0.71857400 2.77165600 0.00772000
H -1.64588600 3.03611600 0.01670200
O -2.20064500 -2.14309200 -0.08380000
3_10
0 1
C 1.14650700 -0.16092600 0.01956800
C -0.65490500 1.45023600 0.00302500
C -1.45367900 -1.17607200 -0.01740100
P 2.97671200 -0.03076200 -0.12721300
H 3.22074700 0.37904000 1.21611400
H 3.21944300 -1.40525100 0.12562900
P 0.34637100 -1.64955200 0.06960400
P -2.11524000 0.53687900 0.01229600

| | | | |
|---|---|---|---|
| O | -2.24699800 | -2.09025900 | -0.07169000 |
| O | -0.75823400 | 2.77441600 | 0.00994300 |
| O | 0.64126800 | 1.10817100 | -0.02192300 |
| H | 0.12634900 | 3.15969000 | -0.02382600 |

3_11
0 1

| | | | |
|---|---|---|---|
| C | -1.16129800 | -0.10712100 | 0.01904000 |
| C | 0.55940700 | 1.66360900 | 0.01812300 |
| C | 1.39934400 | -0.97606100 | -0.00575200 |
| P | -2.99419000 | -0.14487900 | -0.15029000 |
| H | -3.14443300 | -1.48813000 | 0.28648000 |
| H | -3.27005100 | 0.43299900 | 1.12065200 |
| P | -0.29573700 | -1.57896400 | 0.08574000 |
| P | 2.04810700 | 0.61623600 | -0.05374000 |
| O | 2.24198800 | -2.02291400 | -0.02146400 |
| H | 3.15731300 | -1.71561200 | -0.05898600 |
| O | 0.65322400 | 2.85004800 | 0.07515800 |
| O | -0.75774500 | 1.16065300 | -0.02397600 |

3_12
0 1

| | | | |
|---|---|---|---|
| C | 1.17144100 | -0.09624400 | 0.01623100 |
| C | -0.57322400 | 1.65701000 | 0.02491600 |
| C | -1.41214200 | -0.96732400 | -0.00625700 |
| P | 3.00259500 | -0.14603300 | -0.16044300 |
| H | 3.28525400 | 0.44844000 | 1.10105600 |
| H | 3.14743300 | -1.48403500 | 0.29493400 |
| P | 0.28671600 | -1.55419300 | 0.11040900 |
| P | -2.07052600 | 0.61972400 | -0.07550900 |
| O | -2.34146300 | -1.94137400 | -0.03187600 |
| O | -0.65804200 | 2.84147900 | 0.10879800 |
| O | 0.76114700 | 1.16146500 | -0.04164400 |
| H | -1.92405700 | -2.81008600 | -0.00441000 |

3_13
0 1

| | | | |
|---|---|---|---|
| C | -1.36094500 | -1.10368300 | 0.01379200 |
| C | -1.29543700 | 1.39223300 | -0.02256200 |
| C | 1.08961100 | -0.01586000 | 0.01892900 |
| P | 0.30803500 | -1.60484000 | -0.04881500 |
| P | 0.51533500 | 1.59438200 | 0.07432200 |
| O | -2.06786700 | 2.29080800 | -0.08700600 |
| O | -1.91865200 | 0.08359000 | 0.02153300 |
| O | -2.26917300 | -2.06474100 | 0.04700600 |
| H | -3.14632700 | -1.65706600 | 0.04591300 |
| P | 2.92282600 | -0.18115200 | -0.11839500 |
| H | 3.24888000 | 1.15063500 | 0.26067500 |
| H | 3.15066400 | -0.73282000 | 1.17351000 |

3_14
0 1

| | | | |
|---|---|---|---|
| C | -0.62340300 | 1.56994400 | -0.26807800 |
| C | 0.77564800 | -0.07369000 | -0.07693700 |
| C | -1.50418900 | -0.94172200 | 0.21814100 |
| P | -0.53541400 | 0.40017600 | 1.22045700 |
| P | 0.00831800 | -1.70954000 | -0.60086400 |
| P | 2.61971700 | -0.06413400 | 0.14583600 |
| H | 2.67827200 | 1.06634700 | 1.00887700 |
| H | 2.62421100 | -1.00922300 | 1.20861200 |
| O | 0.41168400 | 1.02895200 | -0.96234200 |
| O | -2.66053100 | -1.18935600 | 0.18372700 |
| O | -1.28804300 | 2.48925200 | -0.59372600 |
| H | -0.28501700 | -1.41262000 | -1.95894800 |

3_15
0 1

| | | | |
|---|---|---|---|
| C | -0.57656900 | 1.61560000 | -0.25831900 |
| C | 0.76799200 | -0.07974300 | -0.07068200 |
| C | -1.52484800 | -0.92807900 | 0.20874700 |
| P | -0.54690600 | 0.40248300 | 1.19834400 |
| P | -0.07854800 | -1.57765400 | -0.85938400 |
| P | 2.60392700 | -0.15584500 | 0.20036500 |

| | | | |
|---|---|---|---|
| H | 2.67420000 | 0.94482900 | 1.10042700 |
| H | 2.53499400 | -1.12614300 | 1.23938900 |
| O | 0.47181700 | 1.06707400 | -0.93192600 |
| O | -2.65944200 | -1.25293600 | 0.27734600 |
| O | -1.20639600 | 2.55912900 | -0.58213500 |
| H | 0.26642500 | -2.48625500 | 0.18554500 |

3_16
0 1

| | | | |
|---|---|---|---|
| C | 1.05163700 | 1.43411900 | -0.23300100 |
| C | 1.23805700 | -0.70200300 | 0.08664000 |
| C | -1.12129900 | -0.30865500 | 0.08651000 |
| P | 0.19362200 | 0.44155400 | 1.14794900 |
| P | -0.27426300 | -1.50964000 | -0.75236800 |
| O | 1.76733500 | 0.38711200 | -0.73156000 |
| O | 1.06223200 | 2.54745300 | -0.63106200 |
| O | 2.22382000 | -1.44784600 | 0.64636100 |
| H | 2.65103600 | -1.97575000 | -0.03630500 |
| P | -2.81809500 | 0.29015000 | -0.04218700 |
| H | -3.42643800 | -0.91125500 | -0.49814200 |
| H | -3.18104000 | 0.12152000 | 1.32273500 |

3_17
0 1

| | | | |
|---|---|---|---|
| C | 0.68270300 | 1.52299400 | -0.00310000 |
| C | -1.58756400 | -0.03178400 | -0.00603000 |
| C | 0.58947200 | -0.96273400 | 0.19353300 |
| P | 1.79398200 | 0.15996100 | -0.76732900 |
| P | -0.29006600 | 0.39046100 | 1.20059900 |
| P | -0.93691800 | -1.37716900 | -0.83317500 |
| O | 1.12348700 | -2.08841200 | 0.80656000 |
| H | 1.87936000 | -1.82910700 | 1.34103800 |
| O | -2.74610100 | 0.58319300 | -0.22934900 |
| O | 0.58856000 | 2.68224500 | -0.22950800 |
| H | 2.67407400 | 0.36809100 | 0.34719300 |
| H | -2.89362300 | 1.27515700 | 0.42229100 |

3_18
0 1

| | | | |
|---|---|---|---|
| C | -1.59092400 | -0.01322400 | -0.00217700 |
| C | 0.57734600 | -0.96678000 | 0.18969100 |
| P | -0.96034700 | -1.36682000 | -0.84074900 |
| P | -0.28334500 | 0.39622800 | 1.20019200 |
| O | -2.73638400 | 0.62097100 | -0.22814300 |
| O | 1.24701600 | -2.01171700 | 0.81606200 |
| C | 0.70624500 | 1.51799400 | -0.00679600 |
| P | 1.80219600 | 0.13609400 | -0.74440700 |
| H | 2.66816900 | 0.32341100 | 0.37857200 |
| O | 0.62168100 | 2.67662000 | -0.23921300 |
| H | 0.59915600 | -2.65515200 | 1.11615900 |
| H | -2.85937400 | 1.33428400 | 0.40577500 |

3_19
0 1

| | | | |
|---|---|---|---|
| C | -1.58409900 | -0.07828400 | -0.00851600 |
| C | 0.62649800 | -0.94736600 | 0.16677800 |
| P | -0.88564700 | -1.36159600 | -0.89404800 |
| P | -0.30489400 | 0.36549100 | 1.21380300 |
| O | -2.76414500 | 0.50219200 | -0.20560500 |
| O | 1.28351100 | -2.00879000 | 0.78469000 |
| C | 0.64785800 | 1.53938400 | 0.01673400 |
| P | 1.90493800 | 0.25077300 | -0.52248200 |
| O | 0.45596400 | 2.67205400 | -0.28011000 |
| H | 0.62430800 | -2.64747000 | 1.07024600 |
| H | -2.91354000 | 1.19475800 | 0.44535700 |
| H | 1.62909200 | 0.22663400 | -1.91646800 |

3_20
0 1

| | | | |
|---|---|---|---|
| C | 1.34885000 | 1.00373900 | -0.00782600 |
| C | -1.41563400 | 0.93550700 | 0.01996800 |
| C | 0.02364100 | -1.08578600 | 0.20494900 |
| P | 1.55168300 | -0.68865700 | -0.86086600 |

| | | | |
|---|---|---|---|
| P | -0.00456900 | 0.52777900 | 1.23918500 |
| P | -1.63674600 | -0.81069500 | -0.64370200 |
| O | 0.00613800 | -2.32822000 | 0.83581800 |
| H | 0.77955500 | -2.40306300 | 1.40161100 |
| O | -1.94290900 | 1.96535700 | -0.24073000 |
| O | 1.88105100 | 2.04376200 | -0.20698200 |
| H | 2.49090300 | -1.08429900 | 0.14234400 |
| H | -1.22135400 | -0.50699900 | -1.97059100 |

3_21

0 1

| | | | |
|---|---|---|---|
| C | 1.24241700 | -0.04382000 | 0.28900000 |
| P | 1.67668500 | 1.42658600 | -0.79906300 |
| H | 0.39102700 | 1.57887700 | -1.38573500 |
| H | 1.45269600 | 2.42723500 | 0.19091500 |
| O | 2.27612800 | -0.16568700 | 1.19487700 |
| H | 2.28932200 | -1.06167300 | 1.54400000 |
| P | -0.56487100 | 0.02307100 | 1.19601000 |
| C | -0.79291500 | -1.09506200 | -0.13823900 |
| C | -2.11659200 | 0.46125000 | 0.07796800 |
| O | -2.94086900 | 1.27303600 | -0.11387500 |
| P | 0.73494100 | -1.53170400 | -0.78581100 |
| O | -2.06423900 | -0.81334300 | -0.56707700 |

3_22

0 1

| | | | |
|---|---|---|---|
| C | 1.01464500 | -0.13283900 | 0.30832000 |
| P | -0.43737100 | -0.72250800 | -0.84004300 |
| C | -0.87692200 | 0.95905600 | -0.47054500 |
| C | -2.18412400 | -0.53077300 | 0.01699800 |
| O | -3.05191600 | -1.13918600 | 0.51617800 |
| P | 0.47851800 | 1.74579000 | 0.19327500 |
| O | -2.23011200 | 0.86981900 | -0.27498400 |
| O | 0.79103800 | -0.61189000 | 1.60073300 |
| H | 1.39207100 | -0.15959600 | 2.20051400 |
| P | 2.66249000 | -0.54971300 | -0.46872900 |
| H | 3.43344600 | 0.15070500 | 0.50588500 |
| H | 2.82625600 | -1.81724200 | 0.16200300 |

3_23

0 1

| | | | |
|---|---|---|---|
| C | -0.33158000 | 1.71885800 | -0.22169500 |
| C | 0.79010900 | -0.13537400 | -0.10044500 |
| C | -1.45143500 | -0.82277300 | 0.13702600 |
| P | -0.51803700 | 0.39746900 | 1.14186600 |
| P | -0.26295400 | -1.50894700 | -0.88030000 |
| P | 2.57330100 | -0.51116600 | 0.22035500 |
| H | 2.77091200 | 0.44426800 | 1.25851200 |
| H | 2.31597500 | -1.58731800 | 1.11413200 |
| O | 0.70516000 | 1.11945700 | -0.85884100 |
| O | -2.74427600 | -1.04210100 | 0.32813900 |
| O | -0.83050600 | 2.75494000 | -0.49811600 |
| H | -3.05712100 | -1.73992900 | -0.26023100 |

3_24

0 1

| | | | |
|---|---|---|---|
| C | 1.36563800 | 1.03141500 | -0.01187700 |
| C | -1.45791600 | 0.91404600 | -0.00674500 |
| C | 0.04451800 | -1.06352300 | 0.21348100 |
| P | 1.62303000 | -0.69101900 | -0.79754200 |
| P | -0.02318600 | 0.56208600 | 1.19512400 |
| P | -1.52508400 | -0.80274900 | -0.82211500 |
| O | -0.01674000 | -2.29418000 | 0.85982800 |
| H | 0.76734500 | -2.40391900 | 1.40517500 |
| O | -2.08192800 | 1.90173200 | -0.20585600 |
| O | 1.88448400 | 2.07329800 | -0.23762000 |
| H | 2.50204200 | -1.06329400 | 0.26645800 |
| H | -2.39073800 | -1.29600100 | 0.19641000 |

3_25

0 1

| | | | |
|---|---|---|---|
| C | 1.16206800 | 1.19390300 | 0.01377100 |
| C | -1.51610900 | 0.71340600 | 0.02540500 |

C 0.19251100 -1.08783100 0.17287700
P 1.76680800 -0.45030600 -0.65130900
P -0.08452600 0.48682300 1.26985800
P -1.48281800 -1.02040700 -0.68458700
O 0.31315400 -2.33986000 0.77749600
H 1.14193600 -2.37681200 1.26328500
O -2.18003700 1.66696100 -0.21256300
O 1.43521300 2.31720600 -0.25470800
H 1.41090200 -0.28851700 -2.01822500
H -1.12225900 -0.64764900 -2.00861500
3_26
0 1
C -0.08809400 0.49041700 0.22276600
P -0.87402100 2.12624500 -0.32259100
H -2.21645600 1.66953700 -0.20542200
H -0.80574000 1.87573900 -1.71929500
O -0.48388200 0.38155600 1.56070300
H 0.00996500 -0.33343800 1.97462900
P 1.78638500 0.88188500 0.04715300
P -0.50109100 -1.04151300 -0.86030400
C 2.34145500 -0.71128200 0.03254200
C -1.97155300 -1.32467300 -0.08646900
O 2.85698000 -1.73974300 0.02676400
O -2.97906300 -1.57154500 0.40918200
3_27
0 1
C -1.53753700 -0.81237100 0.04778600
C 1.35278500 -0.42098200 0.31062900
C -0.72768700 1.80101400 0.04500700
O 1.16950000 0.01667100 1.57157700
O -2.46693800 -1.47623600 0.39783800
O 0.02078500 2.54226000 0.51086000
P -1.96288200 0.91679500 -0.66264100
P 0.12153200 -1.67993300 -0.19616200
P 2.61307000 0.11628900 -0.69640100
H 1.83424200 0.68141800 1.79396900
H 0.03795700 -2.33625300 1.06092500
H 2.23987000 -0.70994700 -1.78957300
3_28
0 1
C 0.74749700 1.31030400 0.04384600
C -1.43150000 -0.52036900 0.01674200
C 2.10130800 -1.01277300 0.05205200
O -0.79433300 -1.64151500 -0.36051300
O 0.65360400 2.48849000 -0.13951700
O 2.21133300 -2.01039200 0.60870200
P 2.13243700 0.40526800 -0.86137300
P -0.42218400 0.41114900 1.23500300
P -2.98594000 0.01114800 -0.42091400
H -3.28676300 -1.16408200 -1.19088600
H -1.33927400 -2.11509600 -0.99988800
H -1.30731700 1.51006800 1.35482300
3_29
0 1
C -1.55514700 -0.00006800 -0.34990100
P -2.61511900 0.02379000 1.19784400
H -1.55341500 0.38125100 2.07231000
H -3.04669600 1.36980900 1.03517300
O -2.39120100 -0.23846600 -1.39965300
H -1.89779900 -0.11901500 -2.21789900
P -0.11634400 1.24660200 -0.56221000
O -0.58476300 -1.11426700 -0.16409100
C 0.50446500 -0.32403500 -0.24211000
P 2.06200100 -1.21400400 0.05554800
C 2.94342600 0.21587700 0.25326100
O 3.62388600 1.12416900 0.41064200
3_30
0 1

| | | | |
|---|---|---|---|
| C | -1.28753200 | -1.19699300 | -0.18357000 |
| C | -0.19391700 | 0.55026900 | -0.01663800 |
| C | 2.26307900 | -0.47549400 | -0.05151500 |
| P | -0.41400500 | -0.85043900 | 1.25951000 |
| P | 1.48871600 | 0.84214700 | -0.78724700 |
| P | -0.98422500 | 2.22941000 | 0.24038000 |
| H | -2.13235800 | 1.74431600 | 0.92870300 |
| H | -0.26971800 | 2.52448100 | 1.43322200 |
| O | -1.07920800 | -0.15615200 | -0.98659800 |
| O | 2.97164700 | -1.28502900 | 0.35128500 |
| O | -2.05524200 | -2.16968200 | -0.61771800 |
| H | -2.34256800 | -1.96535500 | -1.51697900 |

