

The Supporting Information

**Aminophosphonates and aminophosphonic acids with tetrasubstituted stereogenic center:
diastereoselective synthesis from cyclic ketimines**

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General

Melting points were determined on the Schmelzpunkt Bestimmer Apotec melting-point apparatus using the standard open capillary method and are uncorrected. ^1H , ^{13}C and ^{31}P NMR spectra were collected on Jeol 400yh, Bruker Avance III 500 and Bruker Avance II 600 instruments. NMR spectra recorded in CDCl_3 , D_2O and DMSO-d_6 were referenced to the respective residual ^1H or ^{13}C signals of the solvents. The reported J values are those observed from the splitting patterns in the spectrum and may not reflect the true coupling constant values. NOESY experiments were carried out at 293K. Infrared spectra ($4000\text{--}400\text{ cm}^{-1}$) were collected on a Perkin Elmer 2000 FTIR spectrophotometer. High resolution mass spectra were collected using electrospray ionization on Waters LCT Premier XE TOF instrument. Optical rotations were measured using an Optical Activity Ltd. Model AA-5 automatic polarimeter; $[\alpha]_D$ values are given in $10^{-1}\text{ deg cm}^2\text{ g}^{-1}$. Chromatographic separations were performed on silica gel 60 (70-230 mesh). Thin layer chromatography was carried out using silica gel 60 precoated plates.

Experimental procedures

Imines

Procedures

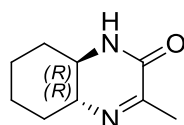
General procedure for synthesis of cyclic imines 1a-e.

(1*R*,2*R*)-1,2-diaminocyclohexane (2.00 mmol, 228 mg, 2.00 equiv) was dissolved in 2-PrOH (4 ml). To the stirred solution was added a ketone ester (1.00 mmol, 1.00 equiv) and the mixture was stirred for 24 hours at room temperature (293 K). The solvent was removed in vacuo and the product was purified by silica gel column chromatography (eluent: $\text{CH}_2\text{Cl}_2/\text{MeOH}$ 97:3 v/v).

Procedure for synthesis of 1f

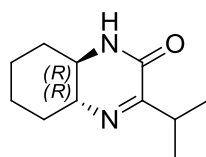
Sodium hydride (60% dispersion in mineral oil, 1.20 mmol, 48.0 mg, 1.20 equiv) was dispersed in anhydrous THF (10 ml) under argon atmosphere. A mixture was cooled to 273 K in an ice bath and then dimethyl-[(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate (1.00 mmol, 262 mg, 1.00 equiv) was added. The mixture was stirred for 30 minutes. The isovaleraldehyde was added (1.00 mmol, 107 μl , 1.00 equiv) and the reaction continued for 30 minutes in 273 K and then for 30 minutes in room temperature. Reaction mixture was washed with Et_2O (20 ml) and saturated NaHCO_3 solution (20 ml). The organic layer was dried (Na_2SO_4), filtered and evaporated under reduced pressure.

Synthesis



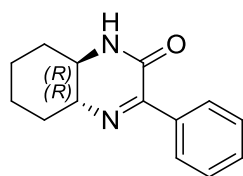
1a 4-methyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

Colorless solid; 148 mg; yield = 89%; mp. 169-170 °C; $[\alpha]_D^{20}$ -178 (c 0.55, CH₂Cl₂); IR (KBr): 573, 773, 1204, 1358, 1450, 1625, 1663, 1686, 2861, 2933, 2949, 3226 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 6.63 (br. s, 1H), 3.11 (td, *J* = 11.5, 3.7 Hz, 1H), 2.97-3.06 (m, 1H), 2.24-2.32 (m, 1H), 2.19 (d, *J* = 2.5 Hz, 3H), 1.83-1.92 (m, 2H), 1.75-1.78 (m, 1H), 1.22-1.44 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 163.0, 159.0, 62.5, 54.5, 31.8, 31.1, 25.3, 23.7, 21.0; HRMS (ESI-TOF) calcd. for C₉H₁₅N₂O [*M*+H]⁺ *m/z*: 167.1184, found: 167.1176.



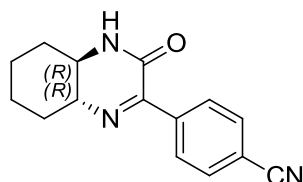
1b 4-isopropyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

Colorless solid; 180 mg; yield = 93%; mp. 125-127 °C; $[\alpha]_D^{20}$ -166 (c 0.67, CH₂Cl₂); IR (KBr): 572, 807, 1068, 1361, 1446, 1627, 1683, 2865, 2930, 3064, 3192 cm⁻¹; ¹H NMR (600 MHz, CDCl₃): δ 6.50 (br. s, 1H), 3.25 (dsep, *J* = 7.0, 1.1 Hz, 1H), 3.02-3.09 (m, 2H), 2.35-2.37 (m, 1H), 1.80-1.94 (m, 3H), 1.33-1.42 (m, 4H), 1.17 (d, *J* = 7.0 Hz, 3H), 1.11 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 169.3, 158.6, 62.4, 54.1, 31.9, 31.1, 30.7, 25.2, 23.7, 20.6, 19.3; HRMS (ESI-TOF) calcd. for C₁₁H₁₉N₂O [*M*+H]⁺ *m/z*: 195.1497, found: 195.1489.



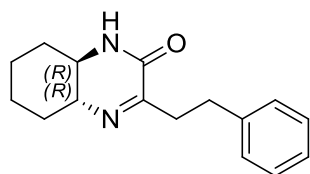
1c 4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

Colorless solid; 130 mg; yield = 57%; mp. 143-144 °C; $[\alpha]_D^{20}$ -239 (c 0.82, CH₂Cl₂); IR (KBr): 688, 696, 739, 809, 1259, 1359, 1446, 1574, 1595, 1683, 2861, 2934, 3084, 3189, 3320, 3480 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.90 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.36-7.44 (m, 3H), 6.99 (br. s, 1H), 3.16-3.23 (m, 2H), 2.38-2.44 (m, 1H), 1.78-1.99 (m, 3H), 1.17-1.54 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 161.6, 158.5, 135.2, 130.4, 129.0 (2C overlapped), 128.1 (2C overlapped), 63.1, 54.1, 31.9, 31.0, 25.3, 23.8; HRMS (ESI-TOF) calcd. for C₁₄H₁₇N₂O [*M*+H]⁺ *m/z*: 229.1341, found: 229.1349.



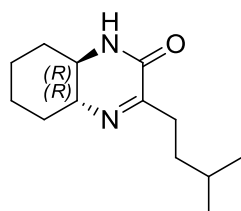
1d 4-((1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl-4-ene)-benzonitrile

Off-white solid; 225 mg; yield = 89%; mp. 184-186 °C; $[\alpha]_D^{20}$ -333 (c 0.48, CH₂Cl₂); IR (KBr): 848, 854, 1254, 1363, 1586, 1673, 2229, 2857, 2940, 3066, 3080, 3185 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 8.04-8.07 (m, 2H), 7.65-7.68 (m, 2H), 6.66 (br. s, 1H), 3.19-3.29 (m, 2H), 2.24-2.45 (m, 1H), 1.81-2.00 (m, 3H), 1.24-1.49 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 159.9, 157.6, 139.1, 131.9 (2C overlapped), 129.7 (2C overlapped), 118.7, 113.7, 63.6, 54.2, 31.7, 31.0, 25.3, 23.7; HRMS (ESI-TOF) calcd. for C₁₅H₁₆N₃O [*M*+H]⁺ *m/z*: 254.1293, found: 254.1299.



1e 4-phenethyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

Pale yellow solid; 180 mg; yield = 70%; mp. 127-128 °C; $[\alpha]_D^{20}$ -110 (c 0.55, CH₂Cl₂); IR (KBr): 499, 711, 756, 1358, 1624, 1678, 2863, 2934, 3064, 3188 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.14-7.28 (m, 5H), 6.52 (br. s, 1H), 2.82-3.03 (m, 6H), 2.29-2.32 (m, 1H), 1.76-1.90 (m, 3H), 1.25-1.41 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 164.9, 158.6, 141.5, 128.7 (2C overlapped), 128.4 (2C overlapped), 126.0, 62.6, 54.4, 35.4, 32.7, 31.2, 31.1, 25.3, 23.8; HRMS (ESI-TOF) calcd. for C₁₆H₂₁N₂O [M+H]⁺ m/z: 257.1654, found: 257.1647.



1f 4-Isopentyl-[(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene]

Yellow solid; 210 mg; 94% yield; mp. 98-101 °C; $[\alpha]_D^{20}$ -36 (c 0.22, CH₂Cl₂); IR (nujol): 1093, 1367, 1456, 1652, 1683, 2924, 3208 cm⁻¹; ¹H NMR (400MHz, CDCl₃): δ 6.00 (br. s, 1H), 3.04-3.08 (m, 2H), 2.59-2.65 (m, 1H), 2.45-2.53 (m, 1H), 2.27-2.31 (m, 1H), 1.75-1.89 (m, 3H), 1.59 (sept., J = 6.72, 1H), 1.20-1.47 (m, 6H), 0.89 (d, J = 6.72, 6H), ¹³C NMR (100MHz, CDCl₃): δ 166.3, 158.9, 62.4, 54.3, 35.7, 31.8, 31.0, 29.7, 28.2, 25.3, 23.8, 22.6, 22.4; HRMS (ESI-TOF) calcd. for C₁₃H₂₃N₂O [M+H]⁺ m/z: 223.1810, found: 223.1805.

Dialkyl aminophosphonic acid esters

Procedures

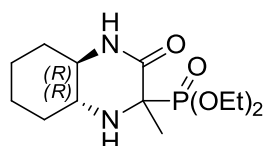
General procedure for synthesis of esters 3aa-cb

Imine (1.00 mmol, 1.00 equiv) was dissolved in toluene (30 ml), mixed with appropriate H-phosphonate (1.00 mmol, 1.00 equiv) and the resulting mixture was stirred for 1 h at 80 °C. After that time the resulting crude product was purified by column chromatography (eluent: CH₂Cl₂/MeOH 98:2 v/v).

Procedure for synthesis of 3fa

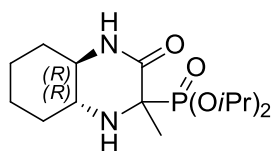
The procedure of esterification of the earlier prepared aminophosphonic acid **4f** employing trimethylsilyldiazomethane (TMSCHN₂) can be found in the literature (Skropeta, D.; Schmidt, R. R. *Tetrahedron: Asymmetry* **2003**, 14, 265–273; Olszewski T. K. *Tetrahedron: Asymmetry* **2016**, 26, 393–399.)

Synthesis



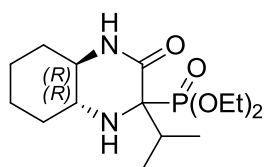
3aa diethyl-[4-methyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

Colorless solid; 237 mg; 78% yield in a diastereomeric ratio = 71:29; IR (KBr): 962, 1026, 1056, 1229, 1451, 1670, 2857, 2929, 3448 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 5.92 (s, dia_{maj} , 1H), 5.85 (s, dia_{min} , 1H), 4.09-4.29 (m, $\text{dia}_{\text{maj}}+\text{dia}_{\text{min}}$, 8H), 3.05-3.16 (m, $\text{dia}_{\text{maj}}+\text{dia}_{\text{min}}$, 2H), 2.96-3.05 (m, $\text{dia}_{\text{maj}}+\text{dia}_{\text{min}}$, 2H), 1.68-2.10 (m, $\text{dia}_{\text{maj}}+\text{dia}_{\text{min}}$, 10H), 1.63 (d, $J = 16.5$ Hz, dia_{min} , 3H), 1.55 (d, $J = 15.9$ Hz, dia_{maj} , 3H), 1.13-1.43 (m, $\text{dia}_{\text{maj}} + \text{dia}_{\text{min}}$, 20H); ^{13}C NMR (100 MHz, CDCl_3): δ 169.7 (dia_{min}), 169.7 (dia_{maj}), 64.3 (d, $J = 6.9$ Hz, dia_{min}), 63.4 (d, $J = 6.9$ Hz, dia_{maj}), 63.2 (d, $J = 7.5$ Hz, dia_{min}), 63.2 (d, $J = 8$ Hz, dia_{maj}), 61.9 (d, $J = 133.2$ Hz, dia_{maj}), 61.8 (d, $J = 162.6$ Hz, dia_{min}), 58.0 (dia_{maj}), 57.8 (dia_{min}), 54.9 (dia_{maj}), 54.4 (d, $J = 10.3$ Hz, dia_{min}), 31.0 (dia_{min}), 31.0 (dia_{maj}), 30.6 (dia_{maj}), 30.4 (dia_{min}), 24.5 (dia_{min}), 24.4 (dia_{maj}), 23.8 (dia_{maj}), 23.8 (dia_{maj}), 23.7 (dia_{min}), 22.1 (dia_{min}), 16.7 (dia_{min}), 16.6 (dia_{min}), 16.6 (dia_{maj}), 16.6 (dia_{maj}); ^{31}P NMR (162 MHz, CDCl_3): δ 25.0 (m, dia_{maj}), 22.4 (m, dia_{min}); HRMS (ESI-TOF): calcd. for $\text{C}_{13}\text{H}_{26}\text{N}_2\text{O}_4\text{P}$ [$M+\text{H}$] $^+$ m/z : 305.1630, found: 305.1626.



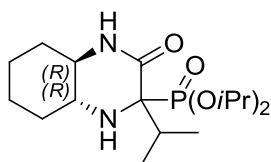
3ab diisopropyl-[4-methyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

Colorless solid; 266 mg; 80% yield in a diastereomeric ratio = 68:32; IR (KBr): 990, 1214, 1227, 1345, 1373, 1455, 1469, 1670, 2861, 2934, 2980, 3197, 3279 cm^{-1} ; ^1H NMR (400MHz, CDCl_3): 6.95-7.05 (s, br, 1H), 4.60-4.74 (m, 2H), 3.02-3.13 (m, 1H), 2.85-2.96 (m, 1H), 1.90-2.30 (br. s, 1H), 1.96-1.75 (m, 4H), 1.44 (d, $J = 15.9$ Hz, 3H), 0.41-0.56 (m, 16H); ^{13}C NMR (100MHz, CDCl_3): 170.1, 72.1 (d, $J = 6.9$ Hz), 71.4 (d, $J = 7.5$ Hz), 61.8 (d, $J = 134.2$ Hz), 57.9, 54.6, 30.7, 30.6, 24.5 (d, $J = 1.7$ Hz), 24.4, 24.2 (d, $J = 2.9$ Hz), 23.9, 23.9 (d, $J = 8.6$ Hz), 23.8 (d, $J = 9.7$ Hz), 22.1; ^{31}P NMR (162MHz, CDCl_3): δ 22.8 (qt, $J = 15.9, 6.5$ Hz); HRMS (ESI-TOF): calcd. for $\text{C}_{15}\text{H}_{30}\text{N}_2\text{O}_4\text{P}$ [$M+\text{H}$] $^+$ m/z : 333.1943, found: 333.1948.



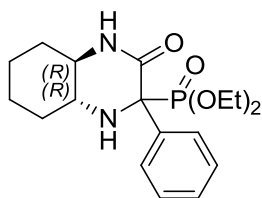
3ba diethyl-[4-isopropyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

Colorless solid; 308 mg; 93% yield in a diastereomeric ratio = 74:26; IR (KBr): 948, 960, 1030, 1052, 1226, 1342, 1454, 1668, 2939, 2980, 3200, 3323 cm^{-1} ; ^1H NMR (400MHz, CDCl_3): 6.22 (br. s, 1H), 6.20 (br. s, 1H), 4.08-4.26 (m, 8H), 2.94-3.08 (m, 3H), 2.63-2.77 (m, 1H), 2.55-2.63 (m, 2H), 2.01 (br. s, 2H), 1.71-1.85 (m, 8H), 1.16-1.38 (m, 20H), 1.04 (d, $J = 6.7$ Hz, 3H), 0.97 (d, $J = 6.7$ Hz, 6H), 0.93 (d, $J = 6.7$ Hz, 3H); ^{13}C NMR (100MHz, CDCl_3): 169.5, 169.4, 69.4 (d, $J = 128.1$ Hz), 68.2 (d, $J = 152.2$ Hz), 63.7 (d, $J = 7.5$ Hz), 63.6 (d, $J = 7.5$ Hz), 63.2 (d, $J = 6.9$ Hz), 62.7 (d, $J = 6.3$ Hz), 57.2 (d, $J = 8.0$ Hz), 57.1 (d, $J = 6.9$ Hz), 56.5, 54.9, 34.2, 33.8, 30.8, 30.7, 30.5, 24.4, 24.3, 23.8, 23.7, 19.6, 19.5, 17.5, 17.3, 17.2, 17.0, 16.7, 16.6, 16.6; $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ 25.6, 21.9; $\text{C}_{15}\text{H}_{29}\text{N}_2\text{O}_4\text{PNa}$ [$M+\text{Na}$] $^+$ m/z : 355.1763, found: 355.1753.



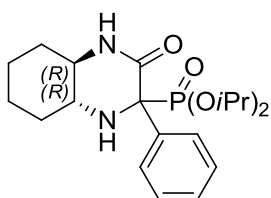
3bb diisopropyl-[4-isopropyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

Colorless solid; 341 mg; 95% yield in a diastereomeric ratio = 83:17; IR (KBr): 806, 1068, 1360, 1447, 1622, 1683, 2866, 2936, 3193 cm^{-1} ; ^1H NMR (400MHz, CDCl_3) : 6.01 (br. s, 1H), 5.93 (br. s, 1H), 4.78 (sept, $J = 6.1$ Hz, 1H), 4.77 (sept, $J = 6.1$ Hz, 1H), 4.09-4.17 (m, 2H), 3.09-3.15 (m, 1H), 2.90-3.08 (m, 3H), 2.76-2.84 (m, 1H), 2.59-2.67 (m, 1H), 1.90 (br. s, 2H), 1.67-1.79 (m, 4H), 1.23-1.39 (m, 36H), 1.01 (d, $J = 6.7$ Hz, 3H), 0.91-0.96 (m, 9H); ^{13}C NMR (100MHz, CDCl_3) : 170.1, 169.9, 72.0 (d, $J = 8.0$ Hz), 71.8 (d, $J = 8.0$ Hz), 71.3, 69.4 (d, $J = 128.7$ Hz, 2C overlapped), 57.2, 57.1, 56.9, 56.7, 54.5, 34.1, 33.8, 30.9, 30.8, 30.6, 24.4 (2C overlapped), 24.39, 24.3 (2C overlapped), 23.9, 23.88 (2C overlapped), 23.8 (2C overlapped), 23.7, 19.6, 19.5, 17.5, 17.4, 17.2, 17.0; $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ 23.6, 20.3; $\text{C}_{17}\text{H}_{33}\text{N}_2\text{O}_4\text{PNa}$ $[M+\text{Na}]^+$ m/z : 383.2076, found: 383.2087.



3ca diethyl-[4-phenyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

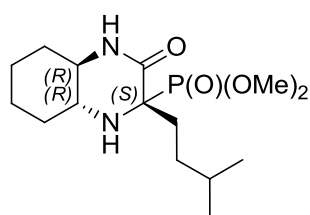
Colorless solid; 325 mg; 89% yield in a diastereomeric ratio = 83:17; IR (Nujol): 1029, 1204, 1342, 1394, 1450, 1674, 2426, 3891 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.97-8.02 (m, 1H), 7.88-7.92 (m, 2H), 7.70-7.75 (m, 1H), 7.23-7.36 (m, 6H), 6.34 (br. s, 1H), 6.32 (br. s, 1H), 4.20-4.27 (m, 2H), 4.10-4.23 (m, 2H), 3.90-4.05 (m, 2H), 3.77-3.85 (m, 2H), 3.17-3.28 (m, 2H), 2.96-3.12 (m, 1H), 2.52 (br. s, 2H), 2.29-2.34 (m, 1H), 1.93-1.96 (m, 2H), 1.56-1.78 (m, 6H) 1.42-1.10 (m, 8H), 1.28 (t, $J = 7.3$ Hz, 3H), 1.25 (t, $J = 7.03$ Hz, 3H), 1.18 (t, $J = 7.3$ Hz, 3H), 1.11 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100MHz, CDCl_3) : 167.7, 167.5, 137.6, 136.4, 128.5, 128.49, 128.1, 128.04, 128.01, 127.9, 127.8, 127.78, 127.3, 127.2, 68.7 (d, $J = 159.7$ Hz), 67.7 (d, $J = 140.2$ Hz) 64.6 (d, $J = 6.9$ Hz), 64.1, 64.0, 63.99, 63.9, 63.8, 58.6, 56.7, 56.0, 53.6 (d, $J = 11.5$ Hz), 30.9, 30.87, 30.6, 30.2, 24.5, 24.4, 23.7, 23.69, 16.5 (q, $J = 9.8$ Hz), 16.4 (q, $J = 10.3$ Hz); $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ 21.3, 19.1; HRMS (ESI-TOF): calcd. for $\text{C}_{18}\text{H}_{28}\text{N}_2\text{O}_4\text{P}$ $[M+\text{H}]^+$ m/z : 367.1787, found: 367.1781.



3cb diisopropyl-[4-phenyl-(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

Colorless solid; 310 mg; 85% yield in a diastereomeric ratio = 85:15; IR (KBr): 986, 1106, 1228, 1345, 1373, 1385, 1447, 1671, 2861, 2934, 2979, 3207 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.89-7.93 (m, 2H), 7.69-7.72 (m, 2H), 7.23-7.35 (m, 6H), 6.11 (br. s, 1H), 6.01 (br. s, 1H), 4.89 (oct., $J = 6.7$ Hz, 1H), 4.75 (oct., $J = 6.7$ Hz, 1H), 4.59 (oct., $J = 6.7$ Hz, 1H), 4.53 (oct., $J = 6.7$ Hz, 1H), 3.21-3.25 (m, 1H), 3.11-3.12 (m, 1H), 2.93-3.02 (m, 1H), 2.48 (br. s, 2H), 2.26-2.32 (m, 1H), 1.66-1.92 (m, 8H), 1.31 (d, $J = 6.1$ Hz, 3H), 1.28 (d, $J = 6.1$ Hz, 3H), 1.27 (d, $J = 6.1$ Hz, 3H), 1.21 (d, $J = 6.4$ Hz, 3H), 1.19 (d, $J = 6.4$ Hz, 3H), 1.18 (d, $J = 6.7$ Hz, 3H), 1.16 (d, $J = 6.7$ Hz, 3H), 1.11-1.44 (m, 8H)

1.01 (d, $J = 6.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 168.2, 167.9 (d, $J = 5.8$ Hz), 138.4, 137.0 (d, $J = 2.9$ Hz), 128.2 (d, $J = 2.3$ Hz), 127.95 (2C overlapped), 127.9 (2C overlapped), 127.85 (d, $J = 1.7$ Hz, 2C overlapped), 127.7 (d, $J = 2.3$ Hz), 127.6 (d, $J = 1.7$ Hz), 127.4 (d, $J = 5.2$ Hz), 72.9 (d, $J = 7.5$ Hz), 72.5 (d, $J = 7.5$ Hz, 2C overlapped), 72.4 (d, $J = 8.0$ Hz), 68.8 (d, $J = 160.3$ Hz), 67.8 (d, $J = 140.8$ Hz), 58.6, 56.9, 55.7, 53.5 (d, $J = 12.1$ Hz), 30.9, 30.8, 30.7, 30.3, 24.5 (d, $J = 5.8$ Hz), 24.4 (3C overlapped), 24.3 (d, $J = 1.7$ Hz), 24.2 (d, $J = 2.9$ Hz), 24.1 (d, $J = 3.5$ Hz), 23.8 (2C overlapped), 23.6 (d, $J = 5.8$ Hz), 23.57 (d, $J = 5.8$ Hz), 23.4 (d, $J = 5.8$ Hz); $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ 19.6, 17.3; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{31}\text{N}_2\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ m/z : 417.1919, found: 417.1917.



3fa dimethyl-[4-isopentyl-(1*R*,4*S*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

Colorless solid; 57 mg; yield = 52% in a diastereomeric ratio >98:2; mp.

139-141 °C; $[\alpha]_D^{20} + 30$ (c 0.10, CH_2Cl_2); IR (KBr): 774, 833, 1037, 1062, 1217, 1351, 1468, 1662, 2868, 2952, 3258 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 5.85 (br. s, 1H), 3.84 (dd, $J = 20.2, 10.4$ Hz, 6H), 3.10-3.16 (m, 1H), 2.56-2.61 (m, 1H), 2.20-2.32 (m, 1H), 1.72-1.89 (m, 6H), 1.53 (non, $J = 6.7$ Hz, 1H), 1.18-1.38 (m, 6H), 0.90 (d, $J = 6.4$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 168.8, 65.3 (d, $J = 158.6$ Hz), 57.2, 56.2 (d, $J = 9.2$ Hz), 55.2 (d, $J = 7.5$ Hz), 54.0 (d, $J = 7.5$ Hz), 33.7, 32.8 (d, $J = 9.8$ Hz), 30.8, 30.7, 28.5, 24.3, 23.6, 22.8, 22.5; $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ 24.2; HRMS (ESI-TOF) calcd. for $\text{C}_{15}\text{H}_{30}\text{N}_2\text{O}_4\text{P}$ $[\text{M}+\text{H}]^+$ m/z : 333.1943, found: 333.1938.

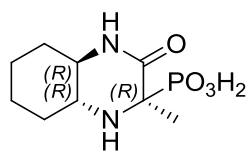
Aminophosphonic acids

Procedures

General procedure for synthesis of acids 4a-f

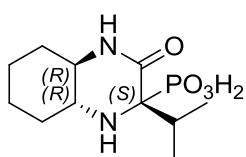
To the solution of imine (1.00 mmol, 1.00 equiv) in CH_2Cl_2 (8 ml) bromotrimethylsilane (1.10 mmol, 0.145 ml, 1.10 equiv) and subsequently tris(trimethylsilyl) phosphite (1.10 mmol, 0.367 ml, 1.10 equiv) were added. The resulting reaction mixture was flushed with argon and stirred for 120 h at room temperature and afterwards the solvent was removed under reduced pressure. The resulting residue was dissolved in methanol (10 ml) and stirred for 12 h at room temperature. After that time the solvent was removed under reduced pressure, and the product was purified by washing with methanol (3 x 2 ml) or by crystallization (abs. EtOH / Et₂O 1:5 v/v), yielding the desired product as a colorless solid.

Synthesis



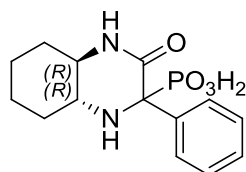
4a [4-methyl-(1*R*,4*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

Colorless solid; 198 mg; yield = 80 % in a diastereomeric ratio >98:2; mp. 270-271 °C; $[\alpha]^{20}_D$ -44 (c 0.43, H₂O); IR (KBr): 821, 932, 1116, 1455, 1467, 1606, 1670, 2924, 2948, 3426 cm⁻¹; ¹H NMR (600 MHz, D₂O): δ 3.55-3.60 (m, 1H), 3.35-3.42 (m, 1H); 1.90-2.01 (m, 2H), 1.65-1.70 (m, 2H), 1.61 (dd, *J* = 12.8, 4.9 Hz, 3H), 1.22-1.46 (m, 4H); ¹³C NMR (151 MHz, D₂O): δ 168.6, 63.0 (d, *J*_{C-P} = 189.9 Hz), 55.3, 54.1, 30.2, 27.1, 23.7, 22.5, 19.3; ³¹P NMR (243 MHz, D₂O): δ 9.7 (q, *J* = 13.1 Hz); HRMS (ESI-TOF) calcd. for C₉H₁₈N₂O₄P [*M*+H]⁺ *m/z*: 249.1004 found: 249.1016.



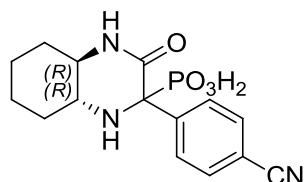
4b [4-isopropyl-(1*R*,4*S*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

Colorless solid; 273 mg; 99% yield in a diastereomeric ratio >98:2; mp. 220-222 °C; $[\alpha]^{20}_D$ -55 (c 0.15, H₂O); IR (KBr): 912, 1042, 1083, 1218, 1342, 1661, 2933, 3425 cm⁻¹; ¹H NMR (400 MHz, D₂O): δ 3.44-3.51 (m, 1H), 3.34-3.40 (m, 1H), 2.80 (dhept, *J*=7.0Hz, *J*=6.7Hz, 1H), 2.07-2.10 (m, 1H), 1.95-1.97 (m, 1H), 1.76-1.79 (m, 1H), 1.66-1.69 (m, 1H), 1.48-1.57 (m, 1H), 1.37-1.56 (m, 3H), 1.02 (d, *J* = 7.3 Hz, 3H), 0.92 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, D₂O): δ 168.1 (d, *J* = 2.3Hz), 71.3 (d, *J* = 126.4 Hz), 56.4, 52.5, 32.2, 30.4, 26.6, 23.6, 22.4, 16.4 (d, *J* = 10.3 Hz), 16.1; ³¹P NMR (162 MHz, D₂O): δ 8.9 (d, *J* = 6.5 Hz); HRMS (ESI-TOF) calcd. for C₁₁H₂₂N₂O₄P [*M*+H]⁺ *m/z*: 277.1317, found: 277.1319.



4c [4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

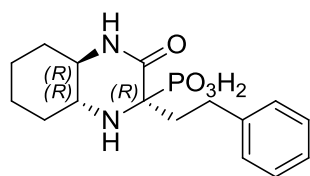
Colorless solid; 248 mg; 80% yield in a diastereomeric ratio >98:2 (diastereomeric ratio of crude product 85:15); mp. 196-198 °C; $[\alpha]^{20}_D$ -35 (c 0.29, H₂O); IR (KBr): 909, 1087, 1239, 1349, 1447, 1460, 1591, 1646, 2865, 2939, 3369 cm⁻¹; ¹H NMR (600 MHz, D₂O): δ 7.36-7.55 (m, 5H), 3.63-3.66 (m, 1H), 3.40-3.45 (m, 1H), 1.99-2.10 (m, 2H), 1.68-1.76 (m, 2H), 0.87-1.40 (m, 4H); ¹³C NMR (151 MHz, D₂O): δ 166.7, 133.8, 129.5, 129.1, 128.3, 69.7 (d, *J* = 185.8 Hz), 55.8, 53.0, 30.3, 27.0, 23.5, 22.5; ³¹P{¹H} NMR (243 MHz, D₂O): δ 8.5; HRMS (ESI-TOF) calcd. for C₁₄H₂₀N₂O₄P [*M*+H]⁺ *m/z*: 311.1161, found: 311.1155.



4d [4-(4-cyanophenyl)-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

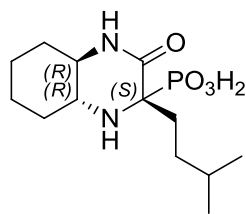
Colorless solid; 251 mg; 75% yield in a diastereomeric ratio >98:2 (diastereomeric ratio of crude product 88:12); mp. 176-178 °C; $[\alpha]^{20}_D$ +18 (c 0.11, H₂O); IR (KBr): 564, 1312, 1335, 1455, 1575, 1669, 2231, 2946, 3421 cm⁻¹; ¹H NMR (400 MHz, D₂O): δ 7.71-7.81 (m, 4H), 3.46-3.57 (m, 1H), 2.81-2.91 (m, 1H), 1.91-2.01 (m, 1H), 1.79-1.88 (m, 1H),

1.55-1.72 (m, 2H), 1.02-1.50 (m, 4H); ^{13}C NMR (100 MHz, D_2O): δ 166.7, 138.0 (d, $J = 4.2$ Hz), 133.1 (2C), 129.7, 129.7, 118.8, 112.6, 69.1 (d, $J = 128.1$ Hz), 54.3 (d, $J = 3.5$ Hz), 53.2, 30.5, 26.6, 23.5, 22.4; $^{31}\text{P}\{^1\text{H}\}$ NMR (243 MHz, D_2O): δ 7.5; HRMS (ESI-TOF): calcd. for $\text{C}_{15}\text{H}_{17}\text{N}_3\text{O}_4\text{P}$ [$M-\text{H}$] $^-$ m/z 334.0957, found: 334.0959.



4e [4-phenethyl-(1*R*,4*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

Colorless solid; 237 mg; 70% yield in a diastereomeric ratio >98:2 (diastereomeric ratio of crude product 89:11); mp. 224-225 °C; $[\alpha]^{20}_{\text{D}} +15$ (c 0.13, DMSO); IR (KBr): 703, 930, 1110, 1458, 1605, 1669, 2938 cm^{-1} ; ^1H NMR (400 MHz, D_2O): δ 7.68 (br. s, 1H), 7.12-7.25 (m, 5H), 3.19-3.22 (m, 1H), 2.96-3.01 (m, 2H), 2.36-2.46 (m, 2H), 2.25-2.28 (m, 1H), 1.62-1.90 (m, 5H), 1.07-1.26 (m, 4H); ^{13}C NMR (100 MHz, D_2O): δ 168.8, 142.9, 128.8 (2C overlapped), 128.7 (2C overlapped), 126.1, 65.4 (d, $J = 125.8$ Hz), 56.2, 55.0, 38.2, 30.9, 30.1, 30.06, 24.6, 23.8; $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, D_2O): δ 17.2; HRMS (ESI-TOF) calcd. for $\text{C}_{16}\text{H}_{24}\text{N}_2\text{O}_4\text{PNa}$ [$M+\text{H}$] $^+$ m/z : 339.1474, found: 339.1462.