3_31

0 1

| | | | |
|---|---|---|---|
| C | 0.86188100 | 0.15291300 | 0.00492600 |
| C | -0.79373800 | 1.11048100 | -0.01181100 |
| C | -1.12698900 | -1.35258200 | 0.00361600 |
| P | -0.43860700 | -0.22114600 | 1.35981200 |
| P | -0.46018300 | -0.20016200 | -1.35234800 |
| O | -1.72039300 | -2.37871100 | 0.00010400 |
| O | 0.56634900 | 1.58826600 | 0.00154800 |
| O | -1.77327200 | 2.02618800 | -0.08108400 |
| H | -1.72539200 | 2.59068800 | 0.69869500 |
| P | 2.59389300 | -0.43174000 | -0.00981800 |
| H | 3.02995200 | 0.43647000 | -1.04829800 |
| H | 3.04050500 | 0.41773700 | 1.04000400 |

3_32

0 1

3_33

0 1

| | | | |
|---|---|---|---|
| C | -1.48427900 | -0.85944100 | -0.11293000 |
| C | 1.48394300 | -0.85990300 | -0.11324500 |
| C | 0.00013100 | 1.61653100 | 0.25776300 |
| P | -0.00018600 | -1.60243400 | 0.74331200 |
| H | -0.00047100 | -2.84183300 | 0.05921800 |
| P | -1.57895500 | 0.97664600 | -0.53443800 |
| H | -2.42977800 | 1.29300800 | 0.55461300 |
| P | 1.57979300 | 0.97655900 | -0.53319500 |
| H | 2.42945600 | 1.29160400 | 0.55715400 |
| O | 2.45701700 | -1.53509700 | -0.30481700 |
| O | -0.00014500 | 2.52083300 | 1.04640000 |
| O | -2.45784200 | -1.53416800 | -0.30354400 |

3_34

0 1

| | | | |
|---|---|---|---|
| C | 0.86808600 | -1.36590200 | 0.18863800 |
| C | 0.86735600 | 1.36632800 | 0.18876500 |
| C | -1.66461300 | -0.00044100 | 0.05466800 |
| O | 1.36982300 | 2.03384800 | 1.04246500 |
| O | 1.37089500 | -2.03329100 | 1.04227700 |
| O | -2.75579900 | -0.00074800 | 0.55210200 |
| P | -0.88048200 | -1.64539900 | -0.42516600 |
| H | -1.36166500 | -2.32871200 | 0.71836200 |
| P | 1.85695900 | 0.00048000 | -0.70207800 |
| H | 0.99390100 | 0.00043900 | -1.83679400 |
| P | -0.88137900 | 1.64505200 | -0.42523200 |
| H | -1.36301700 | 2.32790400 | 0.71839400 |

## 3.5 Isomers of $(HPCO)_4$

**Table S4.** Computed isomers of $(HPCO)_4$. Isomers with a suitable coupling pattern (number of multiplets due to $^1J_{P–H}$ coupling) are shown in bold.

| tetramers | energy [a.u.] | rel. E [kJ mol$^{-1}$] | δ($^{31}$P) ppm | δ($^{31}$P) ppm | δ($^{31}$P) ppm | δ($^{31}$P) ppm |
|---|---|---|---|---|---|---|
| 1 | -1820.17906551 | 70.2 | 22 | 76 | 113 | 117 |
| 2 | -1820.17429888 | 82.7 | 40 | 42 | 82 | 119 |
| 3 | -1820.17464044 | 81.8 | 63 | 70 | 70 | 105 |
| 4 | -1820.18160701 | 63.5 | 88 | 88 | 88 | 88 |
| 5 | -1820.16377872 | 110.3 | 5 | 5 | 39 | 285 |
| 6 | -1820.16266262 | 113.3 | 11 | 48 | 65 | 262 |
| 7 | -1820.16917752 | 96.2 | 22 | 76 | 135 | 186 |
| 8 | -1820.16376120 | 110.4 | 9 | 72 | 144 | 190 |
| 9 | -1820.14093438 | 170.3 | -11 | 67 | 294 | 355 |
| 10 | -1820.15130850 | 143.1 | -18 | -2 | 191 | 259 |
| 11 | -1820.14861646 | 150.1 | -83 | 18 | 176 | 236 |
| 12 | -1820.14637624 | 156.0 | -11 | 59 | 267 | 353 |
| 13 | -1820.14405695 | 162.1 | -12 | 104 | 282 | 325 |
| 14 | -1820.14873532 | 149.8 | -15 | 101 | 263 | 328 |
| 15 | -1820.13623534 | 182.6 | -64 | 37 | 217 | 644 |
| 16 | -1820.16399405 | 109.8 | -67 | 6 | 55 | 300 |
| 17 | -1820.17098224 | 91.4 | -2 | 30 | 114 | 245 |
| 18 | -1820.17803152 | 72.9 | 8 | 69 | 138 | 206 |
| 19 | -1820.16669557 | 102.7 | -53 | 19 | 45 | 276 |
| 20 | -1820.18096250 | 65.2 | 80 | 80 | 97 | 104 |
| 21 | -1820.14772235 | 152.5 | 9 | 233 | 248 | 302 |
| 22 | -1820.13152793 | 195.0 | 11 | 198 | 213 | 275 |
| 23 | -1820.14494191 | 159.8 | 210 | 212 | 234 | 237 |
| **24** | **-1820.12822279** | **203.7** | **-113** | **64** | **223** | **273** |
| **25** | **-1820.13409357** | **188.3** | **-114** | **117** | **198** | **265** |
| **26** | **-1820.16268099** | **113.2** | **-112** | **77** | **184** | **276** |
| **27** | **-1820.14807239** | **151.6** | **-97** | **98** | **103** | **284** |
| **28** | **-1820.12822276** | **203.7** | **-113** | **64** | **223** | **273** |
| **29** | **-1820.14650155** | **155.7** | **-98** | **95** | **148** | **266** |
| **30** | **-1820.15134643** | **143.0** | **-115** | **-40** | **279** | **345** |
| **31** | **-1820.16456257** | **108.3** | **-114** | **18** | **206** | **302** |
| **32** | **-1820.13409381** | **188.3** | **-114** | **117** | **198** | **266** |
| **33** | **-1820.14952168** | **147.8** | **-95** | **-2** | **250** | **271** |
| 34 | -1820.13458024 | 187.0 | -27 | 222 | 265 | 300 |
| **35** | **-1820.18169166** | **63.3** | **-82** | **54** | **127** | **142** |
| **36** | **-1820.18149224** | **63.8** | **-64** | **29** | **180** | **211** |
| **37** | **-1820.18820477** | **46.2** | **-92** | **85** | **95** | **122** |
| **38** | **-1820.18982340** | **42.0** | **-42** | **130** | **163** | **200** |
| **39** | **-1820.18751515** | **48.0** | **-96** | **86** | **116** | **123** |
| **40** | **-1820.18807958** | **46.5** | **-62** | **153** | **161** | **187** |
| **41** | **-1820.18353979** | **58.4** | **-46** | **49** | **174** | **191** |
| 42 | -1820.17663948 | 76.6 | -53 | 15 | 76 | 333 |
| 43 | -1820.19293975 | 33.8 | 13 | 64 | 93 | 173 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 44 | -1820.18856145 | 45.3 | -34 | 72 | 130 | 249 |
| 45 | -1820.18882024 | 44.6 | -8 | 53 | 139 | 229 |
| 46 | -1820.18413378 | 56.9 | 7 | 43 | 173 | 238 |
| 47 | -1820.18936566 | 43.2 | -2 | 43 | 178 | 275 |
| 48 | -1820.16119065 | 117.1 | -22 | 16 | 174 | 223 |
| 49 | -1820.17430162 | 82.7 | 35 | 54 | 198 | 261 |
| 50 | -1820.17498132 | 80.9 | 161 | 162 | 180 | 183 |
| 51 | -1820.17908494 | 70.1 | -8 | 161 | 203 | 216 |
| 52 | -1820.17180368 | 89.3 | 39 | 54 | 250 | 306 |
| 53 | -1820.17312581 | 85.8 | 161 | 161 | 167 | 220 |
| **54** | **-1820.17324232** | **85.5** | **-87** | **128** | **145** | **189** |
| **55** | **-1820.17394115** | **83.6** | **-86** | **111** | **142** | **219** |
| **56** | **-1820.17488443** | **81.2** | **-83** | **130** | **142** | **175** |
| 57 | -1820.17775374 | 73.6 | -15 | 181 | 196 | 214 |
| **58** | **-1820.17237357** | **87.8** | **-75** | **137** | **161** | **195** |
| 59 | -1820.18208705 | 62.3 | 39 | 137 | 171 | 230 |
| 60 | -1820.18003696 | 67.6 | -47 | 149 | 188 | 206 |
| 61 | -1820.16130150 | 116.8 | 35 | 157 | 168 | 294 |
| 62 | -1820.18756699 | 47.9 | 8 | 67 | 78 | 250 |
| 63 | -1820.18702493 | 49.3 | -25 | 58 | 88 | 236 |
| 64 | -1820.18600843 | 52.0 | 19 | 52 | 140 | 192 |
| 65 | -1820.17873855 | 71.1 | 15 | 78 | 107 | 218 |
| 66 | -1820.16632567 | 103.6 | -82 | 91 | 111 | 305 |
| **67** | **-1820.18281240** | **60.4** | **-80** | **65** | **131** | **158** |
| **68** | **-1820.17313341** | **85.8** | **-86** | **121** | **153** | **170** |
| **69** | **-1820.18984181** | **41.9** | **-91** | **67** | **122** | **123** |
| **70** | **-1820.17197831** | **88.8** | **-100** | **8** | **205** | **297** |
| **71** | **-1820.17411616** | **83.2** | **-99** | **-43** | **242** | **284** |
| **72** | **-1820.20361628** | **5.7** | **-96** | **74** | **272** | **278** |
| **73** | **-1820.18900967** | **44.1** | **-75** | **53** | **242** | **288** |
| **74** | **-1820.19053325** | **40.1** | **-78** | **45** | **254** | **268** |
| **75** | **-1820.20580174** | **0.0** | **-101** | **92** | **238** | **297** |
| **76** | **-1820.18736209** | **48.4** | **-119** | **119** | **211** | **246** |
| **77** | **-1820.16396082** | **109.9** | **-125** | **99** | **172** | **209** |
| **78** | **-1820.16317727** | **111.9** | **-114** | **102** | **169** | **176** |
| **79** | **-1820.18326768** | **59.2** | **-121** | **142** | **204** | **266** |
| **80** | **-1820.18303612** | **59.8** | **-101** | **188** | **224** | **255** |
| **81** | **-1820.15384000** | **136.4** | **-102** | **112** | **153** | **236** |
| **82** | **-1820.18731354** | **48.5** | **-166** | **-64** | **37** | **297** |
| 83 | -1820.15943315 | 121.7 | -122 | -83 | 12 | 178 |
| **84** | **-1820.14904278** | **149.0** | **-110** | **-108** | **52** | **272** |
| **85** | **-1820.16673709** | **102.6** | **-74** | **113** | **142** | **197** |
| **86** | **-1820.17420455** | **83.0** | **-113** | **135** | **176** | **263** |
| 87 | -1820.17314002 | 85.8 | 124 | 136 | 288 | 289 |
| 88 | -1820.16478638 | 107.7 | -88 | 311 | 313 | 349 |
| **89** | **-1820.18470047** | **55.4** | **-115** | **135** | **187** | **267** |
| **90** | **-1820.16704565** | **101.8** | **-47** | **123** | **137** | **195** |
| **91** | **-1820.18064786** | **66.0** | **-90** | **54** | **126** | **133** |
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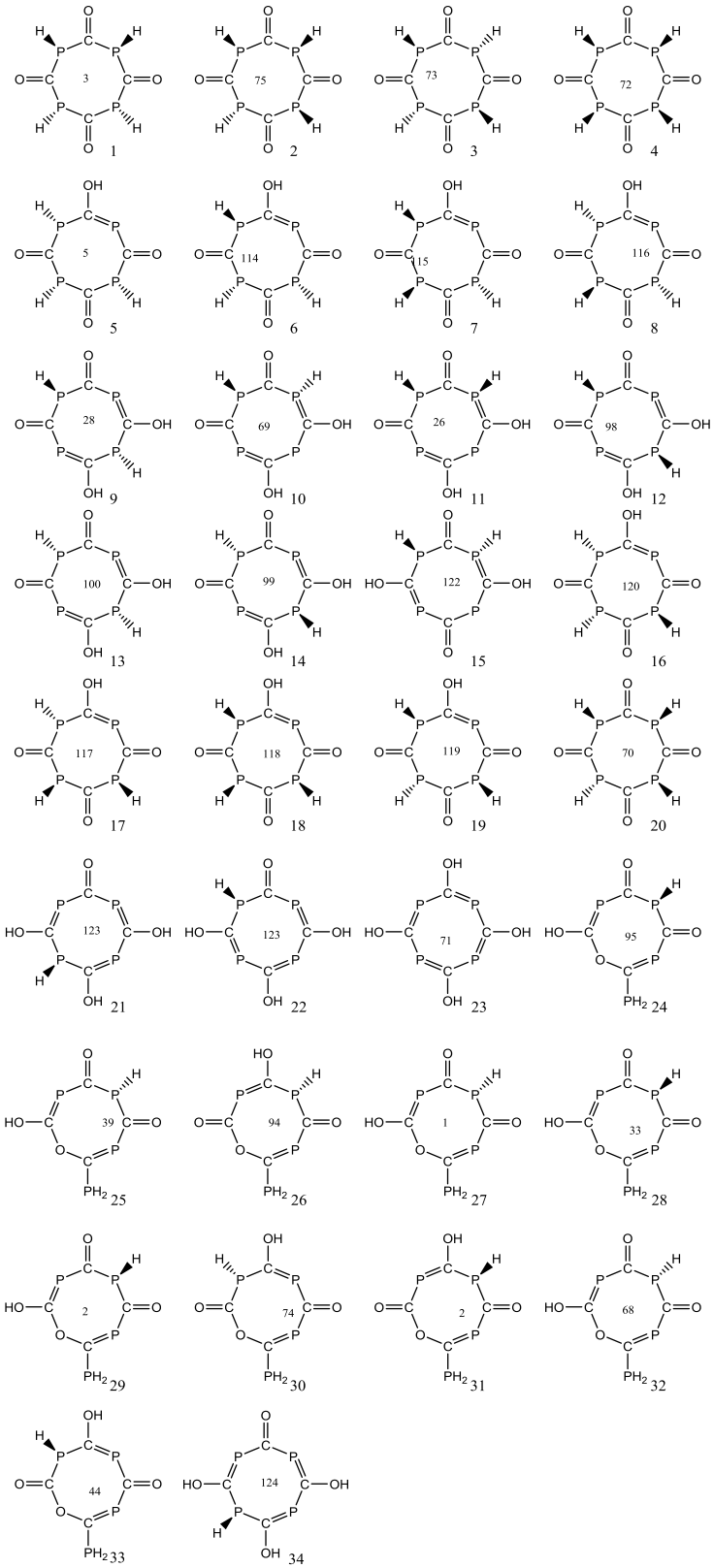

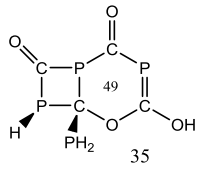

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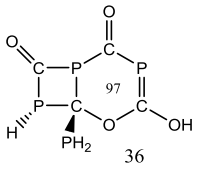

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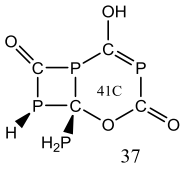

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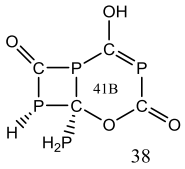

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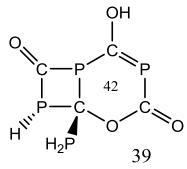

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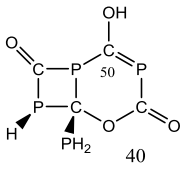

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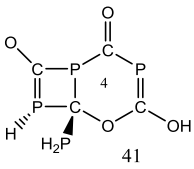

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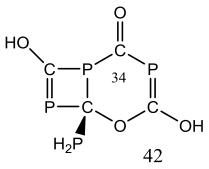

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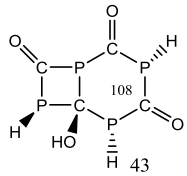

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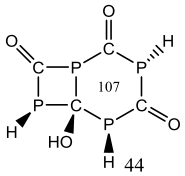

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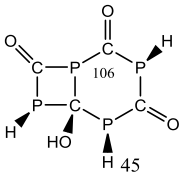

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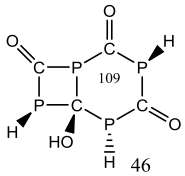

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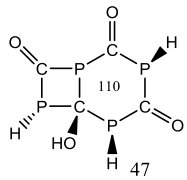

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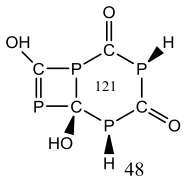

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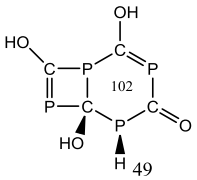

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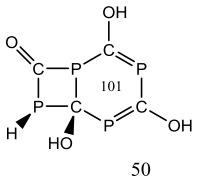

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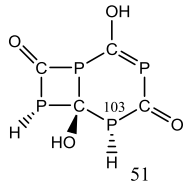

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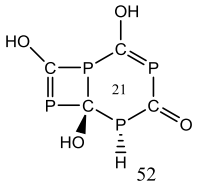

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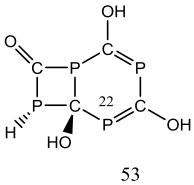

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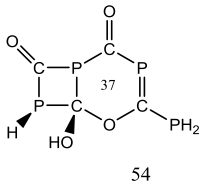