4f [4-isopentyl-(1*R*,4*S*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

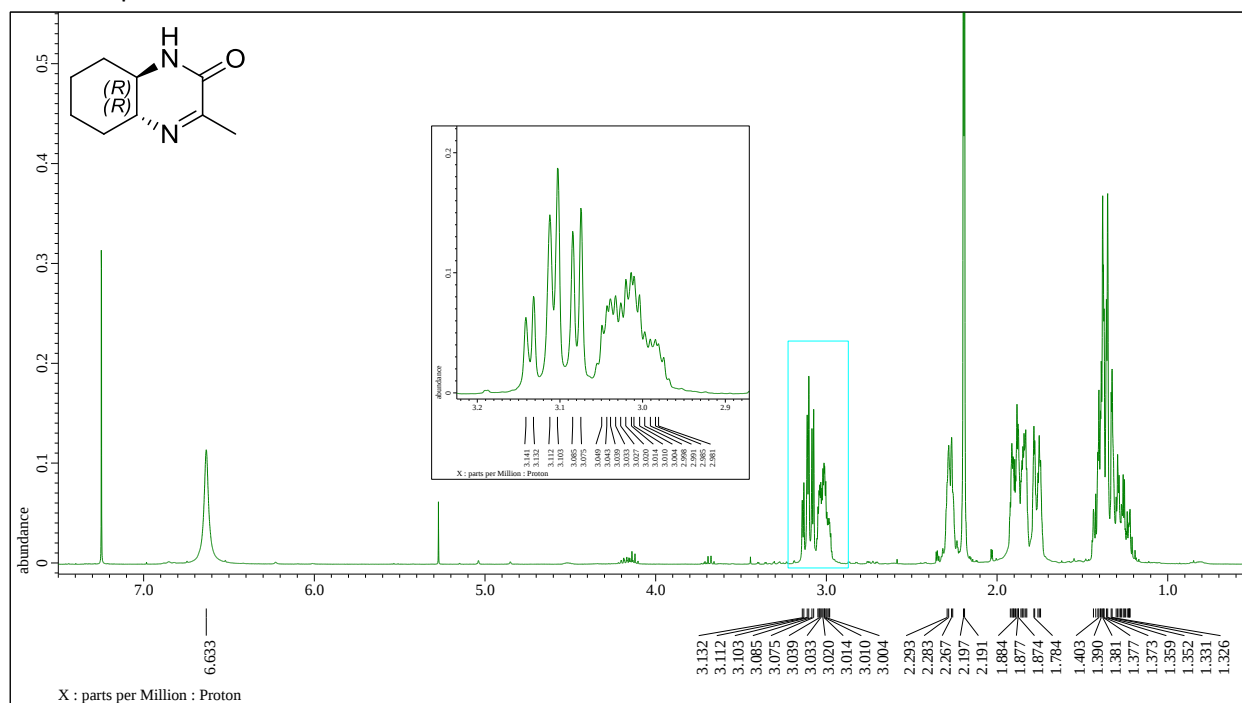
Colorless solid; 198 mg; 65% yield in a diastereomeric ratio >98:2; mp. 226-227 °C; $[\alpha]^{20}_{\text{D}} - 46$ (c 0.54, H_2O); IR (KBr): 922, 1103, 1165, 1353, 1461, 1607, 1672, 2871, 2954, 3203, 3403 cm^{-1} ; ^1H NMR (400 MHz, D_2O): δ 3.52 (dt, $J = 11.0, 4.0$ Hz, 1H), 3.35 (dt, $J = 10.4, 4.0$ Hz, 1H), 1.90-2.16 (m, 4H), 1.64-1.76 (m, 2H), 1.18-1.48 (m, 6H), 1.06 (sep, $J = 4.9$ Hz, 1H), 0.75 (dd, $J = 6.4, 4.0$ Hz, 6H); ^{13}C NMR (151 MHz, D_2O): δ 168.3, 66.8 (d, $J = 126.4$ Hz), 55.9, 52.9, 31.8, 31.6 (d, $J = 4.6$ Hz), 30.4, 27.9, 26.9, 23.6, 22.5, 21.5, 21.5; ^{31}P NMR (162 MHz, D_2O): δ 8.9 (dd, $J = 18.7, 5.6$ Hz); HRMS (ESI-TOF) calcd. for $\text{C}_{13}\text{H}_{25}\text{N}_2\text{O}_4\text{PNa}$ [$M+\text{Na}$] $^+$ m/z : 327.1450, found: 327.1474.