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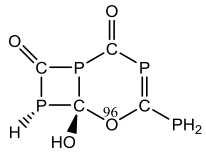

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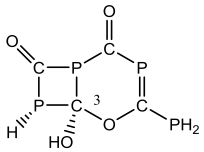

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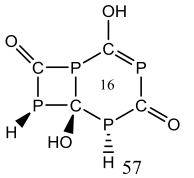

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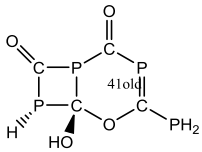

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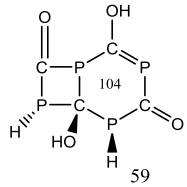

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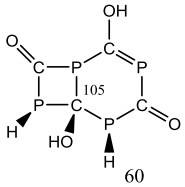

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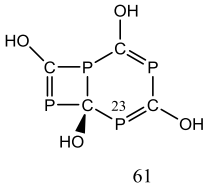

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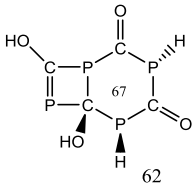

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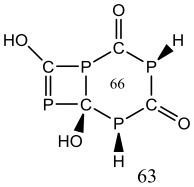

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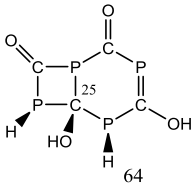

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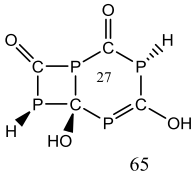

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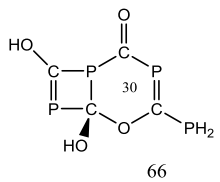

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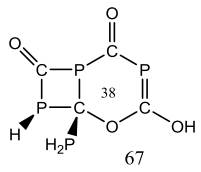

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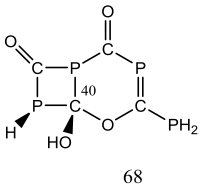

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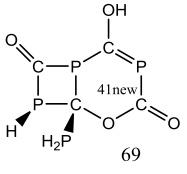

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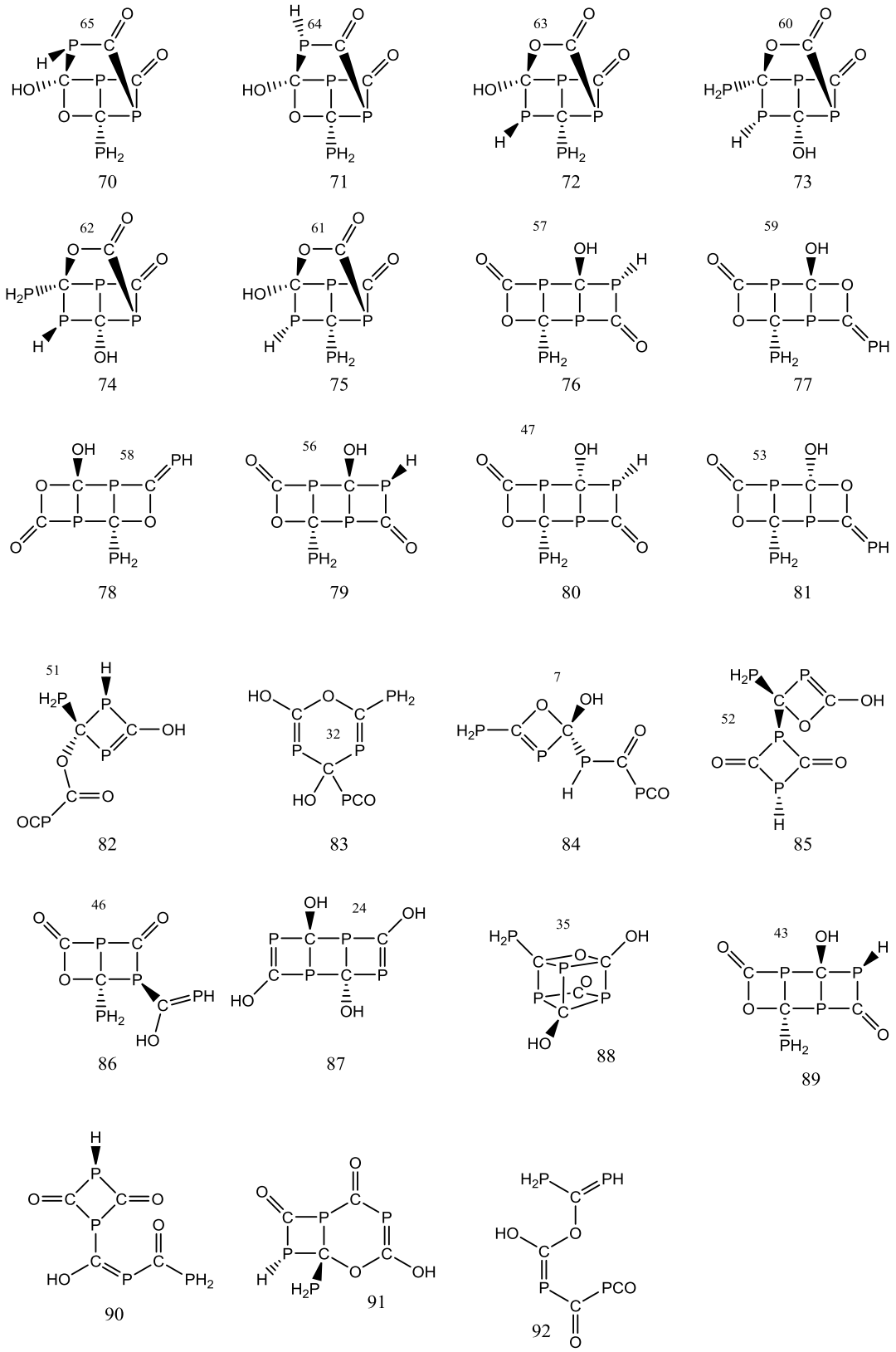


**Figure S37.** Computed isomers of $(HPCO)_4$.

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P -1.29399300 -1.38015500 1.14039300
P 1.76130600 -1.73270300 0.09786800
C 2.09343600 0.10474400 -0.12207900
C -2.16125400 -0.04808200 0.07996800
O 2.99475500 0.43953500 -0.83735100
O -3.34719700 0.07395800 0.13508000
P 1.27635300 1.36298500 1.04296000
H 2.16012200 2.40748400 0.67822400
P -1.14943900 0.94417000 -1.16597600
C -0.11700900 2.04693900 -0.03969200
O -0.29432600 3.23157400 -0.04611200
H 2.15920400 -2.10730800 -1.20727100
H -0.40999400 -0.45298600 1.76642200
H -2.14256500 1.92699100 -1.39679700
4_02
0 1
C -1.93939700 -0.61812100 0.32426900
O -2.42249000 -0.95213100 1.37306000
P -1.16013300 -1.93163900 -0.76543300
P -2.15021900 1.14737600 -0.29669600
C -0.46022700 1.95943500 -0.08645500
C 0.66122700 -1.83169900 -0.21736900
O -0.40603100 3.01221900 0.48120800
O 1.45918400 -2.38939200 -0.91383400
P 1.03351600 1.31536900 -1.07492700
H 1.73762100 2.54070900 -0.98108300
P 1.28774200 -0.93393100 1.32617300
C 2.05136600 0.47159100 0.28017000
O 3.20732800 0.74036300 0.39951400
H -2.68486000 1.65397700 0.91200400
H 0.09628900 -0.21484200 1.60455400
H -0.89436600 -1.11317000 -1.89549500
4_03
0 1
C -1.39215800 -1.54724100 0.08475800
O -1.83031400 -2.41489900 0.78767900
P 0.09734400 -1.84599100 -1.04297100
H 0.19613500 -3.22516300 -0.73121500
P -2.43067600 0.00246700 -0.17071100
C -1.38896700 1.55009600 0.08425600
C 1.55652700 -1.36605800 0.06250000
O -1.82544200 2.41901500 0.78666300
O 2.61036800 -1.89091400 -0.14169800
P 0.10149800 1.84516800 -1.04319500
H 0.20283000 3.22437000 -0.73241000
P 1.43541800 -0.00164300 1.37802900
C 1.55934500 1.36309400 0.06306100
O 2.61403200 1.88658500 -0.14024000
H -3.02669200 0.00329200 1.11181200
H 0.01632000 -0.00016100 1.42784600
4_04
0 1
C -1.54188100 -1.43904400 0.00042800
O -2.41919100 -2.25826200 0.00104400
P -0.05932000 -1.70806300 -1.12549700
H -0.10788300 -3.11974800 -1.05061800
P -1.70828300 0.05931900 1.12539400
C -1.43904600 1.54187900 -0.00048800
C 1.43903600 -1.54187600 -0.00048500
O -2.25823300 2.41922500 -0.00115300
O 2.25820600 -2.41921800 -0.00116300
P 0.05939300 1.70832200 -1.12531700
H 0.10803100 3.11997900 -1.04998300
P 1.70804100 -0.05938600 1.12557200

| | | | |
|---|---|---|---|
| H | 3.11973100 | -0.10802800 | 1.05077800 |
| C | 1.54199200 | 1.43893000 | 0.00049500 |
| O | 2.41946700 | 2.25796400 | 0.00097500 |
| H | -3.11994400 | 0.10789600 | 1.05020800 |

4_05
0 1

| | | | |
|---|---|---|---|
| C | -0.75799700 | -1.32804100 | 0.80050000 |
| O | -0.91888200 | -0.84876500 | 1.88252000 |
| P | 0.93087500 | -2.05837300 | 0.35895600 |
| P | -2.28095900 | -1.23258700 | -0.42946400 |
| C | -1.76086700 | 0.53530800 | -0.56149400 |
| C | 2.00788900 | -0.58521200 | -0.23118000 |
| O | -2.34480700 | 1.29880700 | 0.32135600 |
| O | 2.84458600 | -0.85278300 | -1.04529500 |
| P | -0.25466400 | 0.82158500 | -1.40020800 |
| P | 1.98923600 | 1.08728800 | 0.67046700 |
| C | 0.37739300 | 1.84233000 | -0.00988600 |
| O | -0.21845300 | 2.68125200 | 0.64125400 |
| H | 0.65440600 | -2.46034200 | -0.96981700 |
| H | 2.85109400 | 1.69277200 | -0.28280600 |
| H | -1.57228100 | -1.63246600 | -1.59632600 |
| H | -1.79860600 | 2.11695600 | 0.46636100 |

4_06
0 1

| | | | |
|---|---|---|---|
| C | 1.93619000 | 0.46977200 | 0.46441100 |
| O | 2.32683700 | 0.48237300 | 1.59159200 |
| P | 1.12794600 | 2.02205300 | -0.26723900 |
| P | 2.19430100 | -1.09629100 | -0.64182200 |
| C | 0.50971400 | -1.61298400 | -0.20749400 |
| C | -0.76481100 | 1.79666000 | -0.19057400 |
| O | 0.37033700 | -2.15088200 | 1.01062300 |
| O | -1.39667800 | 2.53042300 | -0.89306300 |
| P | -0.70292900 | -1.12234100 | -1.30978700 |
| P | -1.61779500 | 0.68771600 | 1.09833200 |
| C | -2.01690900 | -0.83771900 | 0.02177900 |
| O | -3.00358500 | -1.48204300 | 0.22290600 |
| H | 1.18100900 | 1.65344400 | -1.63406500 |
| H | -2.89358100 | 1.28120800 | 0.92046200 |
| H | -0.54486500 | -2.42519300 | 1.15453300 |
| H | 2.87418600 | -1.80986000 | 0.38160700 |

4_07
0 1

| | | | |
|---|---|---|---|
| C | 2.18199700 | 0.49214300 | -0.02960900 |
| O | 3.12876800 | 1.08224200 | 0.39307400 |
| P | 0.81891100 | 1.42627700 | -0.99421800 |
| P | 2.18159000 | -1.41051800 | -0.05265700 |
| C | 0.42640800 | -1.53009600 | 0.38986000 |
| C | -0.67512400 | 1.85312700 | 0.09864900 |
| O | 0.16531300 | -1.49898100 | 1.69727400 |
| O | -0.90459800 | 3.01859600 | 0.26412500 |
| P | -0.57695500 | -1.54360100 | -1.00165500 |
| P | -1.90287000 | 0.65449100 | 0.88194700 |
| C | -2.14329600 | -0.78180600 | -0.31193500 |
| O | -3.24581800 | -1.12084600 | -0.64560400 |
| H | -3.06505000 | 1.38225600 | 0.53939600 |
| H | -0.78748500 | -1.46566700 | 1.86518100 |
| H | 2.73084100 | -1.53921500 | 1.24944500 |
| H | 1.42233900 | 2.67460200 | -0.70801100 |

4_08
0 1

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|---|---|---|---|
| C | 2.25309600 | 0.48324400 | -0.07020000 |
| O | 3.25466300 | 1.09844900 | 0.12198200 |
| P | 0.79602700 | 1.37367700 | -0.94591800 |
| P | 2.24776100 | -1.41939100 | 0.24203600 |
| C | 0.42686200 | -1.45058400 | 0.44570100 |
| C | -0.71219500 | 1.81878400 | 0.11962700 |
| O | 0.14180900 | -1.30768000 | 1.74325100 |
| O | -0.91769400 | 2.98476700 | 0.30678000 |

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|---|---|---|---|
| P | -0.53671500 | -1.52447300 | -0.96580700 |
| P | -2.00377600 | 0.63372100 | 0.82336500 |
| C | -2.15969600 | -0.81869000 | -0.35893300 |
| O | -3.23413000 | -1.19084400 | -0.74454900 |
| H | -3.14756500 | 1.36131300 | 0.42503500 |
| H | -0.80362100 | -1.14949400 | 1.89206900 |
| H | 1.37965300 | 2.64042400 | -0.70215700 |
| H | 2.21650400 | -1.67932100 | -1.15696700 |

4_09
0 1

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|---|---|---|---|
| C | 2.28911700 | 0.09124600 | -0.11761600 |
| C | -0.18113000 | 1.42798200 | 0.60291300 |
| C | -2.45236000 | -0.31204000 | -0.19793700 |
| C | -0.04182500 | -1.32850400 | -0.19614500 |
| P | -1.35817100 | -1.44756500 | 0.86476400 |
| P | -1.87059600 | 1.53659500 | -0.25163800 |
| H | -1.43930400 | 1.43708600 | -1.59888200 |
| P | 1.48884800 | 1.58160700 | -0.34662300 |
| P | 1.70733200 | -1.63481300 | 0.27980900 |
| O | -0.13173400 | 1.53789400 | 1.79637400 |
| O | -3.48551300 | -0.59656600 | -0.71320000 |
| O | -0.22167300 | -0.95159900 | -1.47901100 |
| H | 0.59784600 | -0.58713400 | -1.84288400 |
| O | 3.60721900 | -0.00072000 | -0.40822700 |
| H | 3.96997600 | 0.88486000 | -0.54471900 |
| H | 1.53107800 | -1.45634100 | 1.67705100 |

4_10
0 1

| | | | |
|---|---|---|---|
| C | -2.22077400 | 0.14550800 | -0.01739300 |
| C | 0.39287900 | 1.69453300 | -0.23652500 |
| C | 2.30784200 | -0.54109400 | -0.15585300 |
| C | -0.19453200 | -1.54363600 | 0.13624100 |
| P | 0.79822000 | -1.08405400 | -1.15604500 |
| P | 2.04808900 | 1.22134600 | 0.58541700 |
| P | -1.12773400 | 1.35558900 | 0.86518700 |
| P | -2.00035900 | -1.54656800 | -0.22874800 |
| O | 0.30201400 | 2.37112000 | -1.21754900 |
| O | 3.36432100 | -1.07925400 | -0.06197500 |
| O | 0.25585500 | -1.88052100 | 1.36166100 |
| H | -0.49334500 | -2.08360300 | 1.93346300 |
| O | -3.40316100 | 0.65265800 | -0.39840300 |
| H | -3.49006400 | 1.55838500 | -0.07867800 |
| H | 2.84195700 | 1.82786500 | -0.42325700 |
| H | -0.49649700 | 0.45876700 | 1.75260900 |

4_11
0 1

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|---|---|---|---|
| C | -2.15290600 | 0.20816100 | 0.09216300 |
| C | 0.38731300 | 1.72635400 | -0.20098700 |
| C | 2.24167400 | -0.56357400 | -0.10747600 |
| C | -0.23046700 | -1.61601800 | -0.02799400 |
| P | 0.78492300 | -0.98519500 | -1.23431700 |
| P | 2.22991400 | 1.35308400 | 0.17030200 |
| H | 2.07545600 | 1.18675300 | 1.57397600 |
| P | -0.95520500 | 1.23457900 | 1.06396800 |
| H | -0.26104100 | 0.19574800 | 1.71682600 |
| P | -2.03520300 | -1.45060900 | -0.35344700 |
| O | 0.07942200 | 2.40519400 | -1.13617000 |
| O | 3.07368100 | -1.25284900 | 0.38585700 |
| O | 0.19248900 | -2.15985200 | 1.12727700 |
| H | -0.57265500 | -2.38704600 | 1.66837700 |
| O | -3.31293200 | 0.82199800 | -0.18258600 |
| H | -3.34314800 | 1.68118300 | 0.25396700 |

4_12
0 1

| | | | |
|---|---|---|---|
| C | 2.23369400 | 0.11459500 | -0.12361400 |
| C | -0.21973300 | 1.49788900 | 0.56645200 |
| C | -2.42080800 | -0.33851500 | -0.17924100 |
| C | -0.01849600 | -1.41279600 | -0.17144100 |

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|---|---|---|---|
| P | -1.28977600 | -1.37043300 | 0.94637300 |
| P | -1.85466100 | 1.50080200 | -0.39673800 |
| H | -1.33522000 | 1.24526700 | -1.69139400 |
| P | 1.47955200 | 1.62877400 | -0.32067900 |
| P | 1.66191900 | -1.52444400 | 0.53340800 |
| O | -0.25217000 | 1.68595600 | 1.75080600 |
| O | -3.44257200 | -0.68742900 | -0.67812500 |
| O | -0.20085800 | -1.16811900 | -1.48272600 |
| H | 0.64155000 | -0.94262200 | -1.89543300 |
| O | 3.53066600 | -0.02857800 | -0.48980500 |
| H | 3.91192500 | 0.83851600 | -0.68010400 |
| H | 2.29777900 | -2.24331600 | -0.52267300 |

4_13

0 1

| | | | |
|---|---|---|---|
| C | 2.32114500 | 0.09216600 | -0.04405900 |
| C | -0.27114600 | 1.48451400 | 0.49681200 |
| C | -2.46804100 | -0.39166100 | -0.11637800 |
| C | 0.01223700 | -1.31437400 | -0.23202000 |
| P | -1.26492900 | -1.47520400 | 0.86684800 |
| P | -1.81320300 | 1.33924300 | -0.63120200 |
| P | 1.51187700 | 1.57947700 | -0.24093500 |
| P | 1.76385800 | -1.66467000 | 0.17482000 |
| O | -0.36287800 | 1.89945200 | 1.61646500 |
| O | -3.61853500 | -0.65108200 | -0.29304000 |
| O | -0.20089700 | -0.88423400 | -1.49419900 |
| H | 0.61760100 | -0.55160600 | -1.88865900 |
| O | 3.66608200 | 0.05698400 | -0.20049100 |
| H | 4.00960700 | 0.95976300 | -0.23926400 |
| H | -2.63406500 | 1.96990300 | 0.34243400 |
| H | 1.60747000 | -1.65358400 | 1.58651800 |

4_14

0 1

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|---|---|---|---|
| C | 2.27887700 | 0.10107800 | -0.06911900 |
| C | -0.26521600 | 1.51847800 | 0.50448900 |
| C | -2.44465900 | -0.38780500 | -0.14089400 |
| C | 0.01207600 | -1.37612500 | -0.21363100 |
| P | -1.26377900 | -1.44516200 | 0.89529800 |
| P | -1.77046700 | 1.33140900 | -0.67074400 |
| P | 1.51866700 | 1.61646000 | -0.21504900 |
| P | 1.69669300 | -1.57557800 | 0.45745200 |
| O | -0.40262100 | 1.93462400 | 1.61859400 |
| O | -3.58530400 | -0.65510000 | -0.36357100 |
| O | -0.17715800 | -1.02243000 | -1.49994600 |
| H | 0.65789100 | -0.73847000 | -1.89361900 |
| O | 3.60169200 | -0.00047100 | -0.34390200 |
| H | 3.97697400 | 0.88044800 | -0.47327000 |
| H | 2.30012600 | -2.21958500 | -0.66417200 |
| H | -2.63104600 | 1.98393700 | 0.25223700 |

4_15

0 1

| | | | |
|---|---|---|---|
| C | 2.19993000 | 0.27106700 | -0.27128200 |
| O | 2.88170600 | 0.58409900 | -1.18802800 |
| P | 2.00620700 | -1.58196200 | 0.24581500 |
| P | 1.26304700 | 1.63775200 | 0.76195300 |
| C | -0.35998400 | 1.43153000 | -0.05715100 |
| C | 0.17561500 | -1.43199500 | 0.40433100 |
| O | -0.30587400 | 1.86339500 | -1.31422900 |
| O | -0.16525100 | -1.31689200 | 1.68107200 |
| P | -1.91218900 | 1.06805600 | 0.76670500 |
| P | -0.74136700 | -1.21613000 | -1.02201200 |
| C | -2.33526800 | -0.38449000 | -0.32891100 |
| O | -3.42355100 | -0.85462100 | -0.50273200 |
| H | -1.20013300 | 1.85237600 | -1.68479900 |
| H | 0.96212000 | 0.81558300 | 1.87063800 |
| H | -1.00151000 | -0.79231000 | 1.74072700 |
| H | 2.02607800 | -2.01591300 | -1.10406500 |

4_16

0 1

| | | | |
|---|---|---|---|
| C | -0.75590800 | -1.28786600 | 0.81160800 |
| O | -0.88118500 | -0.76167400 | 1.87870100 |
| P | 0.90590800 | -2.06806700 | 0.38488800 |
| P | -2.28834800 | -1.21690100 | -0.40231500 |
| C | -1.74850700 | 0.54259600 | -0.55582700 |
| C | 1.99068400 | -0.61097300 | -0.24007400 |
| O | -2.31224300 | 1.30606100 | 0.34076200 |
| O | 2.75527600 | -0.88107800 | -1.11999900 |
| P | -0.26476600 | 0.82096900 | -1.43372200 |
| P | 2.08173100 | 1.12518900 | 0.55934100 |
| C | 0.42099400 | 1.82487500 | -0.05177200 |
| O | -0.15477800 | 2.65432900 | 0.62451500 |
| H | -1.74266400 | 2.10391100 | 0.49697400 |
| H | 1.47698000 | 0.76725700 | 1.79437800 |
| H | 0.62389700 | -2.50044900 | -0.93278400 |
| H | -1.57619700 | -1.64144600 | -1.55688900 |

4_17

0 1

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|---|---|---|---|
| C | 1.16447900 | 1.44834400 | 0.41766700 |
| O | 1.20394200 | 1.81092800 | 1.55379100 |
| P | -0.29339600 | 1.83333800 | -0.77427700 |
| P | 2.66743400 | 0.43200400 | -0.29128400 |
| C | 1.57864000 | -1.04127400 | -0.07880300 |
| C | -1.83067300 | 1.07887400 | 0.08730700 |
| O | 1.69511100 | -1.61759700 | 1.07801900 |
| O | -2.59063600 | 1.78670700 | 0.68312800 |
| P | 0.29477900 | -1.26633300 | -1.23852600 |
| P | -2.41914700 | -0.70193500 | -0.25684400 |
| C | -0.91603000 | -1.72856000 | 0.07020400 |
| O | -0.73337500 | -2.42575000 | 1.05468600 |
| H | 0.93184100 | -2.23016900 | 1.23457100 |
| H | -0.50284000 | 3.07385700 | -0.10063800 |
| H | 2.29920800 | 0.57379700 | -1.65620800 |
| H | -3.05209700 | -0.85218900 | 1.00100900 |

4_18

0 1

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|---|---|---|---|
| C | 1.90279400 | 1.00345400 | 0.14552600 |
| O | 2.63019300 | 1.69004100 | 0.79173900 |
| P | 0.40161300 | 1.77773000 | -0.77275600 |
| P | 2.47146400 | -0.78610000 | -0.24837100 |
| C | 0.87794300 | -1.58871800 | 0.06146100 |
| C | -1.18994900 | 1.55757100 | 0.27914700 |
| O | 0.66867000 | -2.15297300 | 1.22377600 |
| O | -1.41812800 | 2.30450200 | 1.18065500 |
| P | -0.25464800 | -1.25729400 | -1.21744200 |
| P | -2.59337700 | 0.40450400 | -0.32650400 |
| C | -1.67432100 | -1.18497700 | -0.04015100 |
| O | -1.88354600 | -1.94513100 | 0.88866600 |
| H | -0.29017500 | -2.40019600 | 1.28367900 |
| H | 0.66922900 | 3.00291300 | -0.10748100 |
| H | -3.27769600 | 0.41920500 | 0.91501400 |
| H | 3.04654900 | -1.00001900 | 1.03029900 |

4_19

0 1

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|---|---|---|---|
| C | -0.72906200 | -1.32999900 | 0.78772600 |
| O | -0.91209200 | -0.89382500 | 1.88428400 |
| P | 0.94532000 | -2.06279500 | 0.33727600 |
| P | -2.15616400 | -1.23712900 | -0.55768700 |
| C | -1.76319700 | 0.54496200 | -0.53752300 |
| C | 2.01582000 | -0.57998800 | -0.23951600 |
| O | -2.33467300 | 1.28231000 | 0.37603500 |
| O | 2.78472300 | -0.80866300 | -1.12681500 |
| P | -0.29471900 | 0.84669200 | -1.43522000 |
| P | 2.06470700 | 1.13536600 | 0.59990700 |
| C | 0.40427800 | 1.81378400 | -0.02620600 |
| O | -0.17120500 | 2.65205500 | 0.63823100 |
| H | -1.79239900 | 2.09867200 | 0.51777800 |
| H | 1.44421300 | 0.74196600 | 1.81659400 |

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|---|---|---|---|
| H | -3.19384300 | -1.17310200 | 0.41355400 |
| H | 0.65381100 | -2.44710900 | -0.99284400 |

4_20

0 1

| | | | |
|---|---|---|---|
| C | 1.54358600 | 1.35203800 | -0.10834500 |
| O | 2.45511400 | 1.71304900 | -0.79826000 |
| P | 1.75925900 | -0.05264800 | 1.15142600 |
| H | 3.16321200 | -0.12556200 | 0.97185400 |
| P | 0.00424400 | 2.41596600 | -0.04454700 |
| H | 0.00499000 | 2.81176600 | -1.40179500 |
| C | -1.53873700 | 1.35721600 | -0.10840600 |
| C | 1.44294800 | -1.50279800 | -0.01785000 |
| O | -2.44894200 | 1.72088800 | -0.79863400 |
| O | 2.18239400 | -2.44359000 | -0.01729300 |
| P | -1.75887000 | -0.04631300 | 1.15191700 |
| H | -3.16317400 | -0.11430000 | 0.97326500 |
| P | -0.00272000 | -1.41474300 | -1.22274700 |
| H | -0.00534400 | -2.79919300 | -1.52026000 |
| C | -1.44852600 | -1.49746400 | -0.01754700 |
| O | -2.19156700 | -2.43542100 | -0.01717600 |

4_21

0 1

4_22

0 1

| | | | |
|---|---|---|---|
| C | -0.75436500 | -1.38949500 | 0.70259800 |
| O | -0.77791700 | -1.16254000 | 1.87228300 |
| P | 0.78636300 | -2.00415900 | -0.22076500 |
| P | -2.44854200 | -1.14635900 | -0.28400600 |
| C | -1.79187200 | 0.56180300 | -0.35075500 |
| C | 1.91823000 | -0.72876800 | -0.06132600 |
| O | -2.12145400 | 1.26029100 | 0.73363800 |
| O | 3.17537100 | -1.08415200 | -0.43081200 |
| P | -0.44839200 | 0.81740700 | -1.40703600 |
| P | 1.86387300 | 0.97752900 | 0.63879000 |
| C | 0.54512400 | 1.71461200 | -0.16983100 |
| O | 0.13445100 | 2.95853500 | 0.17762400 |
| H | -1.60766900 | 2.08169000 | 0.76091400 |
| H | -1.90396600 | -1.49604200 | -1.55327100 |
| H | 3.71908100 | -0.29539800 | -0.53092200 |
| H | 0.70669900 | 3.31748800 | 0.87256300 |

4_23

0 1

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|---|---|---|---|
| C | 0.05418500 | 1.75148100 | 0.53793200 |
| O | -0.37950700 | 2.72538000 | 1.35863300 |
| P | -1.07484000 | 1.59965500 | -0.90510500 |
| P | 1.62704400 | 1.11714400 | 0.78055900 |
| C | 1.78990000 | -0.10775900 | -0.56350000 |
| C | -1.75419000 | 0.06628500 | -0.61132700 |
| O | 2.82502400 | 0.21931300 | -1.35788900 |
| O | -2.67334100 | -0.34491300 | -1.51201400 |
| P | 0.98981200 | -1.60346600 | -0.81227500 |
| P | -1.63194700 | -0.96788600 | 0.90420900 |
| C | -0.12476500 | -1.72086100 | 0.63961400 |
| O | 0.23809600 | -2.64664500 | 1.55019900 |
| H | 1.13808500 | -2.93656700 | 1.36249100 |
| H | -2.98432800 | -1.22254500 | -1.26527400 |
| H | 0.29464000 | 2.92933900 | 2.02141900 |
| H | 3.02763300 | -0.51188500 | -1.95720100 |

4_24

0 1

| | | | |
|---|---|---|---|
| C | 2.51806600 | -0.56250600 | -0.03109400 |
| C | 0.03827900 | -1.30978500 | -0.00777800 |
| C | -1.91754900 | -0.11741500 | -0.01923500 |
| C | 0.52468200 | 1.55582300 | 0.28927200 |
| P | 2.12948000 | 1.22147800 | -0.67052500 |
| P | 1.22742400 | -1.23434100 | 1.19898900 |
| P | -1.31032700 | 1.44015600 | -0.29854700 |
| P | -3.75051400 | -0.24013200 | -0.10279300 |

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|---|---|---|---|
| H | -3.78226300 | -1.54751000 | -0.66952900 |
| H | -3.91008300 | -0.72335200 | 1.22705800 |
| O | -1.28957500 | -1.30522700 | 0.30614600 |
| O | 0.27824300 | -1.35147900 | -1.31660800 |
| O | 3.54566700 | -1.08314100 | -0.32306900 |
| O | 0.62103800 | 2.18155600 | 1.31267300 |
| H | -0.54198700 | -1.20100700 | -1.80519000 |
| H | 1.56954400 | 0.73406700 | -1.87933700 |

4_25

0 1

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|---|---|---|---|
| C | -2.20977200 | -0.40296900 | 0.02528600 |
| C | 0.14964400 | -1.74831200 | -0.03207200 |
| C | 1.68331000 | 0.20387900 | -0.11764700 |
| C | -0.34269400 | 1.99644600 | -0.18364100 |
| P | -1.37439400 | 0.88767100 | 1.04460200 |
| P | -1.63554200 | -1.95121400 | -0.46414200 |
| P | 1.55102200 | 1.88833400 | -0.06354300 |
| P | 3.35408600 | -0.55525000 | 0.04255400 |
| H | 3.05570000 | -1.37054500 | 1.16649600 |
| H | 3.14714200 | -1.60798100 | -0.88944400 |
| O | 0.52409300 | -0.46567400 | -0.40560100 |
| O | 0.88315900 | -2.56959700 | 0.41729900 |
| O | -3.51208200 | -0.11370200 | -0.11860700 |
| O | -0.87710500 | 2.86357600 | -0.80289600 |
| H | -3.97267300 | -0.84558100 | -0.55061500 |
| H | -2.48519700 | 1.76989400 | 1.00838000 |

4_26

0 1

| | | | |
|---|---|---|---|
| C | -2.20977200 | -0.40296900 | 0.02528600 |
| C | 0.14964400 | -1.74831200 | -0.03207200 |
| C | 1.68331000 | 0.20387900 | -0.11764700 |
| C | -0.34269400 | 1.99644600 | -0.18364100 |
| P | -1.37439400 | 0.88767100 | 1.04460200 |
| P | -1.63554200 | -1.95121400 | -0.46414200 |
| P | 1.55102200 | 1.88833400 | -0.06354300 |
| P | 3.35408600 | -0.55525000 | 0.04255400 |
| H | 3.05570000 | -1.37054500 | 1.16649600 |
| H | 3.14714200 | -1.60798100 | -0.88944400 |
| O | 0.52409300 | -0.46567400 | -0.40560100 |
| O | 0.88315900 | -2.56959700 | 0.41729900 |
| O | -3.51208200 | -0.11370200 | -0.11860700 |
| O | -0.87710500 | 2.86357600 | -0.80289600 |
| H | -3.97267300 | -0.84558100 | -0.55061500 |
| H | -2.48519700 | 1.76989400 | 1.00838000 |

4_27

0 1

| | | | |
|---|---|---|---|
| C | -2.19354600 | 0.51709900 | -0.14676100 |
| C | 1.53593100 | -0.40432500 | -0.08575400 |
| C | -0.73884900 | -1.88978800 | -0.09632600 |
| H | -0.68431000 | -0.22289300 | 1.74600600 |
| C | 0.24052200 | 1.65003200 | -0.09055900 |
| P | -1.37030100 | 2.21434500 | 0.05381900 |
| P | -1.77523800 | -0.86059200 | 1.10831100 |
| P | 1.14507600 | -2.01725700 | 0.22510300 |
| P | 3.27035900 | 0.20859300 | -0.22085800 |
| H | 3.36658800 | 0.83193700 | 1.05368700 |
| H | 3.82732000 | -1.02337300 | 0.21819900 |
| O | 0.50180500 | 0.41466000 | -0.52605600 |
| O | 1.34352900 | 2.36195900 | 0.13924300 |
| H | 1.10536500 | 3.21089500 | 0.52817800 |
| O | -1.25295900 | -2.50211500 | -0.98314800 |
| O | -3.05834500 | 0.32412000 | -0.94570000 |

4_28

0 1

| | | | |
|---|---|---|---|
| C | 2.51808100 | -0.56256500 | -0.03134200 |
| C | 0.03815400 | -1.30958100 | -0.00778500 |
| C | -1.91767500 | -0.11731500 | -0.01923600 |
| C | 0.52483700 | 1.55567200 | 0.28945100 |