Spectra

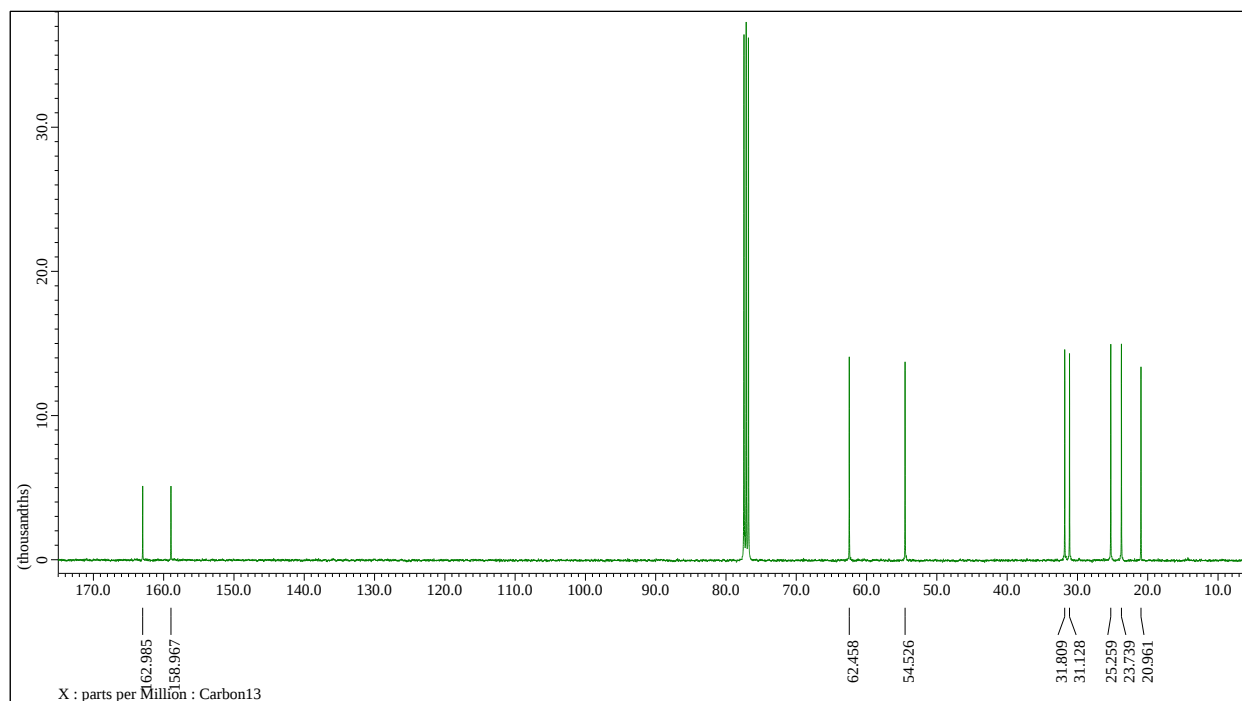
Imines

1a 4-methyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

¹H NMR spectrum of **1a**

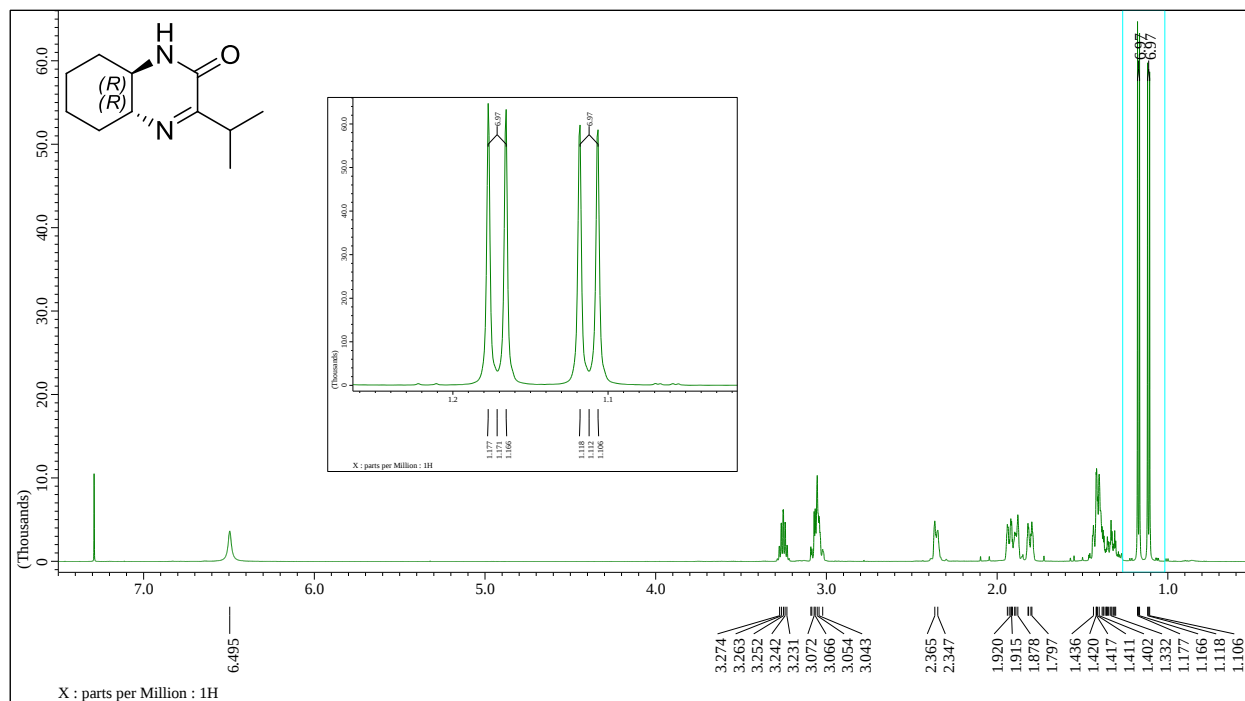


¹³C NMR spectrum of **1a**

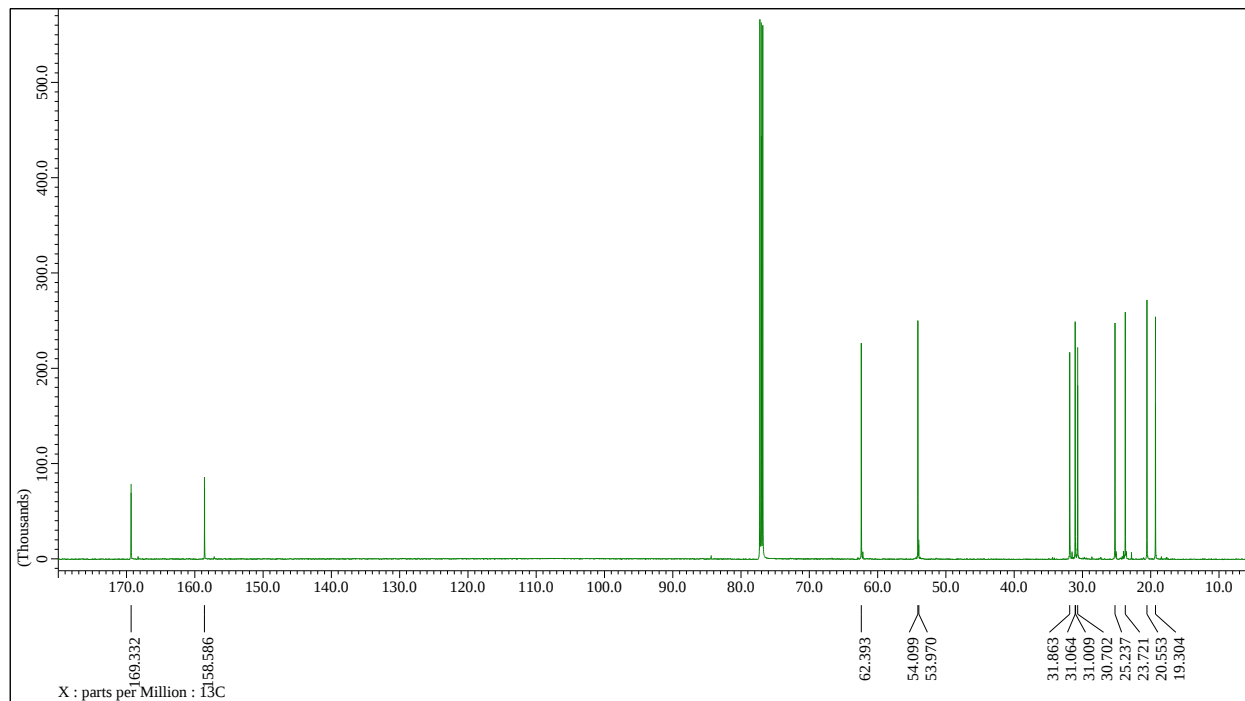


1b 4-isopropyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

¹H NMR spectrum of **1b**

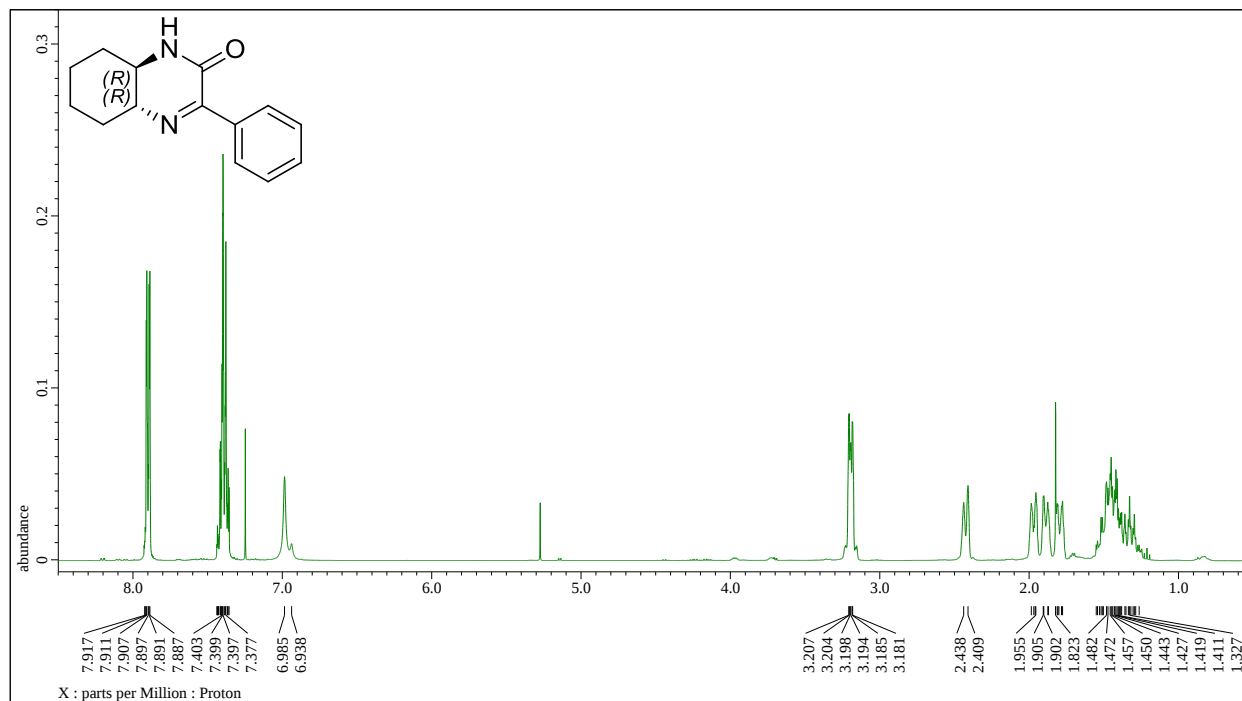


¹³C NMR spectrum of **1b**

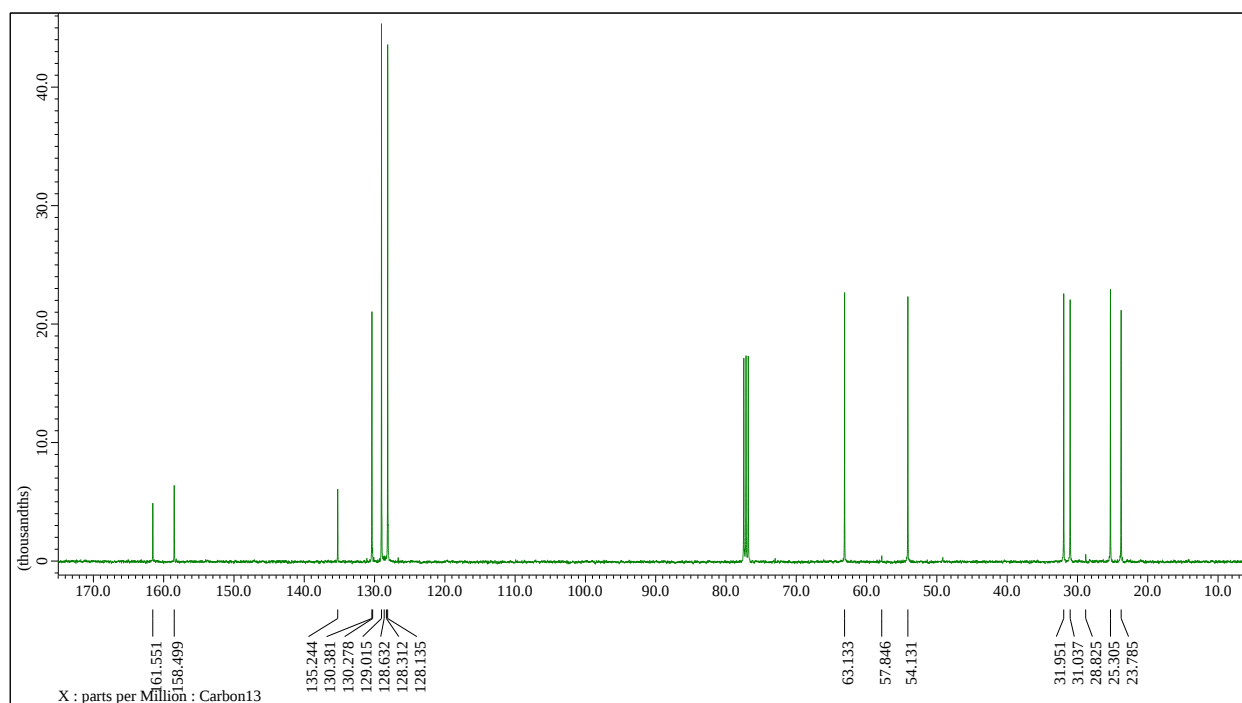


1c 4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

¹H NMR spectrum of **1c**

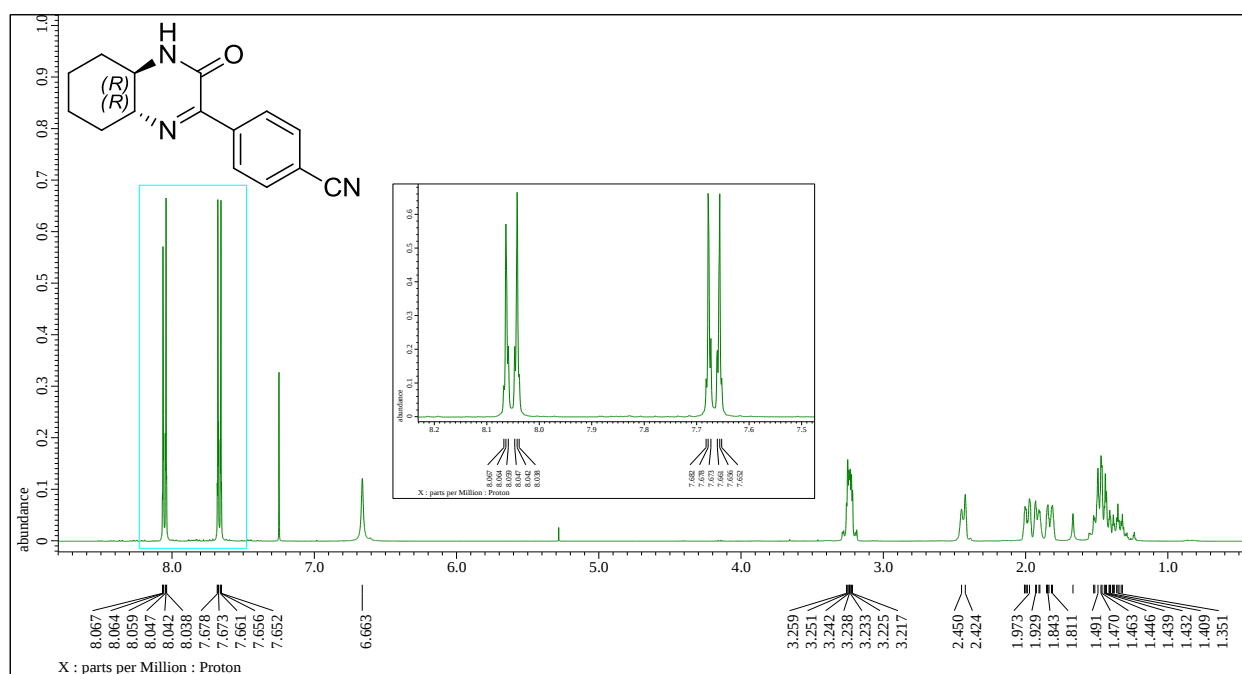


¹³C NMR spectrum of **1c**

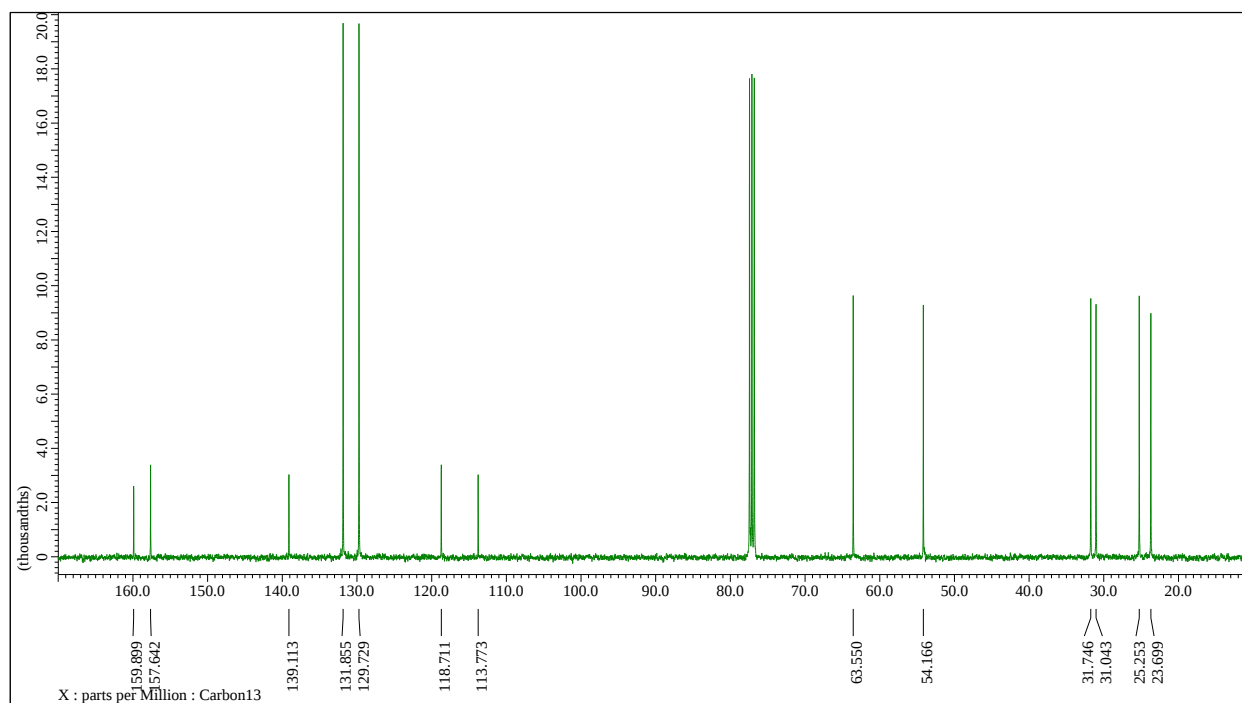


1d 4-((1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl-4-ene)-benzonitrile

^1H NMR spectrum of **1d**

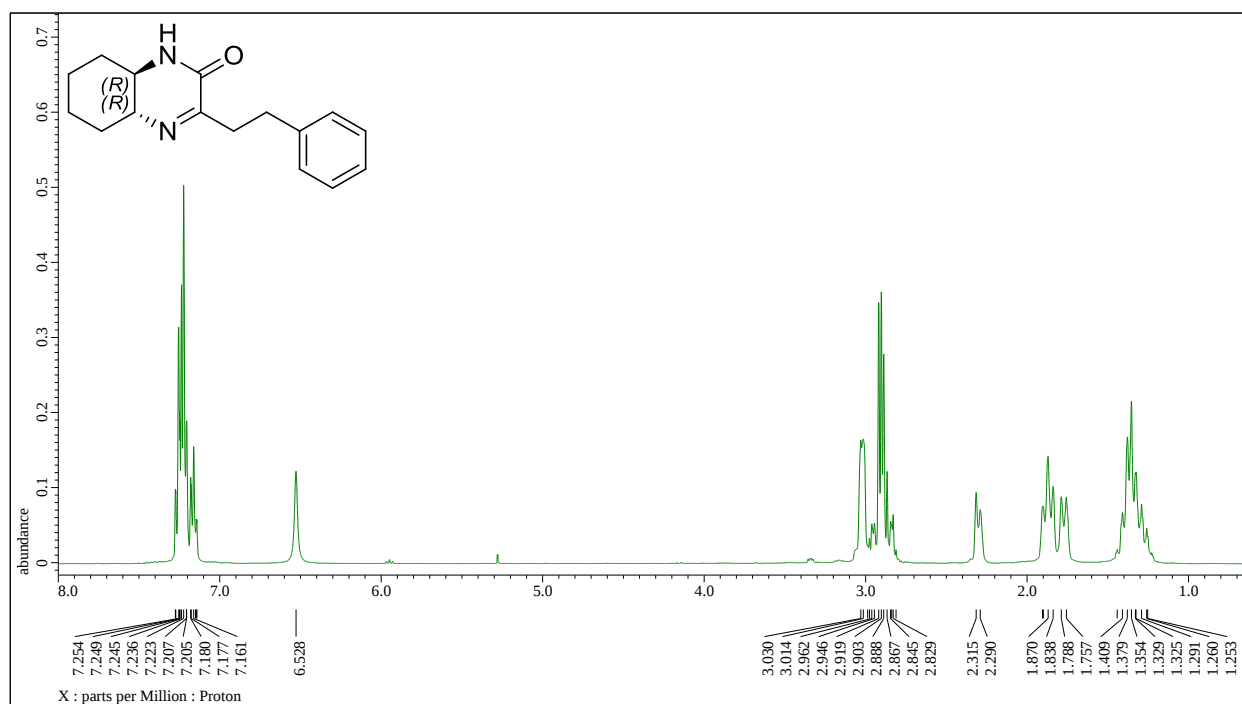


^{13}C NMR spectrum of **1d**

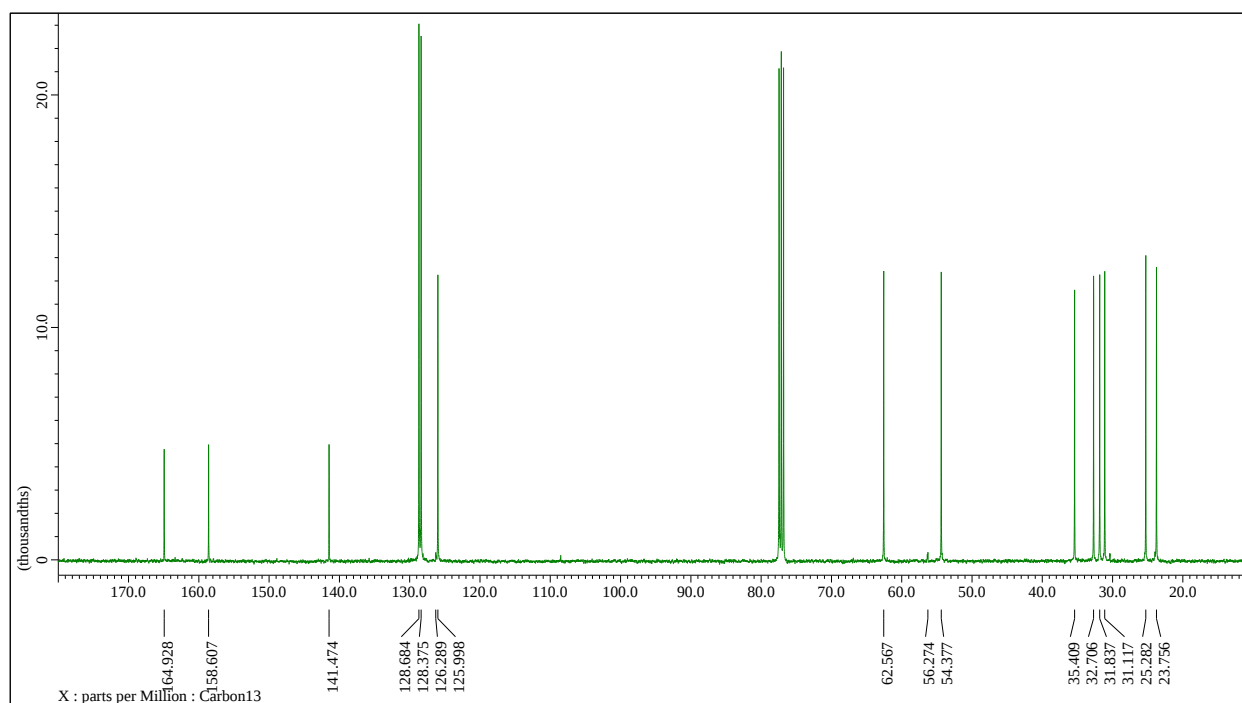


1e 4-phenethyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene

¹H NMR spectrum of **1e**

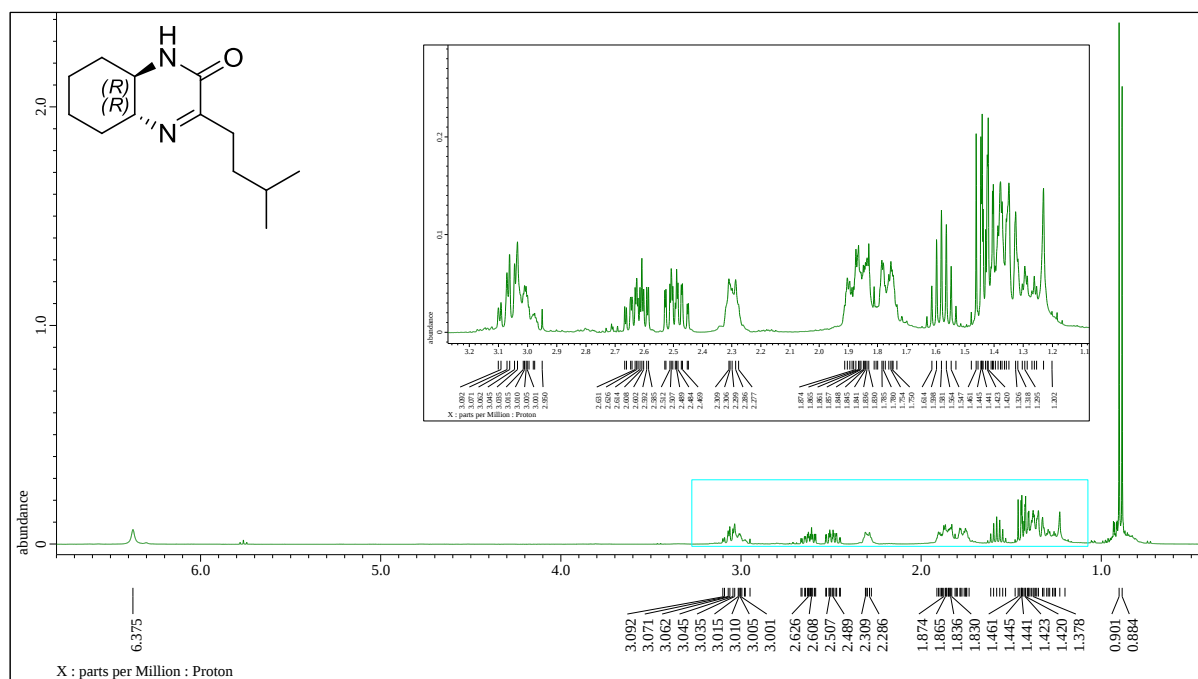


¹³C NMR spectrum of **1e**

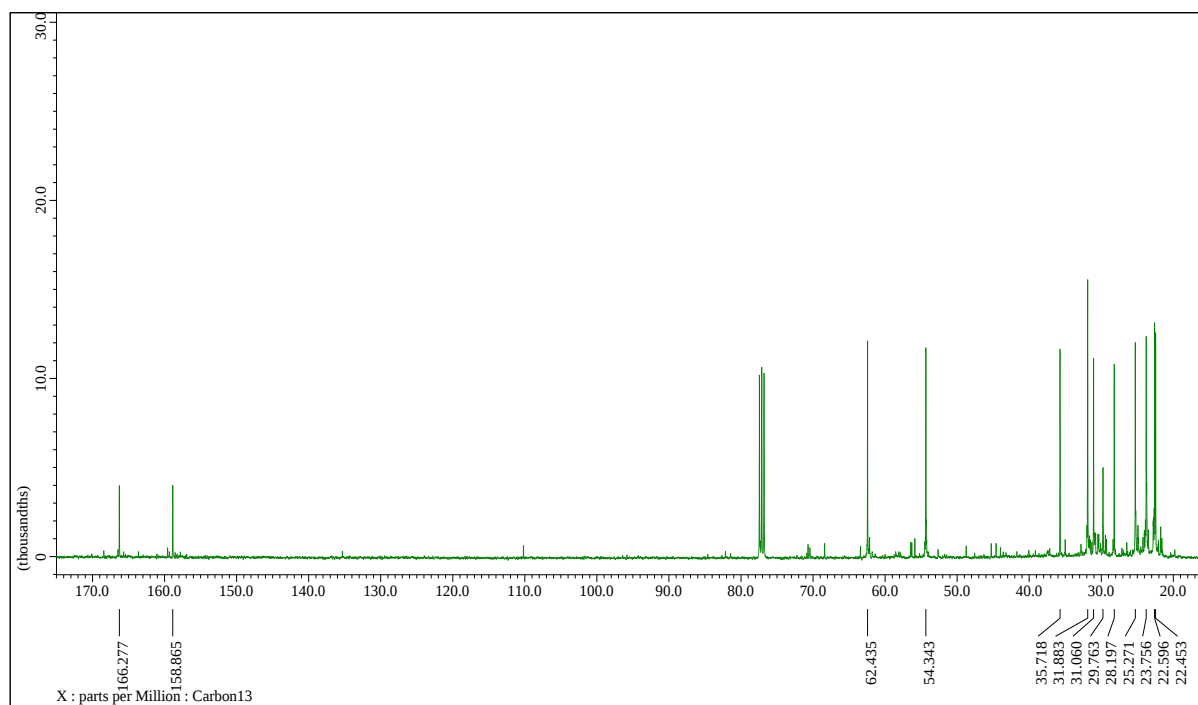


1f 4-Isopentyl-[(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene]