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|---|---|---|---|
| P | 2.12964800 | 1.22139500 | -0.67033000 |
| H | 1.56976700 | 0.73437200 | -1.87936100 |
| P | 1.22749000 | -1.23461600 | 1.19879900 |
| P | -1.31022000 | 1.44027400 | -0.29855100 |
| P | -3.75065700 | -0.24020500 | -0.10299700 |
| H | -3.78197200 | -1.54808900 | -0.66858000 |
| H | -3.91052200 | -0.72234700 | 1.22723500 |
| O | -1.28961400 | -1.30495200 | 0.30648300 |
| O | 0.27784000 | -1.35094700 | -1.31667700 |
| O | 3.54560800 | -1.08322100 | -0.32344900 |
| O | 0.62126100 | 2.18107600 | 1.31307500 |
| H | -0.54233200 | -1.19955900 | -1.80510300 |

4_29

0 1

| | | | |
|---|---|---|---|
| C | -2.24365000 | -0.35689200 | -0.00970100 |
| C | 0.13326000 | -1.60892600 | 0.09579600 |
| C | 1.72558900 | 0.19008800 | -0.17051200 |
| C | -0.40295800 | 1.83295600 | -0.13031500 |
| P | -1.53644900 | 0.92206500 | 1.11120600 |
| P | -1.62466000 | -1.88905600 | -0.45789700 |
| P | 1.48746700 | 1.81573200 | 0.19617600 |
| P | 3.43252400 | -0.49942800 | -0.16086100 |
| H | 3.11239700 | -1.67674300 | 0.56694200 |
| H | 3.31758900 | -1.14102500 | -1.42734200 |
| O | 0.63758000 | -0.54443400 | -0.61705000 |
| O | 0.74360300 | -2.23659600 | 0.90400900 |
| O | -3.48249000 | 0.02332700 | -0.36549900 |
| O | -0.86401300 | 2.46951600 | -1.02683000 |
| H | -0.52578500 | 0.12159000 | 1.69105300 |
| H | 0.13946607 | -2.57602756 | 1.56839201 |

4_30

0 1

| | | | |
|---|---|---|---|
| C | 2.26967400 | -0.17624800 | -0.29311700 |
| C | -0.02564800 | -1.46943700 | 0.18914700 |
| C | -1.82157100 | 0.08593500 | 0.04135400 |
| C | 0.27773500 | 1.70268400 | 0.40112700 |
| P | 1.72214100 | 1.36100000 | -0.77980100 |
| P | 1.66858400 | -1.38353900 | 0.99834400 |
| P | -1.47462900 | 1.66497000 | -0.40997200 |
| P | -3.44992400 | -0.67436800 | -0.32542500 |
| H | -2.93250500 | -1.92212400 | -0.76928300 |
| H | -3.68090600 | -1.13749200 | 1.00218100 |
| O | -0.86756900 | -0.60438100 | 0.80413800 |
| O | -0.26789700 | -2.10644100 | -0.78663300 |
| O | 3.29094900 | -0.67161800 | -1.02241600 |
| O | 0.41003900 | 2.08867600 | 1.52485700 |
| H | 3.55570400 | -1.52869400 | -0.67003100 |
| H | 1.33980900 | -0.44012400 | 1.99930800 |

4_31

0 1

| | | | |
|---|---|---|---|
| C | -2.24365000 | -0.35689200 | -0.00970100 |
| C | 0.13326000 | -1.60892600 | 0.09579600 |
| C | 1.72558900 | 0.19008800 | -0.17051200 |
| C | -0.40295800 | 1.83295600 | -0.13031500 |
| P | -1.53644900 | 0.92206500 | 1.11120600 |
| P | -1.62466000 | -1.88905600 | -0.45789700 |
| P | 1.48746700 | 1.81573200 | 0.19617600 |
| P | 3.43252400 | -0.49942800 | -0.16086100 |
| H | 3.11239700 | -1.67674300 | 0.56694200 |
| H | 3.31758900 | -1.14102500 | -1.42734200 |
| O | 0.63758000 | -0.54443400 | -0.61705000 |
| O | 0.74360300 | -2.23659600 | 0.90400900 |
| O | -3.48249000 | 0.02332700 | -0.36549900 |
| O | -0.86401300 | 2.46951600 | -1.02683000 |
| H | -3.83829500 | -0.58136700 | -1.02867400 |
| H | -0.52578500 | 0.12159000 | 1.69105300 |

4_32

0 1

| | | | |
|---|---|---|---|
| C | -2.52404000 | -0.59012000 | -0.01914000 |
| C | -0.01446100 | -1.29735500 | 0.14310000 |
| C | 1.94226200 | -0.12099400 | 0.01333500 |
| C | -0.55478900 | 1.55260400 | -0.27768700 |
| P | -2.02193200 | 1.05306100 | 0.83620600 |
| P | -1.18413200 | -1.41024700 | -1.07940400 |
| P | 1.32792600 | 1.45411900 | 0.13751100 |
| P | 3.77925100 | -0.21864600 | 0.01448000 |
| H | 3.85189200 | -1.43062400 | 0.76049400 |
| H | 3.87470800 | -0.88797900 | -1.23883500 |
| O | 1.31637000 | -1.34143800 | -0.14189500 |
| O | -0.28326700 | -1.13785000 | 1.43784100 |
| O | -3.66277300 | -0.94114300 | 0.00305400 |
| O | -0.73598200 | 2.29128000 | -1.20803400 |
| H | 0.51791000 | -0.88894700 | 1.91939300 |
| H | -2.92982000 | 1.80163800 | 0.04167500 |

4_33

0 1

| | | | |
|---|---|---|---|
| C | 2.04855500 | -0.33354800 | -0.15033200 |
| C | -0.01192100 | -1.78876500 | 0.14882800 |
| C | -1.68832800 | -0.02027600 | -0.18202800 |
| C | 0.65110400 | 1.92425200 | 0.10187800 |
| P | 1.92205600 | 1.11133600 | -1.02667000 |
| P | 0.99271600 | -0.71882400 | 1.32487300 |
| P | -1.23279500 | 1.57930500 | 0.14155500 |
| P | -3.53964200 | -0.16524300 | -0.19995700 |
| H | -3.58351900 | -0.88379700 | -1.42884600 |
| H | -3.58073300 | -1.35408000 | 0.58526300 |
| O | -1.08114500 | -1.20678800 | -0.47212200 |
| O | 0.28560000 | -2.90522300 | -0.14605300 |
| O | 2.93142000 | -1.26059800 | -0.55449200 |
| O | 0.94047800 | 2.92586600 | 0.69967400 |
| H | 1.75046500 | -1.84625200 | 1.74589700 |
| H | 2.67148200 | -2.13052800 | -0.22544400 |

4_34

0 1

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|---|---|---|---|
| C | -2.30480000 | 0.13447500 | -0.06948900 |
| O | -3.64787600 | 0.14824400 | -0.24317700 |
| P | -1.45356100 | 1.58698500 | -0.33663200 |
| P | -1.84066000 | -1.63664300 | 0.25939600 |
| C | -0.07964500 | -1.38189700 | -0.16904500 |
| C | 0.32641800 | 1.54282900 | 0.38518300 |
| O | 0.01883300 | -1.26554800 | -1.49424700 |
| O | 0.46071800 | 2.13100100 | 1.41998700 |
| P | 1.10119800 | -1.15011700 | 1.03666500 |
| P | 1.95028200 | 1.26040800 | -0.64578200 |
| C | 2.32748700 | -0.28697500 | -0.03845900 |
| O | 3.49724400 | -0.92203500 | -0.21930400 |
| H | 0.88966100 | -0.89247800 | -1.71256100 |
| H | -1.67498700 | -1.52489400 | 1.66711400 |
| H | 4.12669300 | -0.33655100 | -0.65976700 |
| H | -3.94836400 | 1.06054900 | -0.35469900 |

4_35

0 1

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|---|---|---|---|
| C | 0.81731600 | 1.75439200 | 0.49774200 |
| C | -0.51487000 | -0.88972800 | 0.10688700 |
| C | -1.94911900 | 1.08216800 | -0.41511900 |
| C | 1.77179700 | -0.55688500 | -0.65619600 |
| P | 2.38545600 | 0.86271400 | 0.14432200 |
| P | -0.70779900 | 0.77349100 | 0.95591500 |
| P | -2.04403500 | -0.74257100 | -0.99647800 |
| P | -0.44910300 | -2.44259400 | 1.16780900 |
| H | 0.71721800 | -2.05621800 | 1.89050500 |
| H | -1.33278200 | -1.94468800 | 2.16592800 |
| O | 0.56389300 | -1.04683900 | -0.84786400 |
| O | 2.62449800 | -1.34489500 | -1.30000500 |
| O | -2.51390900 | 2.04966200 | -0.79885200 |
| O | 0.77583100 | 2.95426600 | 0.57006600 |

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|---|---|---|---|
| H | -2.99301500 | -1.08850100 | 0.00805900 |
| H | 3.48755600 | -0.91344900 | -1.32462500 |

4_36

0 1

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|---|---|---|---|
| C | 0.63754700 | -0.84910300 | -0.08017900 |
| C | -1.77337700 | -1.02413200 | 0.20438100 |
| C | -0.97923800 | 1.54261700 | -0.57256600 |
| C | 1.52265900 | 1.38644300 | 0.46117000 |
| P | 0.65236200 | 0.75177500 | -1.10621100 |
| P | -2.40627800 | 0.59587000 | 0.06589100 |
| P | 1.33968700 | -0.16926600 | 1.55140300 |
| O | -1.06925900 | 2.73299200 | -0.72848200 |
| O | 2.01844900 | 2.43568500 | 0.69226700 |
| O | -0.58856900 | -1.57320600 | 0.06889800 |
| H | 0.08548300 | 0.33783200 | 2.01189100 |
| P | 1.74472500 | -2.09591400 | -0.94716500 |
| H | 2.89364200 | -1.25615100 | -0.92491100 |
| H | 2.14263200 | -2.82011800 | 0.21316500 |
| O | -2.61269800 | -1.99516400 | 0.54178100 |
| H | -3.50813500 | -1.63592700 | 0.56852900 |

4_37

0 1

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|---|---|---|---|
| C | 1.39369200 | 1.19527700 | 0.51156300 |
| C | -0.78652800 | -0.69637600 | 0.14647300 |
| C | -1.43793100 | 1.60287900 | -0.53278900 |
| C | 1.38003300 | -1.23205200 | -0.89272000 |
| P | 2.48217400 | 0.00308600 | -0.05000600 |
| P | -0.35471600 | 0.96804800 | 0.88190600 |
| P | -2.32681500 | -0.08419300 | -0.77492200 |
| P | -1.08119200 | -2.14673000 | 1.30654600 |
| H | 0.23555200 | -2.14654400 | 1.85218400 |
| H | -1.61182800 | -1.36006100 | 2.36842800 |
| O | 0.01870700 | -1.16893100 | -0.93422800 |
| O | 1.93219900 | -2.06378700 | -1.54936900 |
| O | -1.55489400 | 2.64478000 | -1.07736400 |
| O | 1.81205700 | 2.40344700 | 0.91751100 |
| H | 2.74408300 | 2.52047700 | 0.68901900 |
| H | -3.11972500 | 0.14051800 | 0.38993600 |

4_38

0 1

| | | | |
|---|---|---|---|
| C | 1.33456100 | 1.08253700 | -0.53934500 |
| C | -0.80934800 | -0.71581300 | -0.08143000 |
| C | 1.46215500 | -1.61763000 | 0.25013700 |
| P | 2.42189700 | -0.03115200 | 0.16045100 |
| P | -0.38329800 | 0.84483000 | -1.08679100 |
| P | -2.25100800 | -1.54326800 | -0.96529200 |
| P | -1.11439700 | 0.13854900 | 1.58359600 |
| O | 0.13637100 | -1.76842300 | -0.01507000 |
| O | 2.09342000 | -2.59247900 | 0.53305300 |
| O | 1.70116000 | 2.34650000 | -0.80195700 |
| H | -2.83320300 | -2.14341600 | 0.18754700 |
| H | 2.61633000 | 2.49199000 | -0.52698500 |
| H | -3.10610100 | -0.40499200 | -0.90854100 |
| C | -1.08382300 | 1.67748300 | 0.50600000 |
| O | -1.38917200 | 2.80306800 | 0.70698400 |
| H | -2.53044800 | 0.05324400 | 1.67226900 |

4_39

0 1

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|---|---|---|---|
| C | -1.46366100 | 1.09375800 | -0.54050500 |
| C | 0.82693200 | -0.63876900 | -0.17204300 |
| C | 1.33346800 | 1.65479100 | 0.55382500 |
| C | -1.26297200 | -1.25888900 | 0.95925300 |
| P | -2.45798500 | -0.16363800 | 0.05306100 |
| P | 0.29641400 | 1.00522000 | -0.90471300 |
| P | 2.43753800 | 0.10490100 | 0.51729800 |
| P | 1.12751200 | -2.10298100 | -1.31015600 |
| H | -0.18304600 | -2.12289300 | -1.87211200 |
| H | 1.67133800 | -1.33027800 | -2.37439000 |

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|---|---|---|---|
| O | 0.09128500 | -1.10507900 | 0.95575500 |
| O | -1.74360700 | -2.07455700 | 1.68844100 |
| O | 1.32349200 | 2.63649700 | 1.21105700 |
| O | -1.97680800 | 2.25343200 | -0.98028000 |
| H | 2.21692300 | -0.28887700 | 1.86315700 |
| H | -2.91491500 | 2.30181000 | -0.75197800 |

4_40

0 1

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|---|---|---|---|
| C | -1.33302500 | 1.08290800 | -0.48967600 |
| C | 0.80259200 | -0.72871000 | -0.05439500 |
| C | 1.06128600 | 1.68598700 | 0.38859200 |
| C | -1.47475000 | -1.62692700 | 0.19658600 |
| P | -2.41953900 | -0.02183800 | 0.22092400 |
| P | 0.34768000 | 0.75497400 | -1.13261800 |
| P | 1.11367600 | 0.21948300 | 1.56621500 |
| P | 2.36161900 | -1.59098400 | -0.65451400 |
| H | 1.89952800 | -1.84660600 | -1.97673500 |
| H | 3.04094100 | -0.39307100 | -1.02280100 |
| O | -0.12574500 | -1.78584400 | 0.02137800 |
| O | -2.12343300 | -2.61499200 | 0.37065100 |
| O | 1.29732400 | 2.84268500 | 0.51912000 |
| O | -1.77360100 | 2.34202100 | -0.65456800 |
| H | 2.53492600 | 0.12847100 | 1.61537900 |
| H | -1.05990900 | 2.93617800 | -0.91526600 |

4_41

0 1

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|---|---|---|---|
| C | 0.60753700 | -0.86702400 | -0.07824700 |
| C | -1.80743400 | -0.97148200 | 0.19557000 |
| C | -0.94146000 | 1.57696400 | -0.56192400 |
| C | 1.57132300 | 1.33531500 | 0.45948300 |
| P | 0.66643800 | 0.73743200 | -1.10294400 |
| P | -2.38487900 | 0.67270300 | 0.09492700 |
| P | 1.14219200 | -0.12168100 | 1.57105800 |
| O | -0.99566400 | 2.76925000 | -0.72180600 |
| O | 2.20047900 | 2.32056200 | 0.65666400 |
| O | -0.64763800 | -1.56104700 | 0.02502700 |
| P | 1.68265200 | -2.14975200 | -0.93211800 |
| H | 2.85802800 | -1.34960200 | -0.90928600 |
| H | 2.04899800 | -2.88353900 | 0.23348600 |
| O | -2.67890100 | -1.91634300 | 0.52423400 |
| H | -3.55988600 | -1.52425400 | 0.56676400 |
| H | 2.45081500 | -0.66516100 | 1.68295700 |

4_42

0 1

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|---|---|---|---|
| C | 0.64709500 | -0.88281600 | -0.08161500 |
| C | -1.79535700 | -0.97473200 | 0.28737600 |
| C | -1.01195000 | 1.51153000 | -0.62977500 |
| C | 1.43126000 | 1.25426300 | 0.51610700 |
| P | 0.67191300 | 0.74246100 | -1.06320500 |
| P | -2.44422200 | 0.62448000 | 0.07182700 |
| P | 1.40067100 | -0.15622000 | 1.48500000 |
| O | -1.09316100 | 2.69140500 | -0.86553100 |
| O | 1.92856800 | 2.46747100 | 0.68390400 |
| H | 2.30103400 | 2.56149200 | 1.56882200 |
| O | -0.61706600 | -1.55165500 | 0.12135600 |
| P | 1.63880400 | -2.20082900 | -0.97871600 |
| H | 2.81635000 | -1.41235400 | -1.08375000 |
| H | 2.09723100 | -2.89329900 | 0.18011600 |
| O | -2.67315200 | -1.87491700 | 0.71184100 |
| H | -2.20991200 | -2.71213100 | 0.84608900 |

4_43

0 1

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|---|---|---|---|
| C | -0.79978600 | -0.92210300 | 0.57516200 |
| C | 2.04839800 | -0.79024500 | -0.55136000 |
| C | 0.85251300 | 1.62247600 | 0.27984900 |
| C | -1.93074600 | 0.99358900 | -0.55622800 |
| P | -0.76393500 | 0.92894400 | 0.89643100 |
| P | 2.36587600 | 0.57833200 | 0.68762900 |

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|---|---|---|---|
| P | -2.40563500 | -0.85599700 | -0.49753500 |
| O | 0.92164600 | 2.71801800 | -0.19716500 |
| O | -2.27656600 | 1.86782800 | -1.27780900 |
| O | 2.86716900 | -1.10067800 | -1.37010200 |
| O | -0.91889000 | -1.56075300 | 1.82210800 |
| H | -0.89211700 | -2.51334900 | 1.68439000 |
| P | 0.47562100 | -1.82125000 | -0.46631900 |
| H | -3.26944600 | -0.64186900 | 0.61474700 |
| H | 3.25949100 | 1.29179100 | -0.14895900 |
| H | 0.05401800 | -1.40464400 | -1.75405300 |