¹H NMR spectrum of **1f**



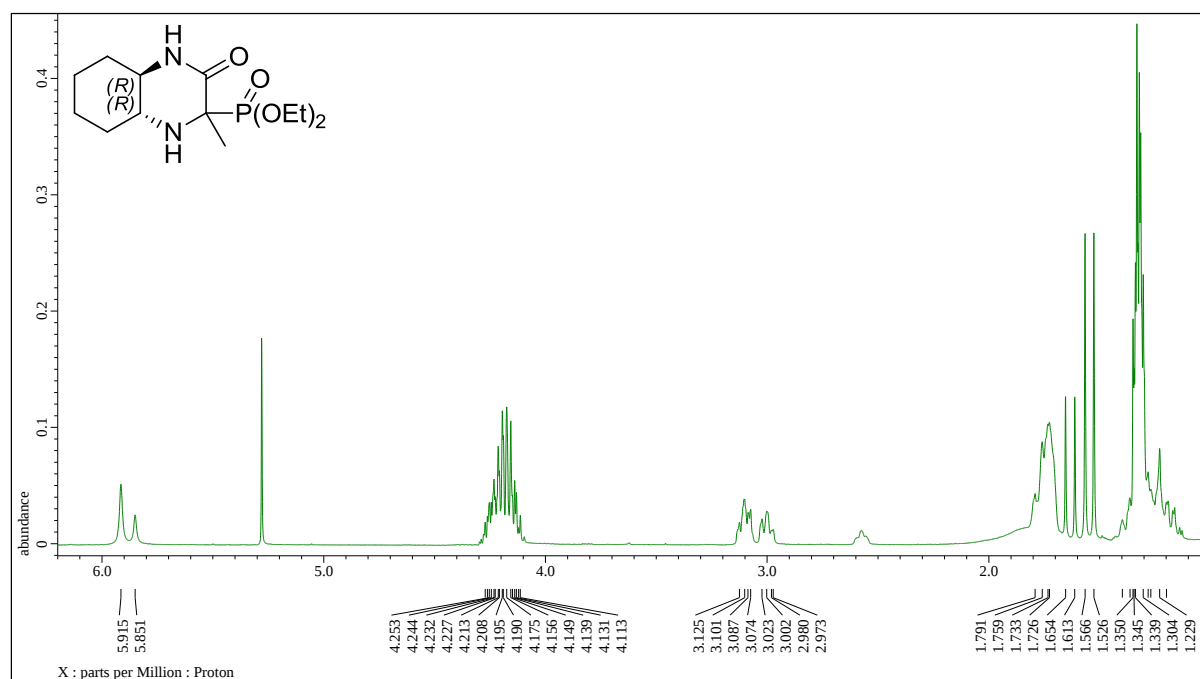
¹³C NMR spectrum of **1f**



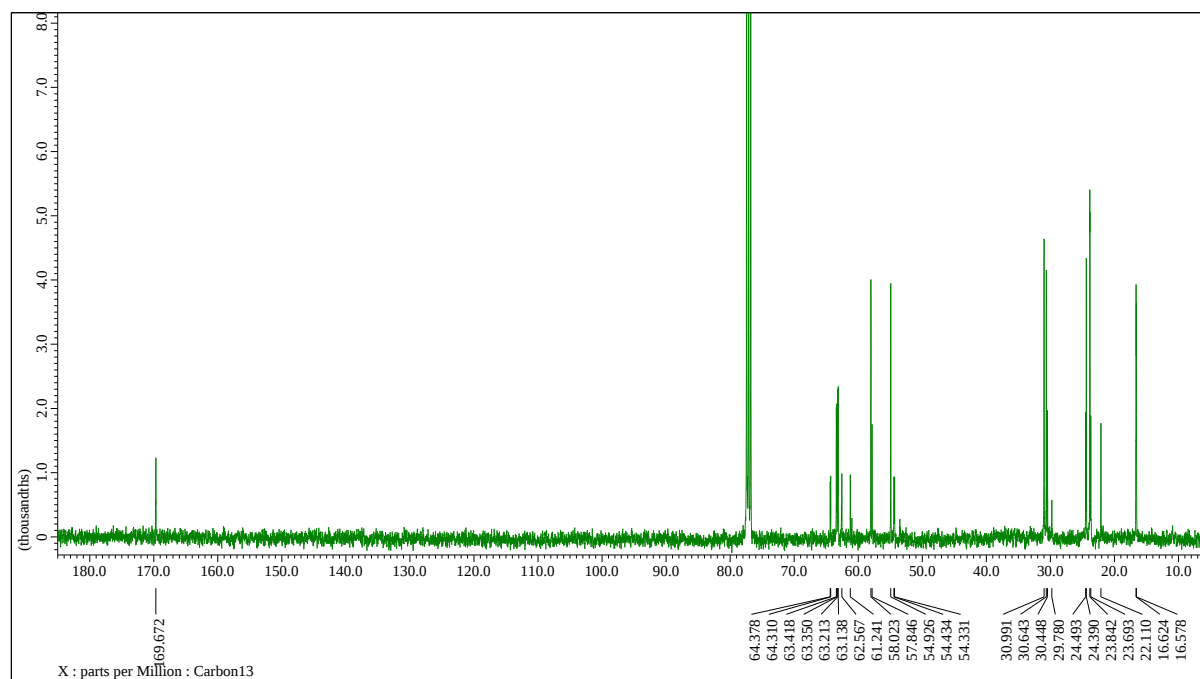
Dialkyl aminophosphonic acid esters

3aa diethyl-[4-methyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

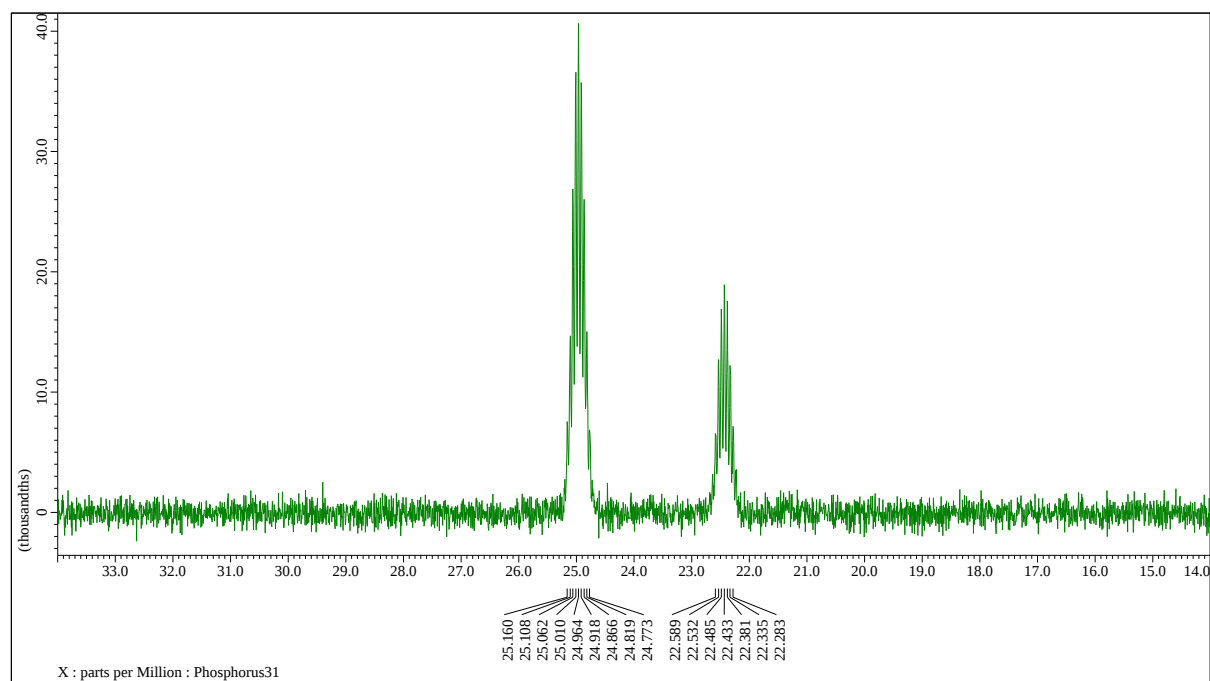
¹H NMR spectrum of **3aa**



¹³C NMR spectrum of **3aa**

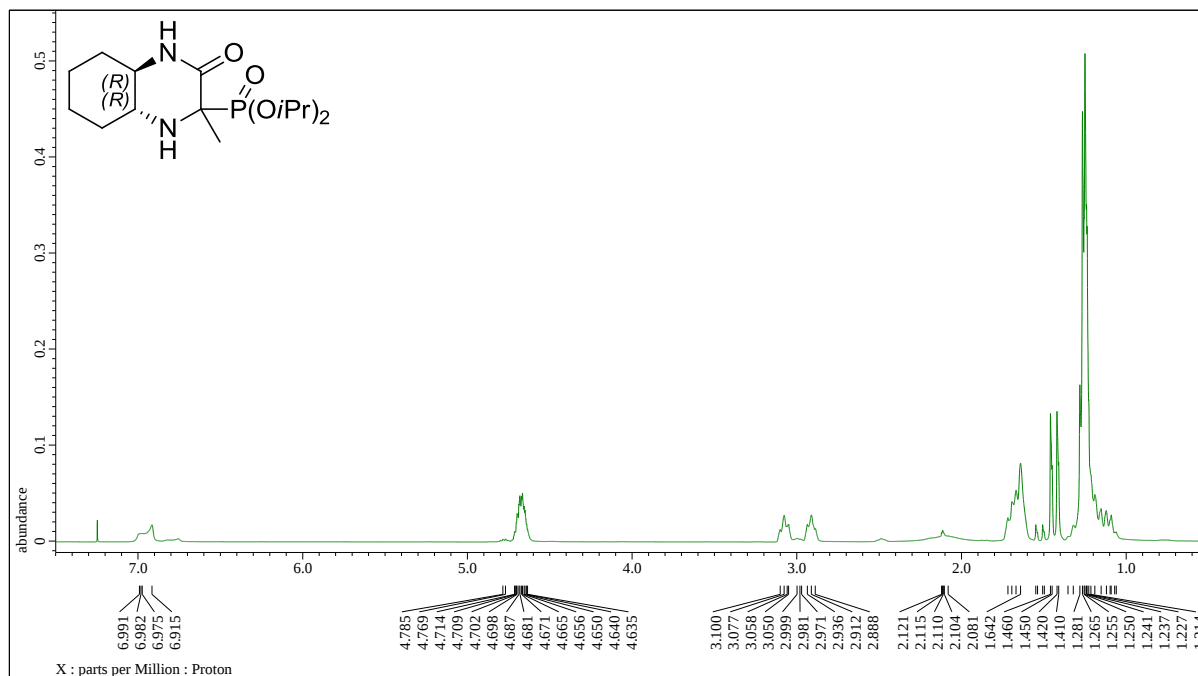


^{31}P NMR spectrum of **3aa**

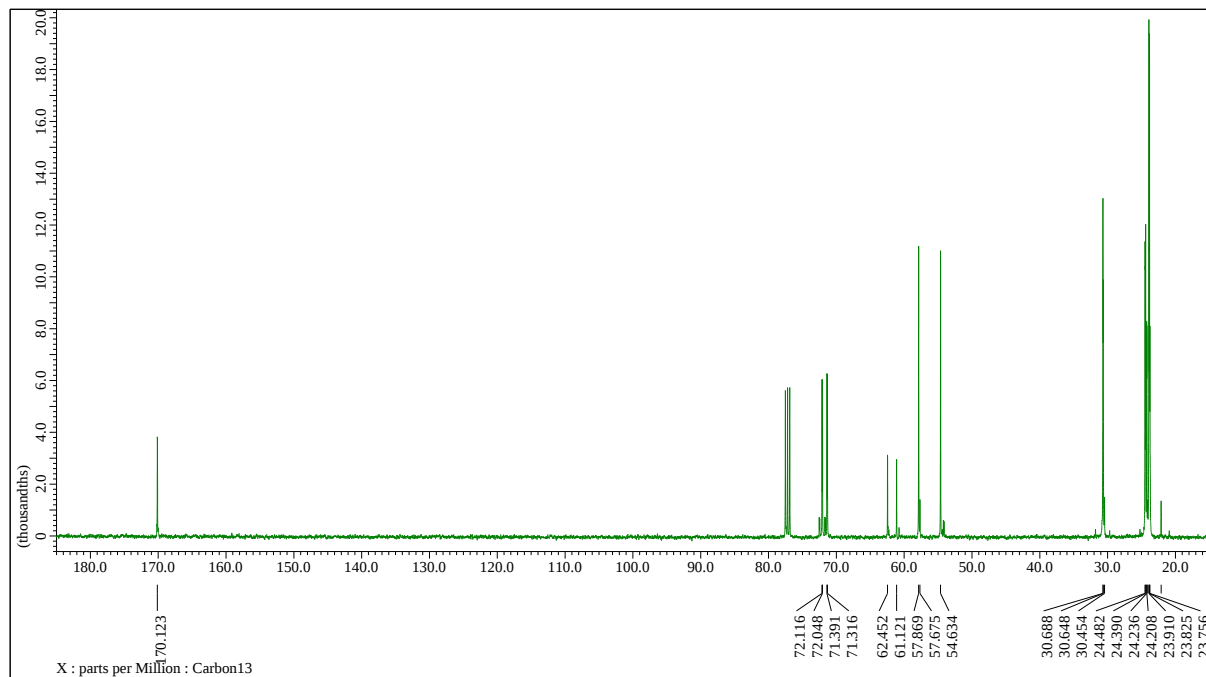


3ab diisopropyl-[4-methyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

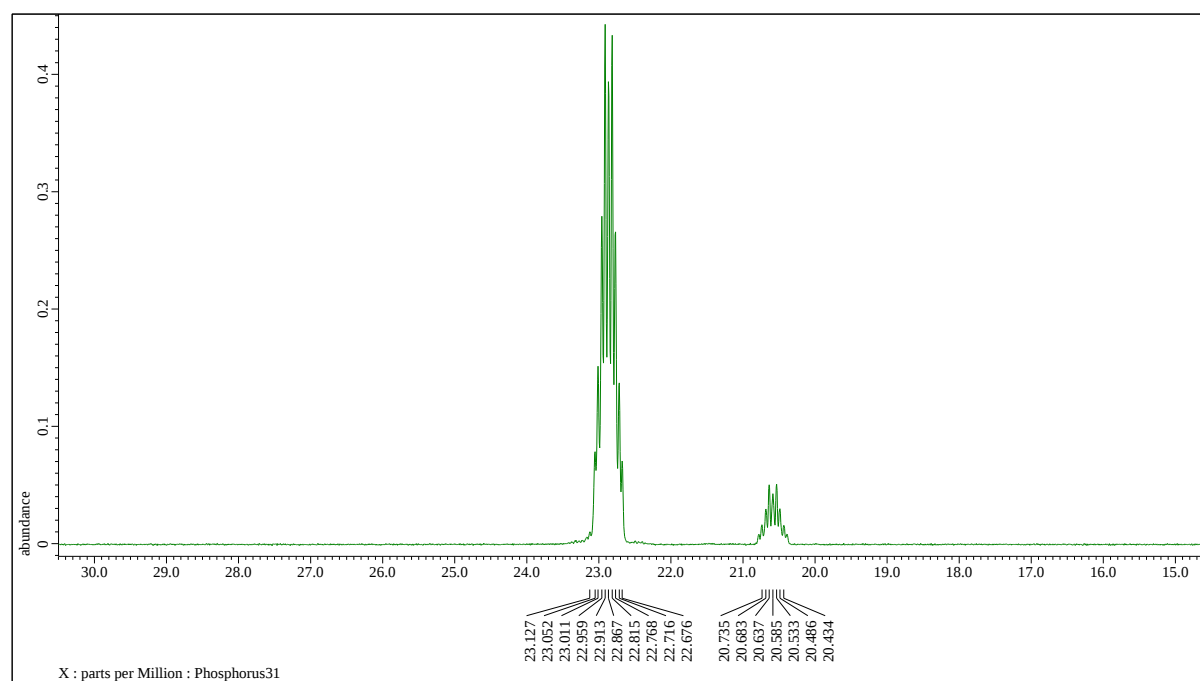
¹H NMR spectrum of **3ab**



¹³C NMR spectrum of **3ab**

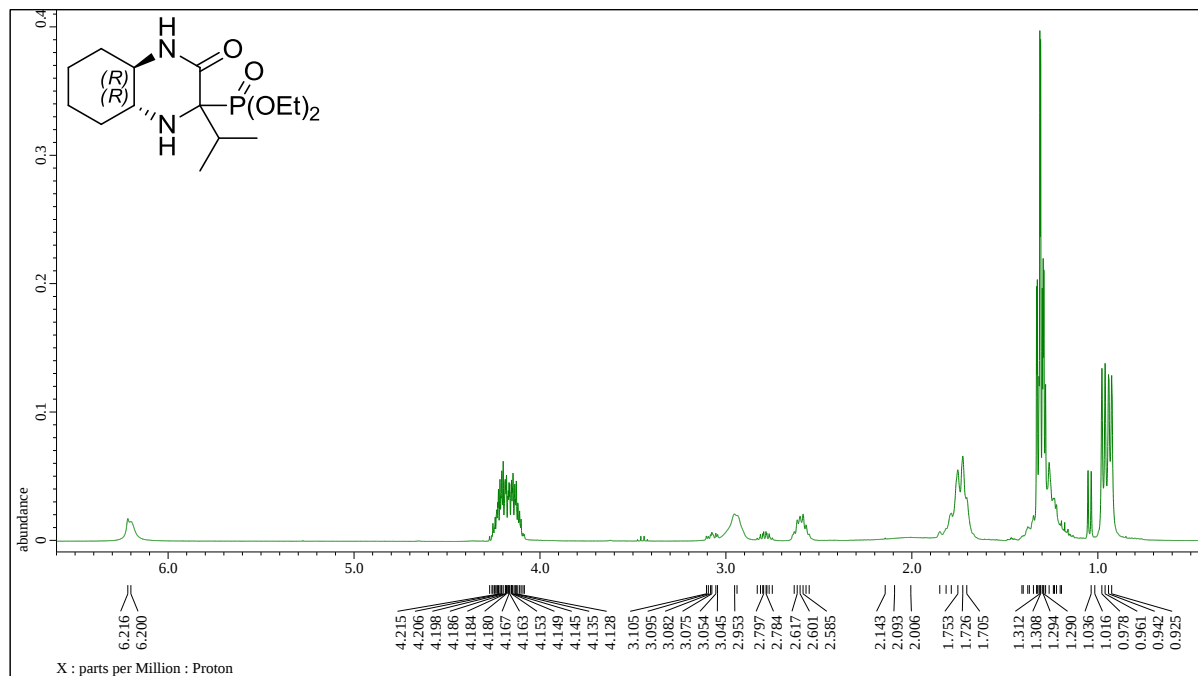


^{31}P NMR spectrum of **3ab**

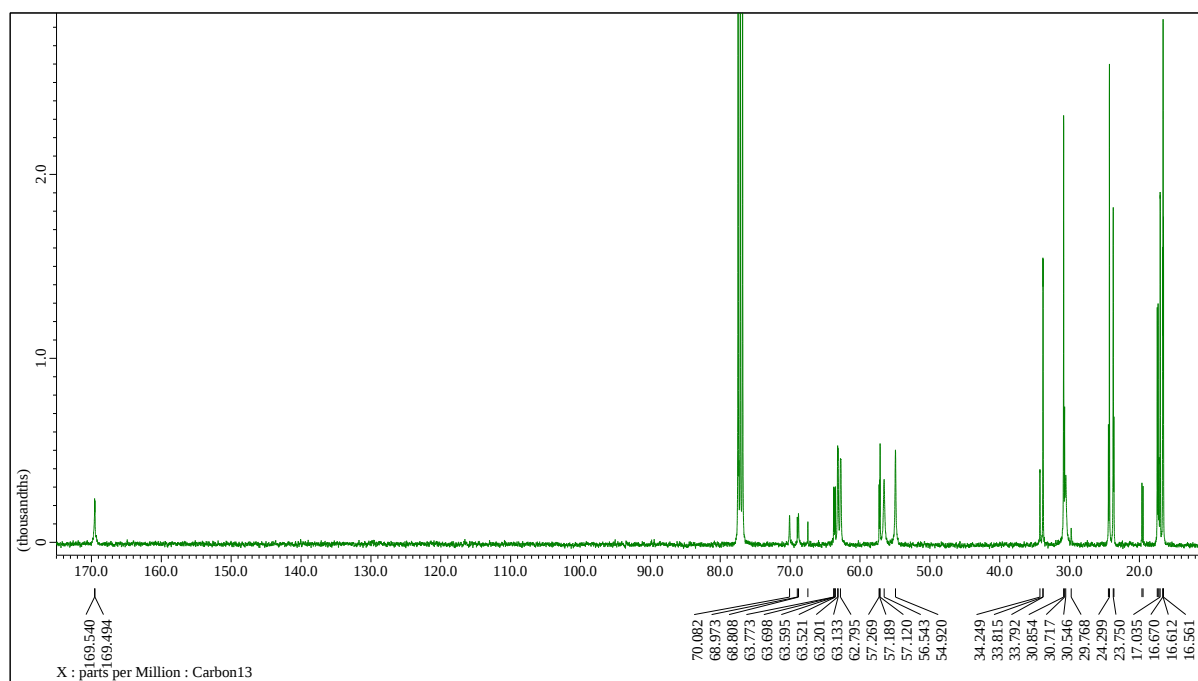


3ba diethyl-[4-isopropyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

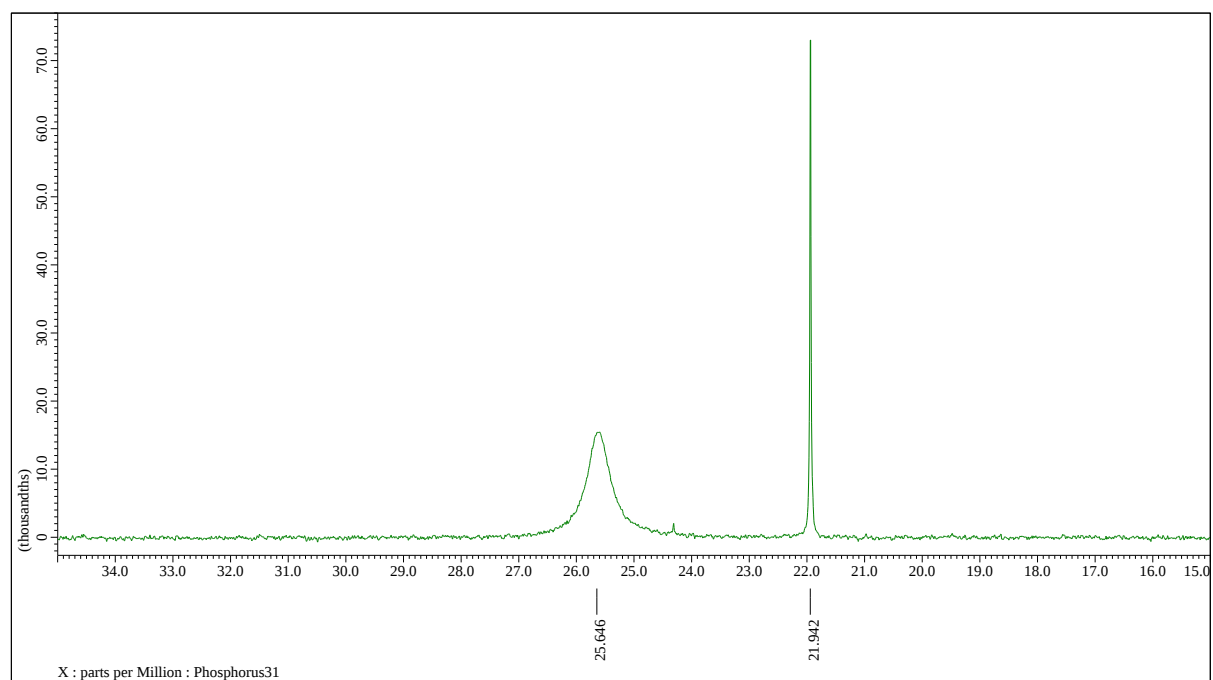
¹H NMR spectrum of **3ba**



¹³C NMR spectrum of **3ba**

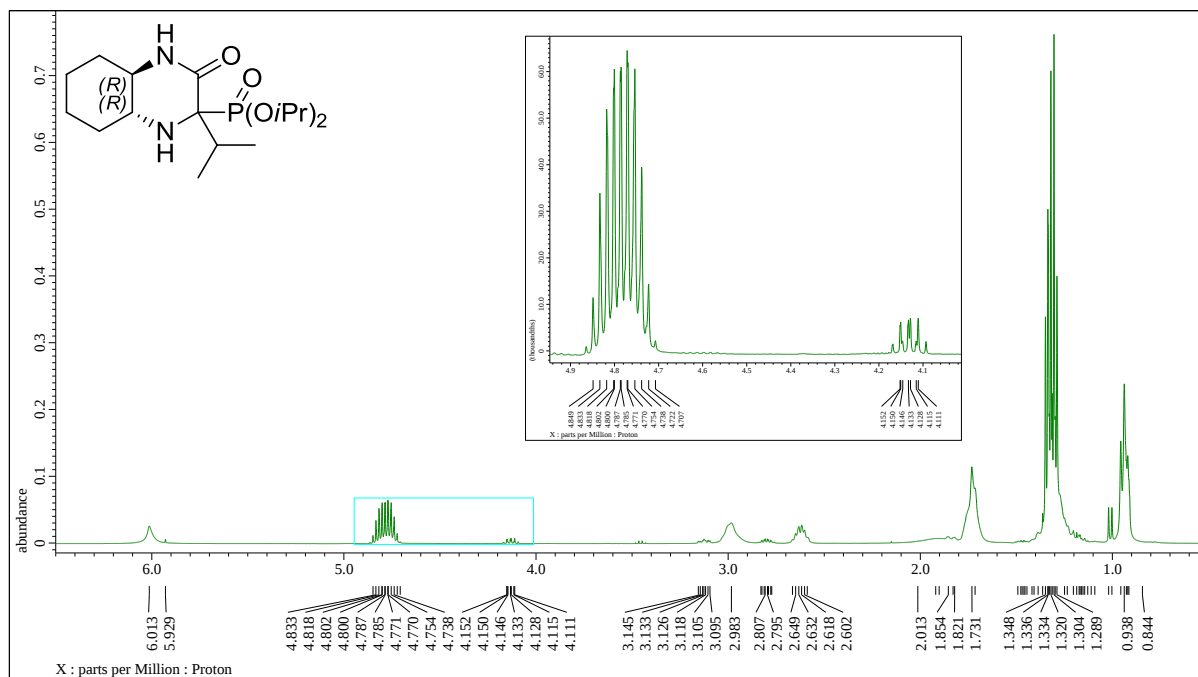


^{31}P NMR spectrum of **3ba**

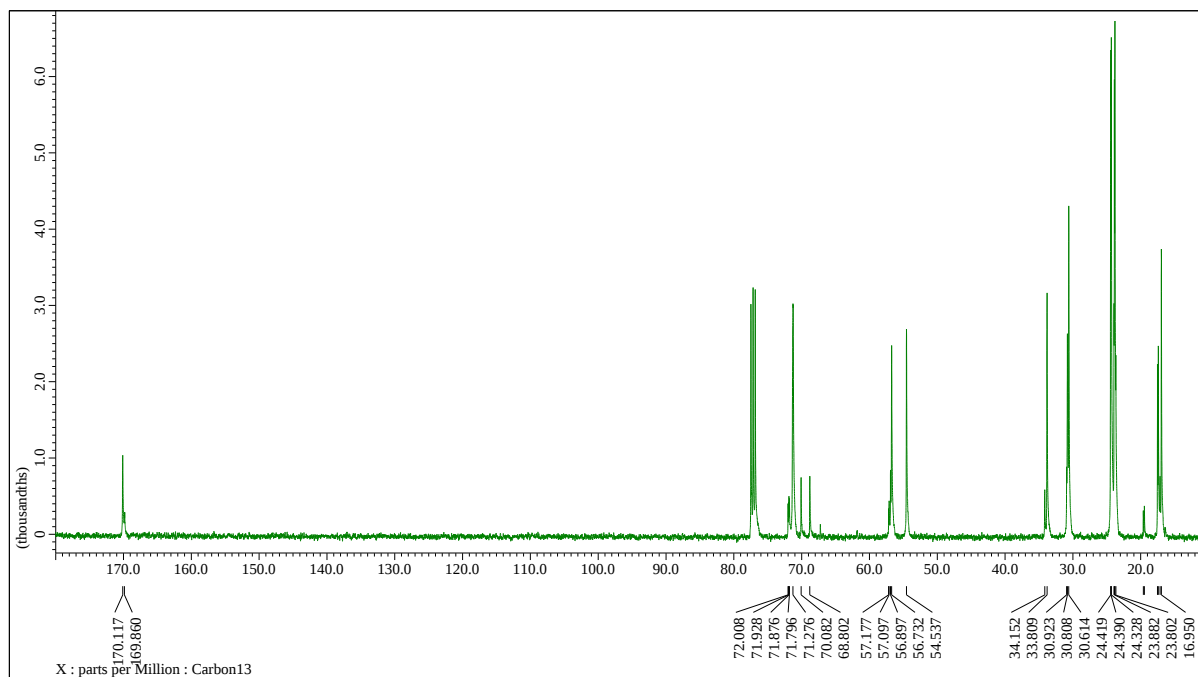


3bb diisopropyl-[4-isopropyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

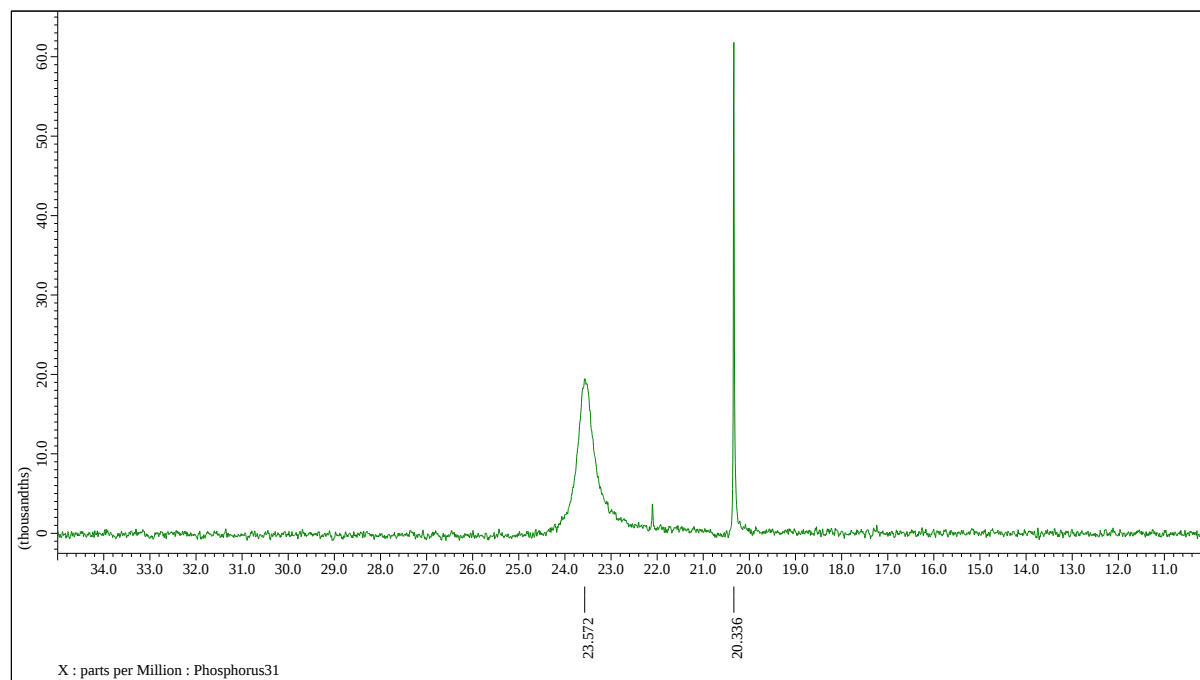
¹H NMR spectrum of **3bb**



¹³C NMR spectrum of **3bb**