4_44

0 1

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|---|---|---|---|
| C | 0.61989200 | -1.15677300 | -0.44183600 |
| C | -2.01104600 | -0.44163500 | 0.57018900 |
| C | -0.37810700 | 1.70371800 | -0.43145600 |
| C | 2.02888900 | 0.69504800 | 0.47617400 |
| P | 0.97045600 | 0.57871200 | -1.10104900 |
| P | -2.18236200 | 1.18371100 | -0.34313800 |
| P | 1.41691500 | -0.89733800 | 1.26747000 |
| O | -0.08135000 | 2.83997800 | -0.18630700 |
| O | 2.79656500 | 1.52092200 | 0.83671000 |
| O | -2.51124700 | -0.63111900 | 1.64079100 |
| O | 1.33947100 | -1.99106500 | -1.32981100 |
| H | 1.30272300 | -2.89577500 | -1.00115500 |
| P | -1.12626800 | -1.84602000 | -0.35224500 |
| H | -1.50413400 | -1.40906700 | -1.65402800 |
| H | 2.58716000 | -1.68447300 | 1.07551500 |
| H | -2.47214900 | 1.99147600 | 0.78459700 |

4_45

0 1

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|---|---|---|---|
| C | 0.43081100 | -1.24020500 | -0.23248700 |
| C | -2.32005200 | -0.10428900 | 0.11135800 |
| C | -0.11300400 | 1.70262000 | -0.41384000 |
| C | 2.22645800 | 0.41793200 | 0.18955700 |
| P | 0.90008900 | 0.31865600 | -1.19400400 |
| P | -1.48803100 | 1.40805600 | 0.82711400 |
| P | 1.40978100 | -0.82561300 | 1.33943100 |
| O | 0.20068300 | 2.82730200 | -0.68933000 |
| O | 3.21200300 | 1.06682500 | 0.27642900 |
| O | -3.48942400 | -0.10834900 | -0.16022700 |
| O | 1.01310700 | -2.26672500 | -1.01957600 |
| H | 1.00019500 | -3.08901200 | -0.51900100 |
| P | -1.36606800 | -1.71977700 | 0.03492800 |
| H | -1.66758900 | -1.92614600 | -1.33529000 |
| H | 2.37844100 | -1.86831500 | 1.28266300 |
| H | -2.38381800 | 2.35486400 | 0.27370900 |

4_46

0 1

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|---|---|---|---|
| C | 0.43246400 | -1.26778100 | -0.32682300 |
| C | -2.23159000 | -0.09864300 | 0.28965300 |
| C | -0.05337500 | 1.68350800 | -0.65624700 |
| C | 2.07765600 | 0.40104800 | 0.51711100 |
| P | 1.13185900 | 0.28891000 | -1.14771900 |
| P | -1.34701000 | 1.50446000 | 0.67923600 |
| P | 1.11799100 | -0.94580600 | 1.42229300 |
| O | 0.17890500 | 2.76765100 | -1.11595700 |
| O | 2.97185100 | 1.10122600 | 0.85169200 |
| O | -3.38029200 | -0.21777000 | 0.62117000 |
| O | 1.10901300 | -2.30628500 | -1.01856700 |
| H | 0.92482900 | -3.14416800 | -0.58378800 |
| P | -1.40272500 | -1.50909600 | -0.62012500 |
| H | 2.15487800 | -1.92217300 | 1.40847000 |
| H | -1.65906700 | -2.44716800 | 0.41774800 |
| H | -2.30911500 | 2.36911300 | 0.10341600 |

4_47

0 1

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|---|---|---|---|
| C | 0.44857300 | -1.24938500 | -0.26355600 |
| C | -2.30281300 | -0.11688500 | 0.13606100 |

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|---|---|---|---|
| C | -0.13427000 | 1.70372500 | -0.44125400 |
| C | 2.17281600 | 0.48136000 | 0.21638000 |
| P | 0.89904800 | 0.32723900 | -1.20517500 |
| P | -1.47882000 | 1.41002400 | 0.82916000 |
| P | 1.63615800 | -1.05892900 | 1.20210100 |
| O | 0.16218400 | 2.82636800 | -0.74169500 |
| O | 3.00481700 | 1.29347800 | 0.42755700 |
| O | -3.47044800 | -0.13385400 | -0.14195600 |
| O | 0.95725700 | -2.26981400 | -1.11770800 |
| H | 1.07840100 | -3.07579600 | -0.60402700 |
| P | -1.33120400 | -1.72011400 | 0.12083200 |
| H | -2.39580300 | 2.34911700 | 0.29888800 |
| H | -1.68235300 | -2.02571300 | -1.21775000 |
| H | 0.78570800 | -0.26321500 | 2.02376400 |

4_48

0 1

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|---|---|---|---|
| C | -1.53321900 | -0.98437400 | 0.79078900 |
| O | -1.88639100 | -0.80207300 | 1.90833700 |
| P | -0.08054100 | -2.13362800 | 0.34841500 |
| P | -2.45357300 | -0.01051900 | -0.64467100 |
| C | -1.05905400 | 1.16775500 | -0.62518900 |
| C | 1.11732700 | -0.91347000 | -0.41087900 |
| O | -1.26279100 | 2.31490100 | -0.05849000 |
| O | 1.83236100 | -1.70669300 | -1.32011200 |
| P | 0.57342100 | 0.75884900 | -1.18803400 |
| P | 2.14799700 | -0.02994900 | 0.92620300 |
| C | 1.34104700 | 1.44506700 | 0.41507900 |
| O | 1.08701800 | 2.56589300 | 0.84234500 |
| H | -0.37081400 | 2.69303700 | 0.28378400 |
| H | -0.65665300 | -2.55579200 | -0.88555200 |
| H | -1.88412100 | -0.77962400 | -1.69378200 |
| H | 2.74386200 | -1.39502400 | -1.32857500 |

4_49

0 1

| | | | |
|---|---|---|---|
| C | -0.39165500 | -1.26116100 | 0.33157500 |
| C | 2.27560700 | -0.35135000 | -0.14253600 |
| C | 0.39414700 | 1.65282600 | 0.12815100 |
| C | -2.14321200 | 0.30028600 | -0.11687800 |
| P | -0.71715700 | 0.46541300 | 0.98393000 |
| P | 2.07678400 | 1.51485800 | -0.13173100 |
| P | -2.13536600 | -1.36109200 | -0.47435500 |
| O | -0.15519600 | 2.86989300 | -0.04533800 |
| O | -2.93102700 | 1.34132800 | -0.40557400 |
| O | 3.32372300 | -0.86216700 | 0.14138400 |
| O | -0.15383800 | -2.09288400 | 1.42844100 |
| H | 0.07731600 | -2.96911900 | 1.10837700 |
| P | 0.89778500 | -1.31514300 | -1.02537300 |
| H | -1.11028100 | 2.84791700 | 0.09304700 |
| H | -3.65742700 | 1.07401900 | -0.98030400 |
| H | 1.38109100 | -2.60633500 | -0.66134200 |

4_50

0 1

| | | | |
|---|---|---|---|
| C | -0.29320700 | -1.32489700 | 0.27557300 |
| C | 2.17112900 | 0.01759400 | -0.13569700 |
| C | -0.07979000 | 1.60400100 | 0.35745800 |
| C | -2.16490400 | 0.21913100 | -0.28755000 |
| P | -0.92757100 | 0.20777600 | 1.16586500 |
| P | 1.47692600 | 1.69191600 | -0.33405100 |
| P | -1.35665600 | -1.16434000 | -1.27961100 |
| O | -0.78553500 | 2.74858900 | 0.36397100 |
| O | -3.03404900 | 0.99980500 | -0.52152200 |
| O | 3.51707000 | 0.03784900 | -0.31198800 |
| H | 3.82962700 | 0.94951500 | -0.34409500 |
| O | -0.76918200 | -2.45323200 | 0.99220900 |
| H | -0.13091900 | -2.66281600 | 1.68463600 |
| P | 1.54916300 | -1.56543800 | 0.03383900 |
| H | -1.73812000 | 2.56623500 | 0.36958000 |
| H | -2.31431900 | -2.16070900 | -0.94080900 |

4_51
0 1
C 0.38042400 -1.30122300 -0.43732900
C -2.11491600 -0.05051700 0.38250200
C -0.05078500 1.64918600 -0.50115200
C 1.97733500 0.28103900 0.65733700
P 1.09228700 0.32583200 -1.04681900
P -1.63076200 1.72900900 0.15228600
P 1.18145400 -1.32923700 1.28699900
O 0.53781900 2.85600100 -0.64283300
O 2.73747400 1.04252100 1.14708500
O -3.04013400 -0.26484300 1.12775700
O 1.05594300 -2.24018900 -1.26538900
H 0.92225000 -3.12321600 -0.90676400
P -1.46352300 -1.47564300 -0.65302800
H 1.39611800 2.78203700 -1.07801500
H -1.67445700 -2.43820400 0.37327600
H 0.18308300 -0.58887300 1.97882800
4_52
0 1
C -1.29111500 0.41764200 -0.68579300
C 1.06915000 1.53835700 0.62360500
C 1.48638600 -0.90152200 -0.60714000
C -0.94279500 -1.34595100 0.88760700
P -0.33847800 -1.19419500 -0.81520100
P 2.40206200 0.31882600 0.14519700
P -2.07475600 -0.07788500 0.98141300
O 2.18627600 -1.95600900 -1.07540600
O -0.55277800 -2.31662900 1.70348400
O 1.23080400 2.20979900 1.60920600
O -2.17457300 0.46172900 -1.78349200
H -2.78437800 1.19521800 -1.66122700
P -0.26729400 1.98735000 -0.62148700
H 1.58662800 -2.56871100 -1.52094200
H -1.00907500 -2.24771700 2.55007800
H -1.06377900 2.66749200 0.34327100
4_53
0 1
C 0.28671400 -1.32129900 -0.29481200
C -2.16330900 0.03324800 0.14734000
C 0.10464800 1.58733900 -0.38212500
C 2.14907900 0.19625600 0.32801300
P 0.96724100 0.18584000 -1.17348500
P -1.45319100 1.70442700 0.29707100
P 1.41140300 -1.29929000 1.23953700
O 0.81806300 2.72767800 -0.41106500
O 2.96378700 1.00984800 0.62955100
O -3.50450500 0.06209500 0.36621700
H -3.81880500 0.97339100 0.35118000
O 0.74110600 -2.36920200 -1.14725500
H 0.43753600 -3.21232600 -0.79343400
P -1.55468400 -1.54489200 -0.06544800
H 1.76841400 2.53944000 -0.35292700
H 0.64093800 -0.40838400 2.03996900
4_54
0 1
C -0.32369000 -1.16699600 0.43122900
C 1.75814800 0.04517000 -0.00480900
C -0.47732800 1.72225700 0.27557900
C -2.38034800 -0.10684100 -0.38197400
P -1.32217100 0.27712100 1.15297100
P 1.30298500 1.67894100 -0.24003600
P -1.14679000 -1.20940800 -1.29153100
O -1.11452600 2.73101200 0.12327100
O -3.46358500 0.26772000 -0.68143800
O 1.09959600 -1.05896700 0.34997000
H -1.84079400 -2.44155900 -1.12863900
O -0.57517100 -2.24043400 1.25177200

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|---|---|---|---|
| H | -0.19970300 | -3.03541600 | 0.85801300 |
| P | 3.54363600 | -0.39395200 | -0.14497300 |
| H | 3.41061800 | -1.16637400 | -1.33392200 |
| H | 3.93376800 | 0.79661900 | -0.81065300 |

4_55
0 1

| | | | |
|---|---|---|---|
| C | -0.31881200 | -1.17972300 | 0.44471400 |
| C | 1.74766700 | 0.06104000 | -0.01726500 |
| C | -0.50022100 | 1.71682000 | 0.29647300 |
| C | -2.36009300 | -0.11106000 | -0.40384500 |
| P | -1.33453600 | 0.25721300 | 1.15440200 |
| P | 1.28066700 | 1.69642000 | -0.22034200 |
| P | -1.23442200 | -1.42851800 | -1.20999100 |
| O | -1.14540400 | 2.72186500 | 0.15670600 |
| O | -3.37437100 | 0.36447400 | -0.78365700 |
| O | 1.09668100 | -1.05552800 | 0.30931400 |
| O | -0.53772900 | -2.23464500 | 1.30120300 |
| H | -0.25204000 | -3.05297600 | 0.87946700 |
| P | 3.53728600 | -0.36186000 | -0.16300400 |
| H | 3.41172700 | -1.12596200 | -1.35817500 |
| H | 3.91585800 | 0.83740700 | -0.81999800 |
| H | -0.53512700 | -0.39911100 | -1.90624500 |

4_56
0 1

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|---|---|---|---|
| C | 2.40566700 | -0.10710400 | -0.35716800 |
| C | -1.77028700 | 0.03378200 | 0.03545800 |
| C | 0.45070700 | 1.74713700 | 0.22806100 |
| C | 0.33634300 | -1.15769700 | 0.41778600 |
| P | 1.18442400 | -1.21095900 | -1.27054500 |
| P | 1.29622300 | 0.32513200 | 1.13350100 |
| P | -1.36556600 | 1.68784000 | -0.14186900 |
| P | -3.48947100 | -0.48048300 | -0.39958500 |
| H | -3.81809600 | -0.96930100 | 0.89647300 |
| H | -4.08239400 | 0.79422800 | -0.20412100 |
| O | -1.08906800 | -1.07227600 | 0.34330900 |
| O | 0.61262400 | -2.31057100 | 1.11553100 |
| H | 0.28404500 | -2.21390100 | 2.01692000 |
| O | 1.08101900 | 2.74495100 | -0.00072700 |
| O | 3.50088900 | 0.25339300 | -0.62859900 |
| H | 1.85401400 | -2.45466500 | -1.11271900 |

4_57
0 1

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|---|---|---|---|
| C | 0.32769300 | -1.35454000 | -0.32511600 |
| C | -2.24390600 | 0.07662000 | 0.27042600 |
| C | 0.01703600 | 1.60736700 | -0.43322200 |
| C | 2.06938400 | 0.25615100 | 0.45970700 |
| P | 0.99503800 | 0.21542100 | -1.11767500 |
| P | -1.57009700 | 1.79938100 | 0.17733400 |
| P | 1.17864900 | -1.13085500 | 1.37255300 |
| O | 0.72290100 | 2.75481100 | -0.49915800 |
| O | 2.93303000 | 1.01527700 | 0.76243700 |
| O | -3.33172200 | -0.03516300 | 0.78285100 |
| O | 0.93745100 | -2.35878300 | -1.12035100 |
| H | 0.61973800 | -3.22077500 | -0.83607900 |
| P | -1.52967900 | -1.52339400 | -0.42185900 |
| H | 1.67565900 | 2.59068300 | -0.53809300 |
| H | -1.73142900 | -2.21132200 | 0.80420700 |
| H | 2.21285600 | -2.08960000 | 1.17767500 |

4_58
0 1

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|---|---|---|---|
| C | -0.31175000 | 1.84316300 | 0.14189200 |
| C | -0.33419000 | -1.06360400 | 0.45024400 |
| C | -2.44975200 | -0.04820400 | -0.34382300 |
| C | 1.72582700 | 0.03469500 | -0.21935800 |
| P | 1.54737500 | 1.69990800 | 0.08521100 |
| P | -1.26167500 | 0.49069800 | 1.01166000 |
| P | -1.76778500 | -1.80666300 | -0.57218700 |
| O | 0.78657000 | -0.91948600 | -0.42595800 |

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|---|---|---|---|
| O | -3.33504000 | 0.52015800 | -0.89024400 |
| O | -0.87161600 | 2.82748900 | -0.25668900 |
| H | -1.21989900 | -1.50544600 | -1.84865400 |
| O | 0.04441000 | -1.76340400 | 1.57498400 |
| H | 0.36659700 | -2.63245300 | 1.31183600 |
| P | 3.39365700 | -0.72806600 | -0.34781100 |
| H | 3.28889700 | -1.08559000 | -1.72141800 |
| H | 4.11542600 | 0.47097600 | -0.58533400 |

4_59

0 1

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|---|---|---|---|
| C | -0.48914200 | -1.26212400 | 0.29161800 |
| C | 2.28005100 | -0.33574900 | -0.09723900 |
| C | 0.37134100 | 1.63172500 | 0.16325400 |
| C | -2.12146800 | 0.57740900 | -0.09765700 |
| P | -0.67578200 | 0.44175000 | 1.08542600 |
| P | 2.01338700 | 1.50774200 | -0.27914700 |
| P | -2.18076000 | -1.22563900 | -0.61706500 |
| O | -0.21200900 | 2.83564600 | 0.05567100 |
| O | -2.70151700 | 1.55759900 | -0.46982500 |
| O | 3.35928900 | -0.76489300 | 0.20887400 |
| O | -0.50799600 | -2.14465100 | 1.38870700 |
| H | -0.53046700 | -3.04959700 | 1.06422000 |
| P | 0.99049500 | -1.50163700 | -0.85565800 |
| H | -1.18049500 | 2.75103800 | -0.00630300 |
| H | -1.71497800 | -0.92768800 | -1.92722300 |
| H | 1.46900400 | -2.64415200 | -0.16130400 |