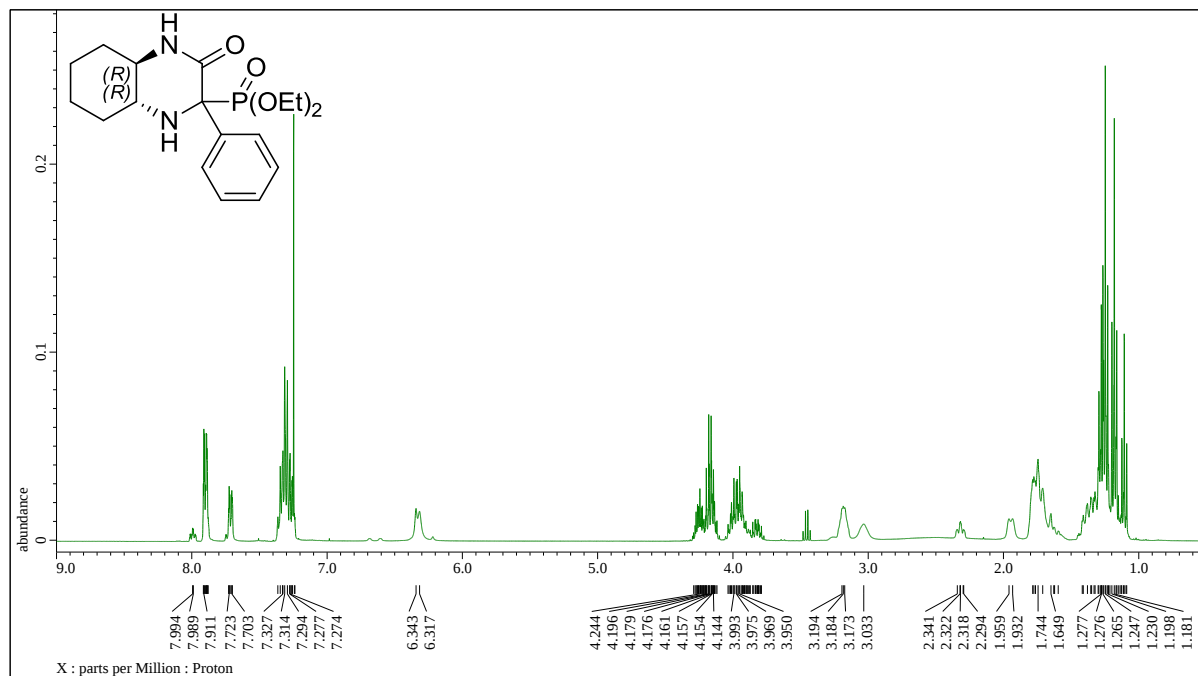


^{31}P NMR spectrum of **3bb**

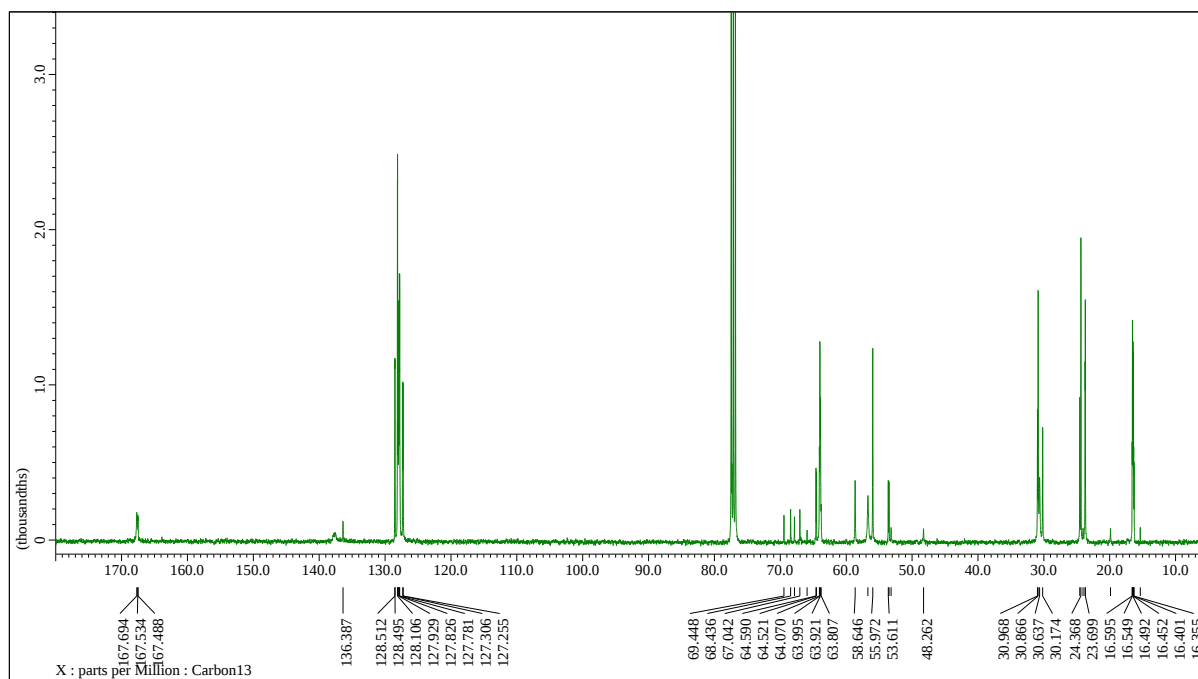


3ca diethyl-[4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

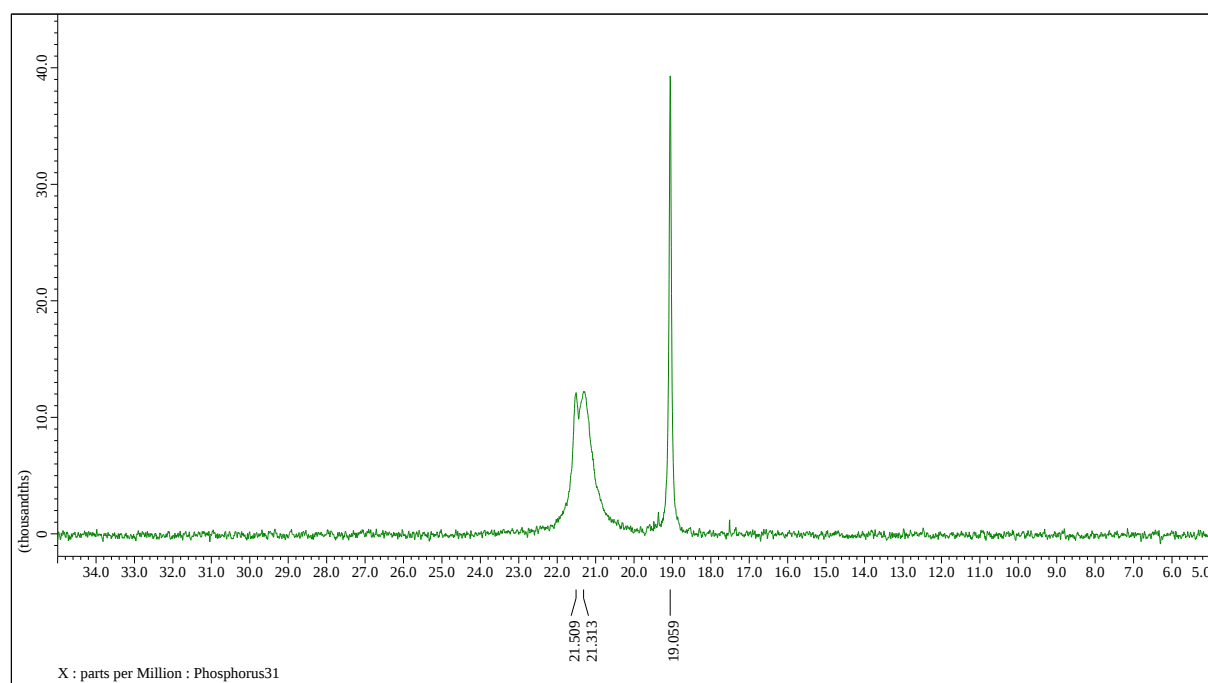
¹H NMR spectrum of **3ca**



¹³C NMR spectrum of **3ca**

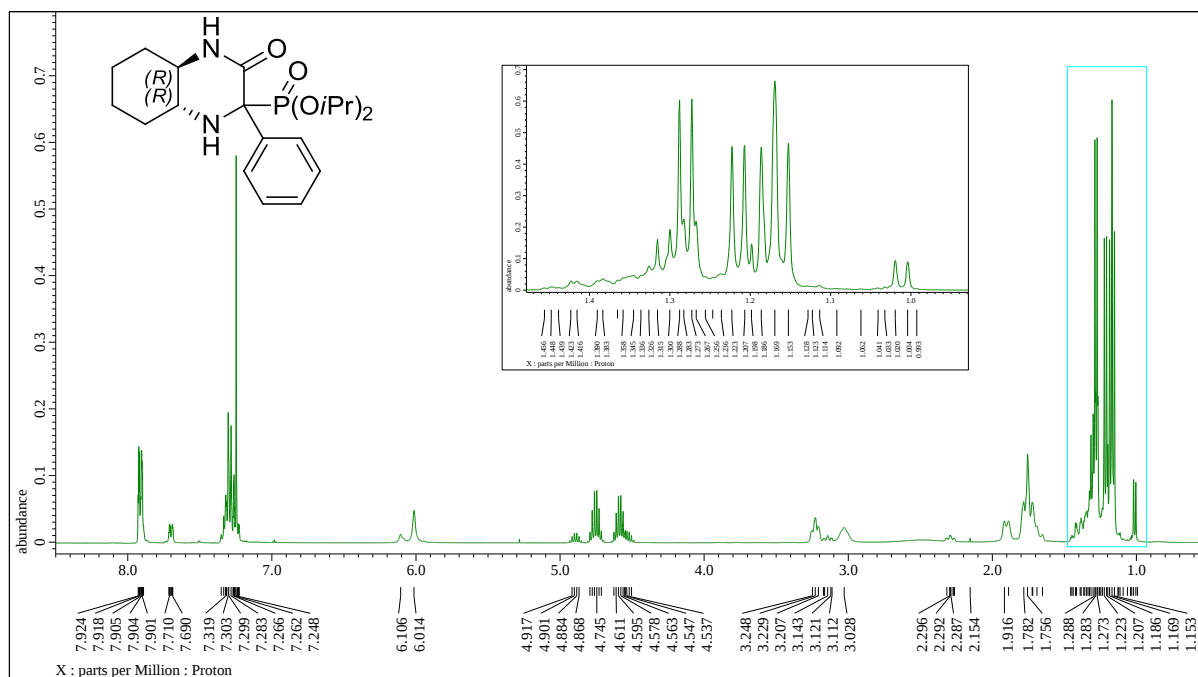


^{31}P NMR spectrum of **3ca**

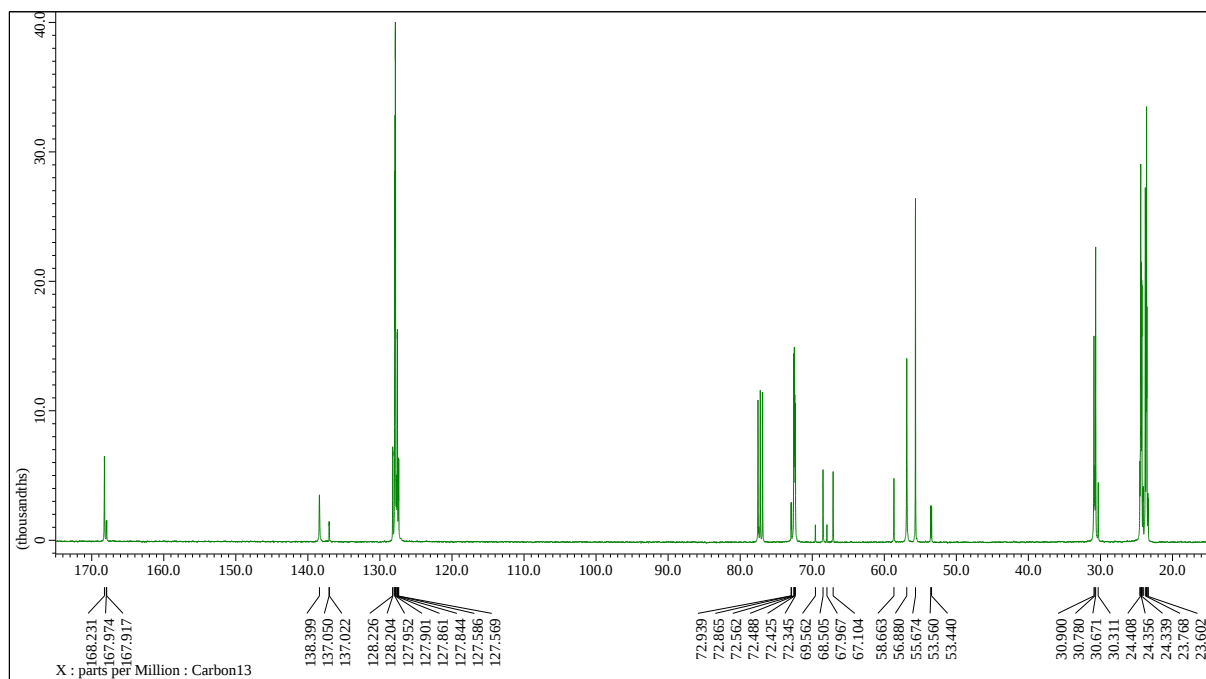


3cb diisopropyl-[4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

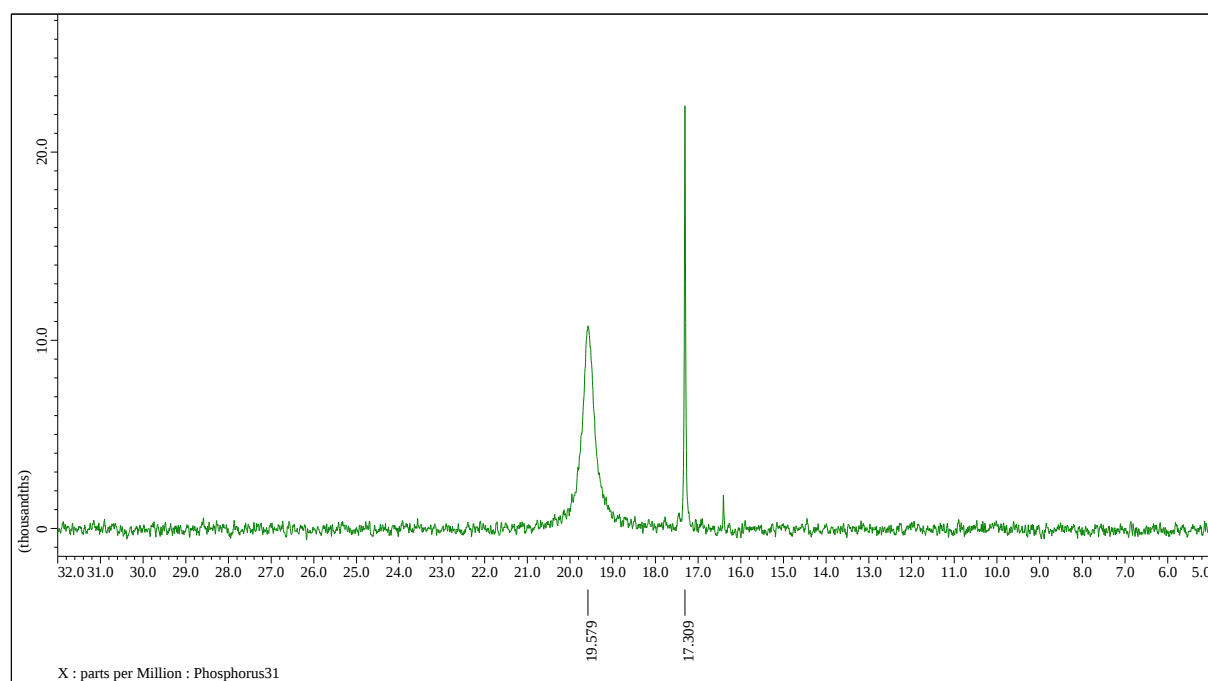
¹H NMR spectrum of **3cb**



¹³C NMR spectrum of **3cb**

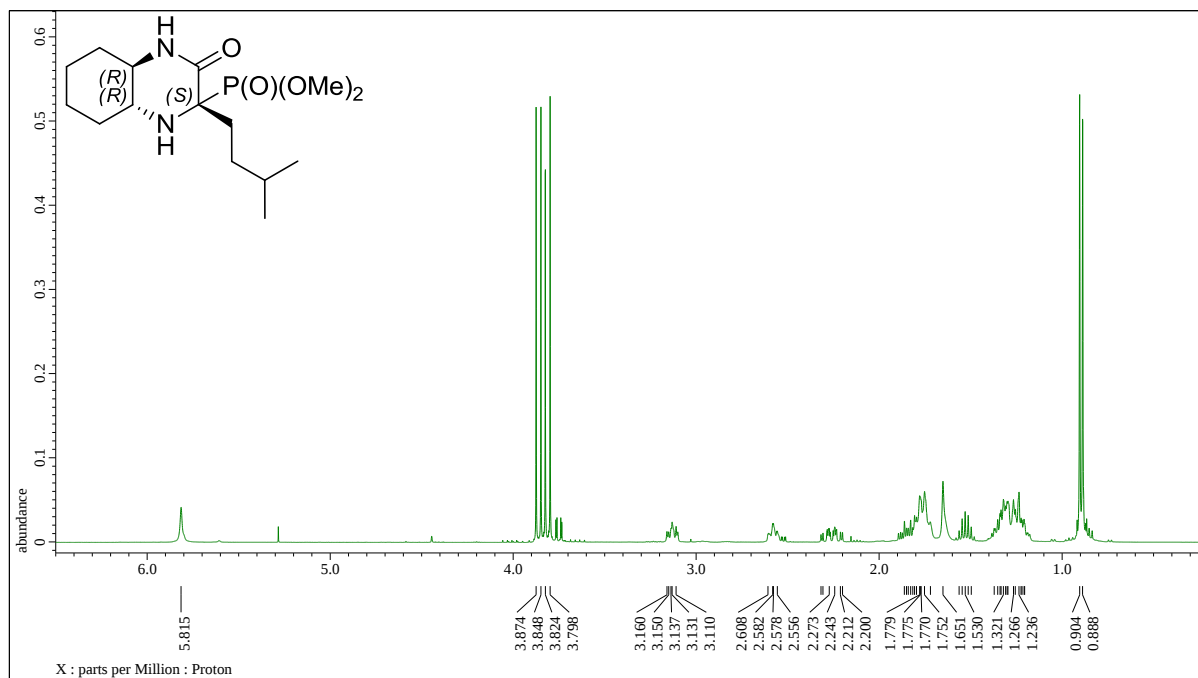


^{31}P NMR spectrum of **3cb**