4_60

0 1

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|---|---|---|---|
| C | -0.34139900 | -1.33026300 | 0.24518500 |
| C | 2.33999900 | 0.04876100 | -0.14326000 |
| C | 0.05511700 | 1.60401900 | 0.26416500 |
| C | -2.17579400 | 0.30743300 | -0.16922000 |
| P | -0.81315200 | 0.24810100 | 1.15358400 |
| P | 1.62539000 | 1.74495600 | -0.39484300 |
| P | -1.52790900 | -1.09521700 | -1.23464900 |
| O | -0.66366600 | 2.74136000 | 0.26500100 |
| O | -3.04722000 | 1.10941700 | -0.31599200 |
| O | 3.53928700 | -0.04130900 | -0.06418900 |
| O | -0.75121000 | -2.34841400 | 1.13805800 |
| H | -0.59373600 | -3.20443200 | 0.72630300 |
| P | 1.44759900 | -1.61854800 | -0.23600300 |
| H | -1.61480200 | 2.56771200 | 0.34497400 |
| H | 1.84785800 | -1.96839000 | 1.08015300 |
| H | -2.50330800 | -2.05239000 | -0.83702600 |

4_61

0 1

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|---|---|---|---|
| C | -0.56649800 | -1.20093800 | 0.57011100 |
| C | 2.06990600 | -0.41420200 | -0.30297300 |
| C | 0.33813800 | 1.67894900 | 0.42345900 |
| C | -1.94358400 | 0.36054900 | -0.60365400 |
| P | -1.02334400 | 0.56815900 | 0.94925600 |
| P | 1.93434800 | 1.38377100 | -0.07956700 |
| P | -1.83836200 | -1.32082900 | -0.85751000 |
| O | -0.00152500 | 2.97957700 | 0.52278900 |
| O | -2.54859000 | 1.37008400 | -1.22405900 |
| O | 3.30755700 | -0.73219500 | -0.77404500 |
| H | 3.81341300 | 0.07274900 | -0.93511700 |
| O | -0.86522800 | -1.96226100 | 1.71786600 |
| H | -0.45925200 | -2.83048600 | 1.62140800 |
| P | 1.05587300 | -1.77447100 | -0.15353500 |
| H | -0.83553800 | 3.06307800 | 1.00386300 |
| H | -2.97183300 | 1.05742300 | -2.03188500 |

4_62

0 1

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|---|---|---|---|
| C | -0.48215400 | -1.10829200 | 0.40438300 |
| C | 2.29277100 | -0.50770500 | -0.29553600 |
| C | 0.44678400 | 1.68733100 | 0.00461800 |
| C | -2.25297100 | 0.42279900 | -0.10789900 |

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|---|---|---|---|
| P | -0.82363300 | 0.67545900 | 0.95882400 |
| P | 2.19230200 | 1.19916900 | 0.54157600 |
| H | 2.86157800 | 1.87007400 | -0.51344800 |
| P | 0.71228500 | -1.19806500 | -1.02654900 |
| P | -2.22648600 | -1.27052600 | -0.33967700 |
| O | 3.36094100 | -1.02916400 | -0.44579600 |
| O | 0.19348000 | 2.62984400 | -0.68998000 |
| O | -3.08495000 | 1.39238200 | -0.45923300 |
| H | -3.80633400 | 1.03806700 | -0.99189600 |
| O | -0.29036100 | -2.04308700 | 1.42104300 |
| H | 0.61662000 | -1.99267100 | 1.73606600 |
| H | 1.05164600 | -2.57061000 | -0.88499100 |

4_63

0 1

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|---|---|---|---|
| C | 0.36779600 | -1.15207500 | -0.22618400 |
| C | -2.17993200 | -0.46970300 | 0.15913500 |
| C | -0.35934600 | 1.73167900 | 0.02296000 |
| C | 2.23482900 | 0.34455200 | -0.09481400 |
| P | 0.69044800 | 0.55681200 | -1.00659500 |
| P | -2.25363600 | 1.40270000 | -0.05431000 |
| P | -0.75533100 | -1.00791300 | 1.27267600 |
| P | 2.16939400 | -1.30275300 | 0.35282900 |
| O | -2.94467200 | -1.22222200 | -0.38300100 |
| O | 0.07457600 | 2.68145200 | 0.60433000 |
| O | 3.13572300 | 1.30674300 | 0.04144700 |
| H | 3.89647900 | 0.98575500 | 0.53913400 |
| O | 0.02609800 | -2.16831500 | -1.10810000 |
| H | -0.92987200 | -2.17116600 | -1.24081900 |
| H | -1.11329800 | -2.38500000 | 1.30104300 |
| H | -2.33030200 | 1.32976000 | -1.47234400 |

4_64

0 1

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|---|---|---|---|
| C | -0.57513800 | -1.03762400 | 0.44960000 |
| C | 2.11342700 | -0.45976500 | -0.28591400 |
| C | 0.53680700 | 1.75422400 | 0.13209600 |
| C | -2.21989500 | 0.66478400 | -0.28440900 |
| P | -0.82147300 | 0.74998300 | 0.95453000 |
| P | 2.30713700 | 1.14220900 | 0.27299700 |
| P | -2.32241200 | -1.24552300 | -0.32810800 |
| O | 0.29543300 | 2.85511600 | -0.27747000 |
| O | -2.83930900 | 1.49592200 | -0.85867600 |
| O | 3.15680300 | -1.29492800 | -0.40959800 |
| H | 3.97259600 | -0.84556700 | -0.15035500 |
| H | -2.99557800 | -1.26493600 | 0.92882000 |
| O | -0.27206400 | -1.80782500 | 1.57285000 |
| H | -0.13351900 | -2.71876400 | 1.29920600 |
| P | 0.59268300 | -1.18935800 | -1.00530900 |
| H | 0.95938300 | -2.54638200 | -0.77440500 |

4_65

0 1

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|---|---|---|---|
| C | -0.68195500 | -0.90553600 | 0.57955100 |
| C | 1.94204400 | -0.72371900 | -0.45502100 |
| C | 0.70178700 | 1.70170000 | 0.21796000 |
| C | -2.09308800 | 0.79945600 | -0.56031400 |
| P | -0.86346100 | 0.93770300 | 0.84355300 |
| P | 2.21980000 | 0.65063700 | 0.72063900 |
| P | -2.37995800 | -1.07544900 | -0.33135100 |
| O | 0.80409000 | 2.77370500 | -0.29549800 |
| O | -2.55218600 | 1.58695600 | -1.31665800 |
| O | 3.00436500 | -1.12186900 | -1.17999700 |
| H | 3.70622200 | -0.46391900 | -1.14535500 |
| H | -3.17101800 | -0.82198100 | 0.82872900 |
| O | -0.59397800 | -1.54888600 | 1.82527400 |
| H | -0.30529700 | -2.45458700 | 1.67487800 |
| P | 0.49964800 | -1.60420900 | -0.71188000 |
| H | 3.11859800 | 1.35960200 | -0.13068100 |

4_66

0 1

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|---|---|---|---|
| C | -0.30532300 | -1.23069600 | 0.49521000 |
| C | 1.74395100 | 0.07703000 | -0.00607300 |
| C | -0.47609300 | 1.75075000 | 0.36283600 |
| C | -2.15586000 | -0.19729500 | -0.50116600 |
| P | -1.36629200 | 0.24489500 | 1.08517900 |
| P | 1.30996100 | 1.73163800 | -0.11343700 |
| P | -1.25534100 | -1.51683000 | -1.11016100 |
| O | -1.11789700 | 2.76395900 | 0.26277700 |
| O | -3.22362600 | 0.44948200 | -0.93590600 |
| H | -3.50962100 | 0.09633800 | -1.78693200 |
| O | -0.42167900 | -2.33602200 | 1.30387800 |
| H | -0.02485900 | -2.13990700 | 2.15963500 |
| O | 1.11181900 | -1.04793700 | 0.31223900 |
| P | 3.44618300 | -0.38937200 | -0.55389400 |
| H | 4.03456800 | 0.88379100 | -0.33522700 |
| H | 3.85327000 | -0.92975700 | 0.69847400 |

4_67

0 1

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|---|---|---|---|
| C | -0.49506400 | -0.90166300 | 0.10780300 |
| C | 1.79785500 | -0.49501800 | -0.64996000 |
| C | 0.77858200 | 1.76628600 | 0.48024100 |
| C | -1.97573600 | 1.03077100 | -0.41026500 |
| P | -0.72742600 | 0.75524300 | 0.96097100 |
| P | 2.38189800 | 0.94517800 | 0.11769100 |
| P | -2.03256200 | -0.80045300 | -0.98110500 |
| O | 0.68837000 | 2.96459100 | 0.54578400 |
| O | -2.55881900 | 1.98573400 | -0.79770500 |
| O | 2.71430200 | -1.23846000 | -1.25363000 |
| H | 2.28470100 | -2.03305000 | -1.59665400 |
| H | -2.96743900 | -1.15519900 | 0.03082800 |
| P | -0.22994900 | -2.33253800 | 1.28805000 |
| H | -1.38066400 | -2.07841100 | 2.08132300 |
| H | -0.86172600 | -3.33829600 | 0.50055300 |
| O | 0.58263400 | -1.00046000 | -0.86533200 |

4_68

0 1

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|---|---|---|---|
| C | -0.38820700 | -1.05106700 | 0.49750500 |
| C | 1.72492900 | -0.02774500 | -0.16102900 |
| C | -0.23690100 | 1.87471600 | 0.16518200 |
| C | -2.41468100 | 0.01386400 | -0.45493900 |
| P | -1.28788900 | 0.54576400 | 0.94575400 |
| P | 1.61191000 | 1.63766000 | 0.18591000 |
| P | -1.73097300 | -1.75703000 | -0.65985200 |
| O | -0.73110300 | 2.89504300 | -0.23118900 |
| O | -3.27943800 | 0.57868500 | -1.03623500 |
| H | -2.54718200 | -2.25384900 | 0.39631700 |
| O | 0.77116500 | -0.97046400 | -0.34043400 |
| O | -0.07056500 | -1.73587700 | 1.64922900 |
| H | 0.27549700 | -2.60185100 | 1.40771300 |
| P | 3.34155400 | -0.75185200 | -0.65562000 |
| H | 4.13695400 | 0.31359500 | -0.15793400 |
| H | 3.48439600 | -1.57374200 | 0.49975300 |

4_69

0 1

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|---|---|---|---|
| C | -0.79237600 | -0.69696900 | 0.14724500 |
| C | 1.37157200 | -1.23084700 | -0.90367500 |
| C | 1.39181600 | 1.18507000 | 0.51817100 |
| C | -1.43557000 | 1.59724000 | -0.54760300 |
| P | -0.36123000 | 0.97116100 | 0.88105800 |
| P | 2.47612700 | -0.00555200 | -0.05036500 |
| P | -2.33179500 | -0.08817200 | -0.77029200 |
| O | 1.81296800 | 2.39086600 | 0.93005200 |
| O | -1.53665000 | 2.63423000 | -1.10459500 |
| O | 1.91977000 | -2.05121000 | -1.57733700 |
| H | -3.11675400 | 0.15751800 | 0.39367000 |
| P | -0.90056300 | -2.06833100 | 1.42077700 |
| H | -1.91869600 | -1.45964700 | 2.20633300 |
| H | -1.79945400 | -2.90190500 | 0.69830200 |

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|---|---|---|---|
| O | 0.00878700 | -1.16967200 | -0.93596100 |
| H | 2.74518200 | 2.50676000 | 0.70192100 |

4_70

0 1

| | | | |
|---|---|---|---|
| C | -0.31310300 | -0.91359800 | 1.56584000 |
| C | -0.35436700 | 1.45726800 | -0.02885900 |
| C | 1.17858000 | -0.04330100 | -0.24795500 |
| C | -1.46008000 | -0.94993400 | -0.93437000 |
| P | 0.13969500 | -1.65975900 | -0.12264500 |
| P | 0.66294600 | 0.71693200 | 1.42232600 |
| O | -2.06560100 | -1.59882500 | -1.73069500 |
| O | -0.95945800 | -1.34706500 | 2.46303500 |
| P | 2.94633000 | -0.38719900 | -0.64310800 |
| H | 2.74713500 | -0.62184600 | -2.03252000 |
| H | 3.32488700 | 0.97333000 | -0.81138900 |
| O | -0.37567900 | 2.82590800 | 0.06584600 |
| H | -0.70044700 | 3.19136400 | -0.76502800 |
| O | 0.56594300 | 0.99329700 | -1.01937600 |
| P | -2.06987400 | 0.72417700 | -0.33013900 |
| H | -2.18583800 | 1.25577300 | -1.64600700 |

4_71

0 1

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|---|---|---|---|
| C | -0.43761600 | -1.09285000 | 1.37144000 |
| C | -0.17791400 | 1.50457200 | 0.11805400 |
| C | 1.20066700 | -0.12275000 | -0.25841300 |
| C | -1.62032900 | -0.71833700 | -0.90768500 |
| P | 0.00691500 | -1.60645900 | -0.41469400 |
| P | 0.67634600 | 0.44121600 | 1.48155900 |
| O | -2.54089800 | -1.38613200 | -1.27103000 |
| O | -1.17048900 | -1.57736500 | 2.16776700 |
| P | 2.94630100 | -0.59504300 | -0.62332200 |
| H | 2.81262900 | -0.58090400 | -2.04010000 |
| H | 3.47096300 | 0.72413900 | -0.54558200 |
| O | -0.02333900 | 2.82526200 | 0.45470100 |
| H | -0.31946400 | 3.37196000 | -0.28296400 |
| O | 0.73867500 | 1.06928100 | -0.90156400 |
| P | -1.83899600 | 1.13631000 | -0.65529200 |
| H | -2.64307500 | 0.97227600 | 0.50550000 |

4_72

0 1

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|---|---|---|---|
| C | -0.33470200 | -1.43124700 | 1.10220700 |
| C | -0.91599500 | 1.25665800 | 0.35324000 |
| C | 1.13924100 | 0.10263500 | -0.22414900 |
| C | -1.55134100 | -0.63768400 | -1.04021300 |
| P | 0.15001300 | -1.42277800 | -0.75079800 |
| P | 0.32063200 | 0.31010500 | 1.49314600 |
| P | 0.52212200 | 1.77628500 | -0.78980200 |
| O | -1.88920800 | 0.47436100 | -0.34264700 |
| O | -2.34824700 | -1.16957600 | -1.74578900 |
| O | -0.84393800 | -2.25172800 | 1.78448300 |
| H | -0.04446900 | 1.45954600 | -2.06222800 |
| P | 2.95328300 | -0.30792700 | -0.22542500 |
| H | 3.18200300 | -0.11664400 | -1.61798500 |
| H | 3.41896100 | 0.98744400 | 0.13525000 |
| O | -1.60666500 | 2.19728900 | 1.05635900 |
| H | -2.26600800 | 2.58945500 | 0.47238300 |

4_73

0 1

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|---|---|---|---|
| C | 1.35747300 | -0.54176100 | 1.27762200 |
| C | -1.17359500 | -0.12048200 | 0.00840000 |
| C | 0.71294100 | 1.35954300 | -0.21677400 |
| C | 0.58425600 | -1.45434100 | -1.00450400 |
| P | 1.85451100 | -0.12150200 | -0.53167300 |
| P | -0.08676700 | 0.69350400 | 1.36790800 |
| P | -0.87150000 | 1.28341500 | -1.25024800 |
| P | -2.96285800 | -0.49482900 | 0.38543600 |
| H | -2.69975500 | -1.36163400 | 1.48386400 |
| H | -3.15884800 | 0.64622000 | 1.21202700 |

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|---|---|---|---|
| O | -0.69218200 | -1.34343000 | -0.55306800 |
| O | 0.93620800 | -2.43321900 | -1.57855700 |
| O | 1.51063600 | 2.49597900 | -0.22351000 |
| O | 1.81144700 | -1.29934500 | 2.06439800 |
| H | -1.56227100 | 2.25338000 | -0.45542700 |
| H | 1.00476100 | 3.23557800 | 0.12563600 |

4_74

0 1

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|---|---|---|---|
| C | 1.32426400 | -0.56178200 | 1.28898000 |
| C | -1.18107400 | -0.09768900 | 0.00062600 |
| C | 0.75168400 | 1.34095500 | -0.23162900 |
| C | 0.57128300 | -1.45594700 | -1.00756300 |
| P | 1.86460400 | -0.16682700 | -0.50290400 |
| P | -0.08824200 | 0.70460700 | 1.38022000 |
| P | -0.89438100 | 1.40385800 | -1.11701600 |
| P | -2.97466700 | -0.45856000 | 0.36914800 |
| H | -2.74179000 | -1.29065700 | 1.50111900 |
| H | -3.17911700 | 0.71380500 | 1.14683600 |
| O | -0.70719300 | -1.31630100 | -0.57528900 |
| O | 0.90053900 | -2.43319300 | -1.60000000 |
| O | 1.58046200 | 2.45504300 | -0.23151300 |
| O | 1.73899600 | -1.32952400 | 2.08824600 |
| H | -0.65222400 | 0.73967100 | -2.35551700 |
| H | 1.06405400 | 3.22960300 | 0.01182200 |

4_75

0 1

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|---|---|---|---|
| C | -0.39296800 | -1.43134200 | 1.10205100 |
| C | -0.86799200 | 1.28294800 | 0.34940200 |
| C | 1.13988300 | 0.05771300 | -0.20823900 |
| C | -1.57920600 | -0.58849200 | -1.03390800 |
| P | 0.10388600 | -1.42849000 | -0.75941900 |
| P | 0.31918600 | 0.29332300 | 1.48235000 |
| P | 0.52015400 | 1.69013200 | -0.91256700 |
| O | -1.87696300 | 0.53644200 | -0.33523100 |
| O | -2.40121700 | -1.10532100 | -1.72020900 |
| O | -0.92903600 | -2.24315200 | 1.77318900 |
| H | 1.22454200 | 2.49548500 | 0.03120600 |
| P | 2.94096400 | -0.39107400 | -0.22607300 |
| H | 3.17996700 | -0.13598200 | -1.60668000 |
| H | 3.43313700 | 0.87605000 | 0.19825200 |
| O | -1.50811400 | 2.27800000 | 1.02231100 |
| H | -2.17617100 | 2.65336600 | 0.43653400 |

4_76

0 1

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|---|---|---|---|
| C | 2.17718300 | -0.85005900 | -0.07680600 |
| C | 0.79984800 | 0.81673700 | 0.11260600 |
| C | -0.60291900 | -1.28531500 | 0.06978200 |
| P | 0.65522900 | -0.58714500 | -1.16806900 |
| P | -0.54425900 | 0.22528800 | 1.29583400 |
| P | 1.01746200 | 2.63544700 | -0.18524700 |
| H | 1.83470900 | 2.48143500 | -1.34190800 |
| H | -0.18366600 | 2.79634300 | -0.92635900 |
| O | 2.04216300 | 0.28814600 | 0.66715300 |
| O | -0.26992300 | -2.56863200 | 0.45701500 |
| O | 3.04635000 | -1.64271100 | 0.01680300 |
| H | -0.96500800 | -2.92553200 | 1.01852300 |
| P | -2.38754300 | -0.99401100 | -0.46690700 |
| C | -2.02144300 | 0.71412500 | 0.20335200 |
| O | -2.51995900 | 1.77661800 | 0.00001000 |
| H | -2.30442500 | -0.74620600 | -1.86586400 |

4_77

0 1

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|---|---|---|---|
| C | 2.47155700 | -0.15147800 | -0.01186000 |
| C | 0.60380300 | 0.94535300 | 0.11908700 |
| C | 0.00933800 | -1.47035500 | -0.04454900 |
| P | 1.02074600 | -0.36131500 | -1.20282400 |
| P | -0.47995500 | -0.12274200 | 1.25676600 |
| P | 0.16745300 | 2.72890200 | -0.13042900 |

H 0.96639800 2.91526300 -1.29468000
H -1.01788100 2.45724100 -0.86670900
O 1.92361200 0.85129500 0.73809300
O 0.52820800 -2.69728200 0.14947600
O 3.54596100 -0.61905900 0.13168300
H -0.05053200 -3.20374600 0.73087500
C -1.88424100 -0.46192100 0.10766500
O -1.33896200 -1.51197200 -0.57422200
P -3.41304000 0.22747100 -0.05695300
H -3.79933800 -0.60695100 -1.15019200
4_78
0 1
C 2.39075500 -0.59103100 0.07810900
C 0.40659700 -1.44347700 -0.07416800
C 0.06724500 1.02089600 0.11659400
P 0.97630000 -0.18374200 1.25997200
P -0.54176500 -0.24389800 -1.19565000
O 1.74026300 -1.55311100 -0.64496700
O 3.50693600 -0.23792300 -0.08448700
C -1.91387500 0.18093700 -0.03835600
O -1.26201000 1.12316000 0.70144000
P -3.51199500 -0.33985900 0.06450000
H -3.82153000 0.49054000 1.18552100
P 0.87238500 2.62063500 -0.32170800
H -0.28789200 3.18111400 -0.92407700
H 0.63973000 3.23723900 0.93955300
O -0.17816000 -2.64491300 0.09783300
H 0.38526000 -3.20757900 0.64067900
4_79
0 1
C 2.15480900 -0.90457400 -0.06005600
C 0.83835100 0.81351300 0.10674100
C -0.62580400 -1.25673500 0.07287500
P 0.65691300 -0.58880100 -1.17121200
P -0.54107500 0.24760200 1.26218300
P 1.10297800 2.62483600 -0.18860500
H 1.86770200 2.46377200 -1.37962500
H -0.12249100 2.82437400 -0.87991300
O 2.05920900 0.24491700 0.67150100
O -0.32544800 -2.54550700 0.46870900
O 2.98809000 -1.73223500 0.04935500
H -0.97276100 -2.84026500 1.11621900
P -2.36128400 -0.92919200 -0.65246200
H -3.02460400 -1.36577500 0.53947200
C -2.02204700 0.75200800 0.19302200
O -2.55718700 1.80481900 0.05790900
4_80
0 1
C 0.47314100 1.61285200 -0.88117000
C 1.24620300 -0.18886900 0.05396800
C -1.06847100 0.16539200 1.07489000
P 0.48836300 1.27764100 0.98104600
P -0.11507900 -1.40414400 0.57391300
P 2.98104100 -0.83764300 0.13627200
H 3.62119500 0.42795800 0.27601900
H 2.95618900 -1.09414500 1.53492600
O 1.06330700 0.43924300 -1.25210700
O -1.77572900 0.24021500 2.26952300
O 0.12490100 2.47913400 -1.60422200
C -1.23249800 -1.25122700 -0.96601400
P -2.28370600 0.22402500 -0.37964300
H -3.20058600 -0.66440600 0.25542900
O -1.25990400 -1.88001000 -1.96831000
H -1.16693600 0.17486000 3.01068100
4_81
0 1
C -0.60303400 0.51177100 1.74181200
C -1.16677400 -0.41080700 -0.13847400

| | | | |
|---|---|---|---|
| C | 0.56499000 | 1.31751500 | -0.71028900 |
| P | -1.12838100 | 1.44955600 | 0.18384700 |
| P | 0.25001100 | -0.43725300 | -1.44838300 |
| P | -2.62548200 | -1.46429300 | -0.58864200 |
| H | -3.60250100 | -0.72411000 | 0.13787100 |
| H | -2.88750300 | -0.79552900 | -1.81668100 |
| O | -0.76358400 | -0.73757700 | 1.21703000 |
| O | 1.00652200 | 2.41599900 | -1.37954400 |
| O | -0.26512200 | 0.77433400 | 2.83996300 |
| C | 1.64766400 | -0.47943900 | -0.26021700 |
| P | 2.65305000 | -1.71679300 | 0.26947600 |
| H | 3.37304300 | -0.89061600 | 1.18562400 |
| O | 1.64302900 | 0.84549300 | 0.09146900 |
| H | 0.25512300 | 2.92177600 | -1.69963000 |

4_82

0 1

| | | | |
|---|---|---|---|
| C | -3.08303700 | 1.22522300 | 0.17560500 |
| C | 0.64502600 | -0.29551300 | 0.38638500 |
| C | 2.54786900 | 0.69089400 | -0.60202700 |
| C | -1.51652700 | -0.74019600 | -0.51224800 |
| P | -3.27920000 | -0.19111600 | -0.73047700 |
| P | 1.60401400 | -0.58944300 | -1.22359100 |
| P | 1.57625500 | 1.28532200 | 0.81895000 |
| P | 0.73160800 | -1.62163600 | 1.71448000 |
| H | 0.50202900 | -2.74101100 | 0.86935200 |
| H | 2.14625900 | -1.75304400 | 1.67209800 |
| O | -0.74301300 | 0.08826000 | 0.21048700 |
| O | -1.13668800 | -1.76680700 | -1.00138600 |
| O | 3.68633400 | 1.26343500 | -0.97700200 |
| O | -3.07180800 | 2.20705200 | 0.76526200 |
| H | 2.39978500 | 0.78934600 | 1.87841600 |
| H | 4.02319800 | 0.83982000 | -1.77549300 |

4_83

0 1

| | | | |
|---|---|---|---|
| C | 1.19773900 | -0.42616900 | 1.92304700 |
| C | -0.44766300 | 1.75853700 | -0.12323000 |
| C | -1.47493700 | -0.40552800 | -0.23990400 |
| C | 1.28322200 | -0.32738400 | -0.71679100 |
| P | 2.28488800 | -0.99625900 | 0.77257900 |
| P | 1.11886700 | 1.53359400 | -0.77797100 |
| P | -0.25226300 | -1.36952800 | -0.88535600 |
| P | -3.11952200 | -1.18908200 | -0.07052400 |
| H | -3.30402400 | -0.88096400 | 1.30830900 |
| H | -3.87971300 | -0.06778600 | -0.51291800 |
| O | -1.42469100 | 0.89327700 | 0.20037800 |
| O | -0.83990000 | 3.00254400 | 0.15276800 |
| O | 0.49294900 | -0.06613100 | 2.75796100 |
| O | 2.18216100 | -0.70453300 | -1.75783300 |
| H | -1.79007200 | 2.99224600 | 0.31999100 |
| H | 1.85994000 | -0.32235400 | -2.58122600 |

4_84

0 1

| | | | |
|---|---|---|---|
| C | -1.73402600 | -0.35093600 | 0.05479500 |
| C | 1.54442500 | 0.10882100 | -1.16900000 |
| C | 2.02899700 | -1.06041100 | 1.19297400 |
| C | -0.69084800 | 1.43899000 | 0.16149600 |
| P | -1.27293000 | 0.29693600 | 1.56941200 |
| P | 1.80768400 | -1.59091800 | -0.39211800 |
| O | -1.28800400 | 2.66900400 | 0.17720900 |
| H | -1.04770300 | 3.14877400 | -0.62432500 |
| O | 2.22777100 | -0.83099600 | 2.30061700 |
| P | -2.42032700 | -1.90397700 | -0.59869800 |
| H | -3.12590100 | -2.23651000 | 0.58730300 |
| H | -3.53724100 | -1.30505900 | -1.24626200 |
| O | -1.29323300 | 0.55313300 | -0.84997100 |
| O | 1.66886300 | 0.18545000 | -2.35696500 |
| P | 1.17124600 | 1.63124800 | -0.11608800 |
| H | 1.01127200 | 2.46196000 | -1.26305700 |

4_85
0 1
C 1.82998100 -1.03172100 0.63006100
C 0.89957900 0.59340600 -0.23610000
C -1.32238400 -1.26189200 -0.65023300
P 2.23752600 -0.55275800 -0.96970500
P -0.72258500 0.47943400 -1.12411500
P 1.29020900 2.36980800 0.22286500
H 2.66899400 2.12114900 0.48034100
H 1.53124700 2.78217900 -1.11703300
O 0.88318700 -0.17402300 1.03568000
O -0.98967600 -2.32752200 -1.05580700
O 2.22327800 -1.95684500 1.47262600
C -1.99696300 0.92678900 0.21004400
P -2.60231800 -0.81410200 0.67508600
H -3.76008700 -0.84696200 -0.15227400
O -2.32457100 1.98675900 0.63653600
H 1.71835500 -1.87854400 2.29208600
4_86
0 1
C -1.47563900 -1.13830100 -0.96286200
C -0.91291900 0.72634300 -0.02240700
C -0.08431300 -1.14634200 1.35067200
P -1.88684200 -0.67083900 0.82993600
P 0.62486300 0.56384100 1.04285900
P -1.48867700 2.46168100 -0.35056100
H -2.83025800 2.12984100 -0.68973500
H -1.79040400 2.75528500 1.00802000
O -0.83695800 0.01591000 -1.29026000
O 0.35547600 -2.16240300 1.76378800
O -1.67063500 -2.06363600 -1.66717100
C 2.10570300 0.44846700 -0.02799300
P 2.34313500 -0.88518500 -1.04159200
H 3.61666000 -0.44335700 -1.51789300
O 2.97991500 1.47313700 0.09043200
H 2.69743200 2.07070200 0.79121500
4_87
0 1
C -0.41807100 -1.23019900 0.19403700
C 2.24714300 -0.24689700 -0.23898100
C 0.39851600 1.19310500 -0.13139000
C -2.22964100 0.26381900 0.15011300
P -0.70703200 0.36271600 1.16033700
P -2.17888700 -1.31384900 -0.49476400
O -3.14327800 1.21024400 -0.03146000
O 3.14019600 -1.22932400 -0.21437100
O 0.11355600 -2.29526000 0.90259500
H 0.02016400 -3.09306200 0.37473400
P 0.67939200 -0.39521100 -1.15782400
P 2.17019300 1.29368600 0.50319400
H -2.78803200 2.05788700 0.25775100
H 3.87649900 -0.99451900 0.36208200
O -0.22383800 2.33718600 -0.62380700
H 0.35560700 2.75783100 -1.26503300
4_88
0 1
C 1.20050600 -0.02602000 -0.06213800
C -0.34303500 1.47795700 0.04421100
C -0.91167900 -0.74793300 1.51786300
C -1.04496900 -0.69248100 -0.98651800
P 0.12575700 -1.62765100 0.19442900
P -1.90173200 0.36825000 0.34660600
P 0.21201800 0.58869200 -1.56770300
O -1.75862500 -1.32990000 -1.98565700
O 0.81722500 1.08298400 0.75987600
P 3.01467100 -0.32066300 0.12281200
H 3.09140000 -1.29413600 -0.90976300
H 3.45022500 0.74840400 -0.71382400

| | | | |
|---|---|---|---|
| O | -0.63040300 | 2.78734600 | 0.22508000 |
| H | 0.17543000 | 3.29654700 | 0.07784800 |
| H | -2.39005500 | -1.93551700 | -1.58776500 |
| O | -0.86477800 | -0.79216400 | 2.70205500 |

4_89
0 1

| | | | |
|---|---|---|---|
| C | -0.62012700 | -1.25788000 | 0.06541500 |
| C | 2.16204900 | -0.88894000 | -0.05462500 |
| C | 0.84465300 | 0.82265800 | 0.11531300 |
| C | -2.03576200 | 0.74173300 | 0.19348300 |
| P | -0.54383300 | 0.22716700 | 1.24579800 |
| P | -2.35456100 | -0.93536200 | -0.66616800 |
| O | -2.59465500 | 1.78412900 | 0.09711400 |
| O | 2.98104700 | -1.73243800 | 0.06012600 |
| H | -3.02062300 | -1.39159500 | 0.51244100 |
| O | -0.38003500 | -2.49113900 | 0.64140900 |
| H | -0.43755500 | -3.18166000 | -0.02582300 |
| P | 0.68346500 | -0.56021400 | -1.17971600 |
| P | 0.95414800 | 2.60470900 | -0.34815300 |
| H | 1.47977500 | 3.03969300 | 0.90042900 |
| H | 2.23374700 | 2.48800000 | -0.95923700 |
| O | 2.06257900 | 0.25140200 | 0.68613100 |

4_90
0 1

| | | | |
|---|---|---|---|
| C | -1.56032300 | -0.40111700 | 1.22918800 |
| C | 1.63187000 | -0.56074400 | -0.04348000 |
| C | 0.23506000 | 1.86673800 | 0.02135000 |
| C | -1.62322100 | -0.33066700 | -1.21152100 |
| P | -2.18826100 | -1.70630300 | -0.01448600 |
| P | -1.42697200 | 1.06693500 | 0.04632500 |
| P | 1.84768100 | 1.29477900 | -0.01091000 |
| P | 3.26490600 | -1.46506900 | 0.09745000 |
| H | 2.92914700 | -2.47242400 | -0.84241100 |
| H | 3.97563900 | -0.63796300 | -0.81212300 |
| O | 0.59864400 | -1.19050700 | -0.05908300 |
| O | -1.49210400 | -0.33939400 | -2.38866200 |
| O | 0.12406400 | 3.20727000 | 0.02943500 |
| O | -1.37006300 | -0.47712400 | 2.39577100 |
| H | -3.53790600 | -1.24157400 | 0.03106100 |
| H | -0.81182400 | 3.44961400 | 0.05487300 |

4_91
0 1

| | | | |
|---|---|---|---|
| C | 1.00682800 | 1.62729400 | 0.57672400 |
| C | -0.62454800 | -0.82579600 | 0.14388300 |
| C | -1.76032400 | 1.27388600 | -0.46999500 |
| C | 1.63580500 | -0.70253100 | -0.73033100 |
| P | 2.44486000 | 0.57200700 | 0.13580500 |
| P | -0.64499900 | 0.85203900 | 0.99260900 |
| P | -2.28390800 | -0.53645200 | -0.73169700 |
| P | -0.60671600 | -2.39664900 | 1.17508600 |
| H | 0.55676400 | -2.06751400 | 1.93073500 |
| H | -1.49886700 | -1.89627200 | 2.16312800 |
| O | 0.36790900 | -1.02530300 | -0.89076000 |
| O | 2.35705400 | -1.54074500 | -1.46443500 |
| H | 3.26491300 | -1.21504200 | -1.50520600 |
| O | -2.05979300 | 2.28117200 | -1.01539800 |
| O | 1.11973400 | 2.81656200 | 0.71669600 |
| H | -1.78716000 | -0.67596000 | -2.05622300 |

4_92
0 1

| | | | |
|---|---|---|---|
| C | 1.97435100 | -0.92563400 | -0.28646400 |
| C | -1.66874100 | 0.74497000 | -0.17240700 |
| C | 2.49026000 | 1.50943200 | 0.39119900 |
| C | -0.65728200 | -1.48929400 | -0.13626800 |
| P | 0.80018600 | -2.40222000 | -0.11960400 |
| P | 1.94403800 | 0.18347000 | 1.27826100 |
| P | -1.08370500 | 2.30355000 | -0.50107800 |
| P | -3.39717200 | 0.22634400 | 0.23003100 |

| | | | |
|---|---|---|---|
| H | -3.15720000 | -0.27293400 | 1.53934400 |
| H | -3.77236100 | 1.51869600 | 0.67779900 |
| O | -0.68446100 | -0.19635400 | -0.41683600 |
| O | -1.86682200 | -2.02365700 | 0.03325000 |
| H | -1.78187900 | -2.94569200 | 0.30026100 |
| O | 2.86174900 | 2.41122900 | -0.21209900 |
| O | 2.71880500 | -0.81035600 | -1.21030900 |
| H | -2.30447000 | 2.94901800 | -0.15996500 |

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