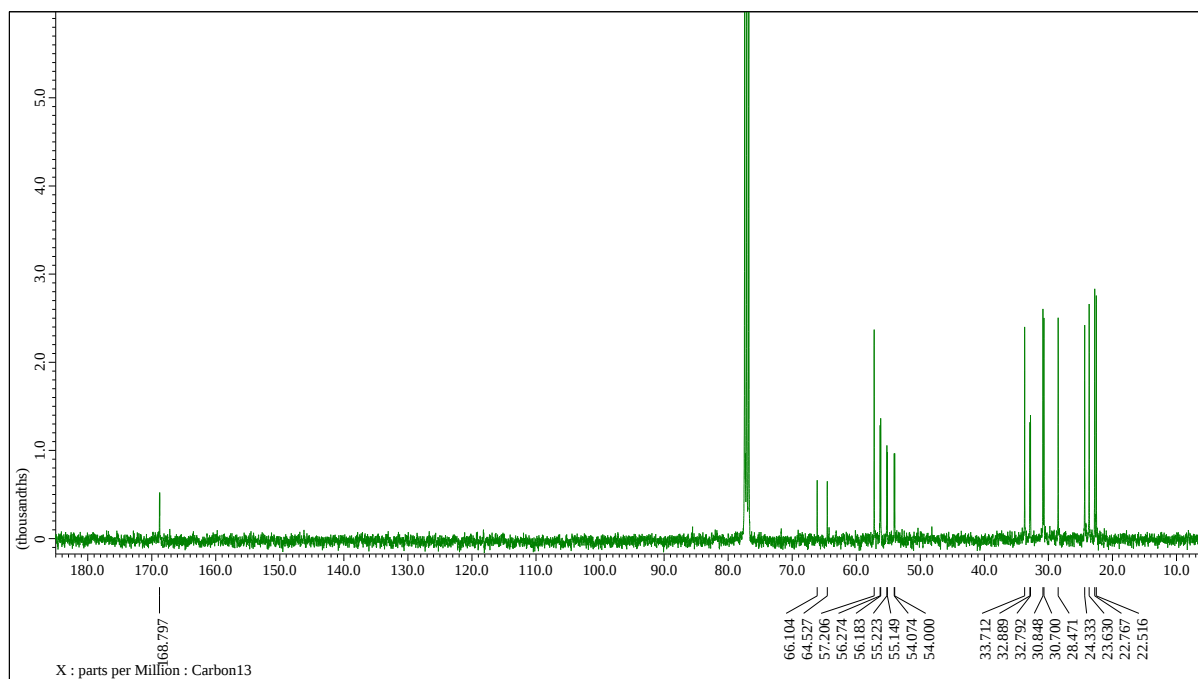


3fa dimethyl-[4-isopentyl-(1*R*,4*S*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonate

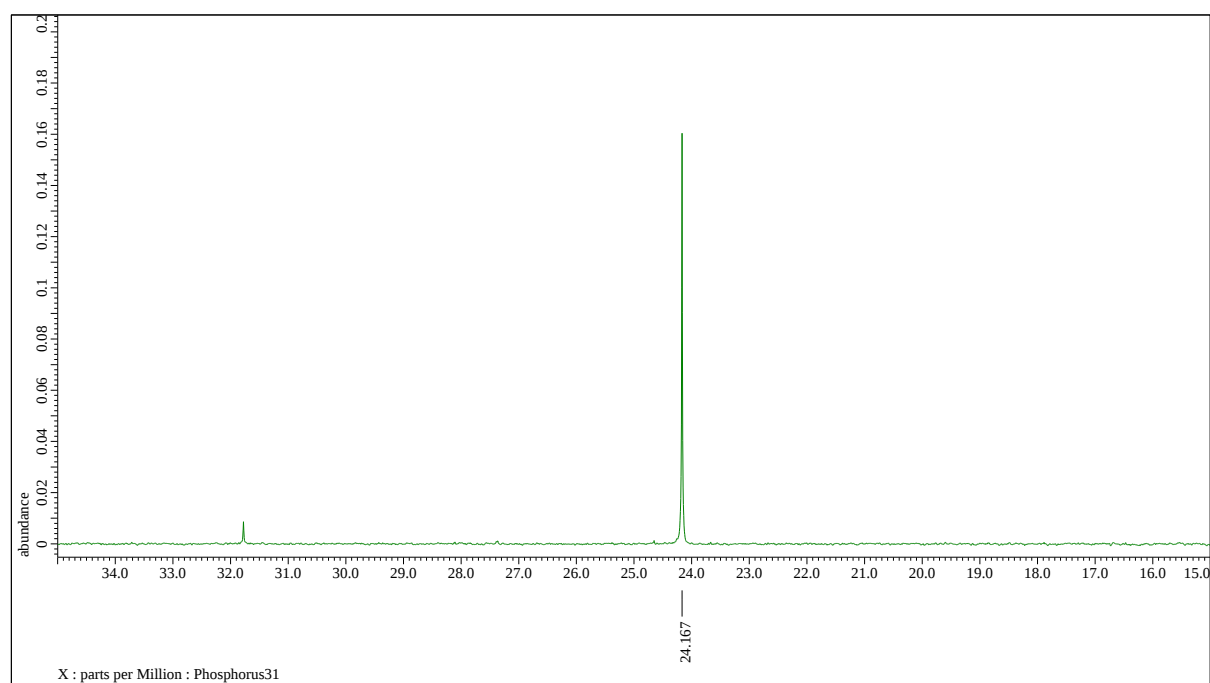
¹H NMR spectrum of **3fa**



¹³C NMR spectrum of **3fa**



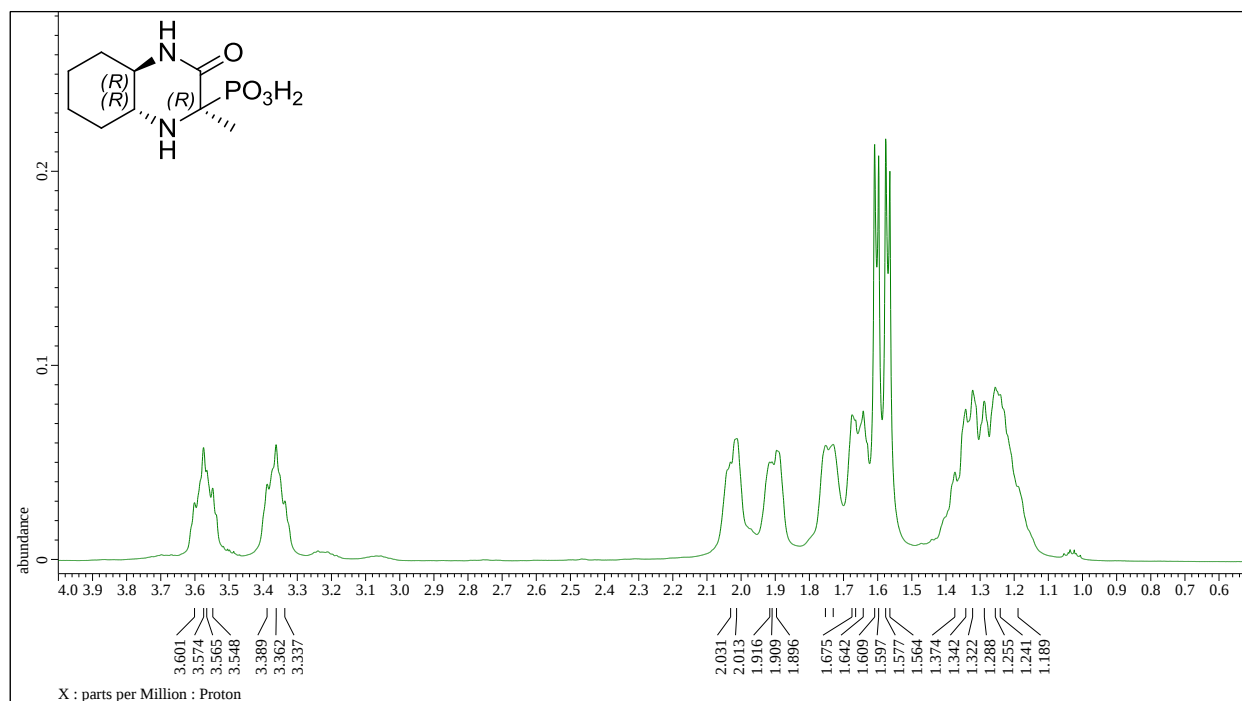
^{31}P NMR spectrum of **3fa**



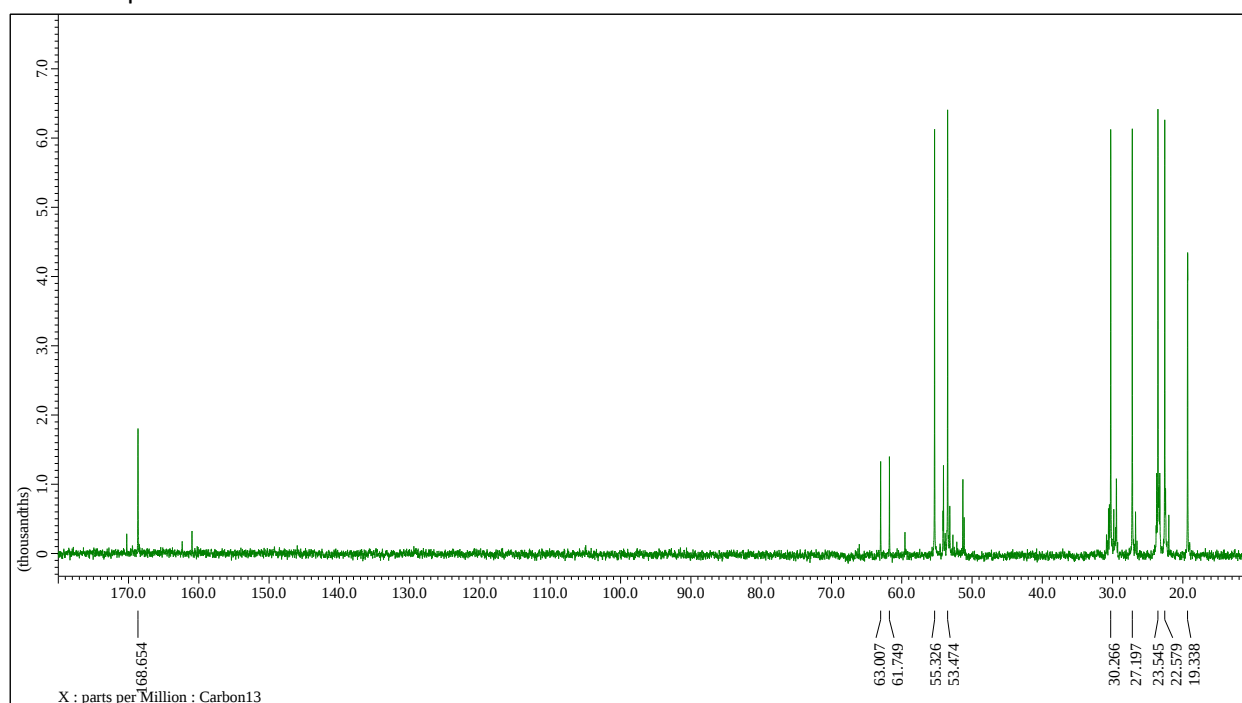
Aminophosphonic acids

4a [4-methyl-(1*R*,4*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

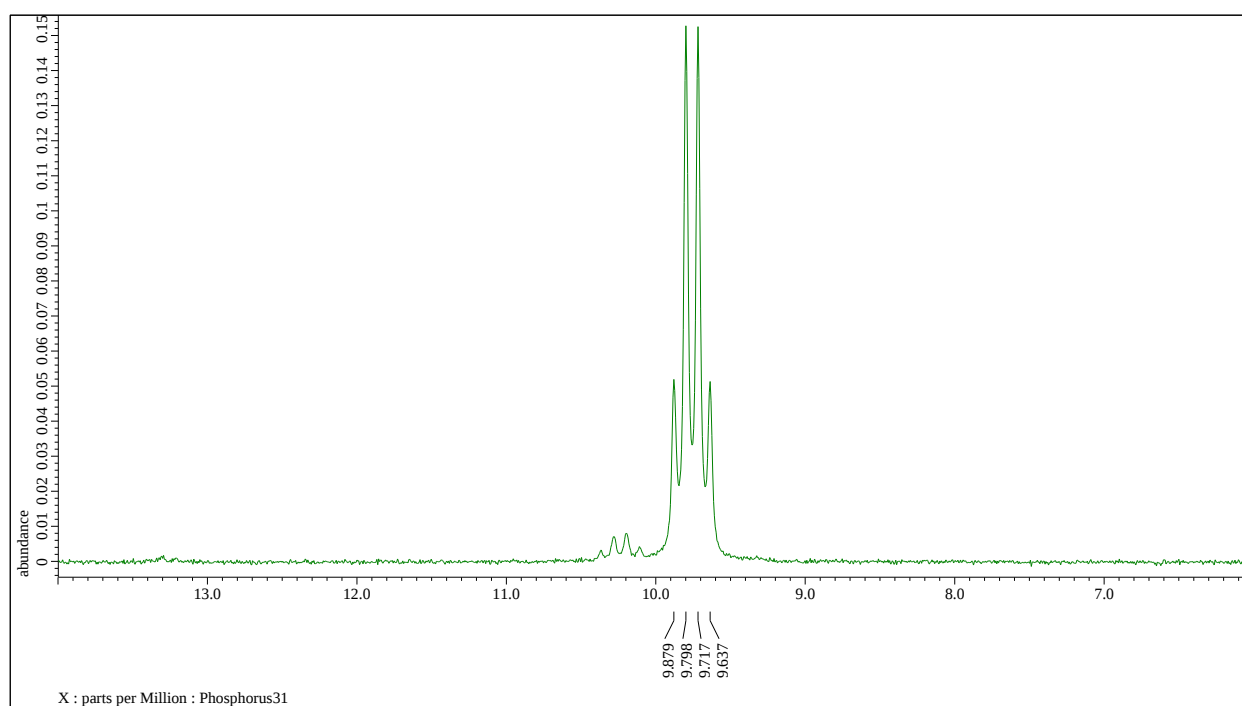
¹H NMR spectrum of **4a**



¹³C NMR spectrum of **4a**

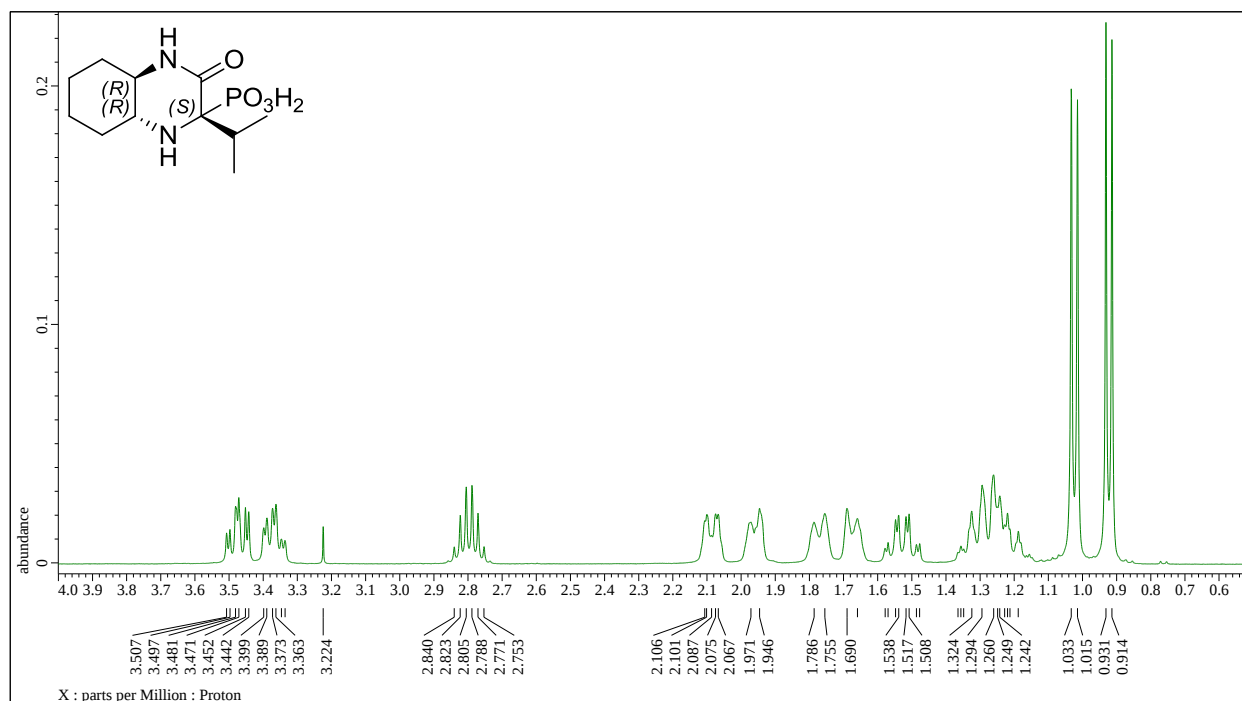


^{31}P NMR spectrum of **4a**

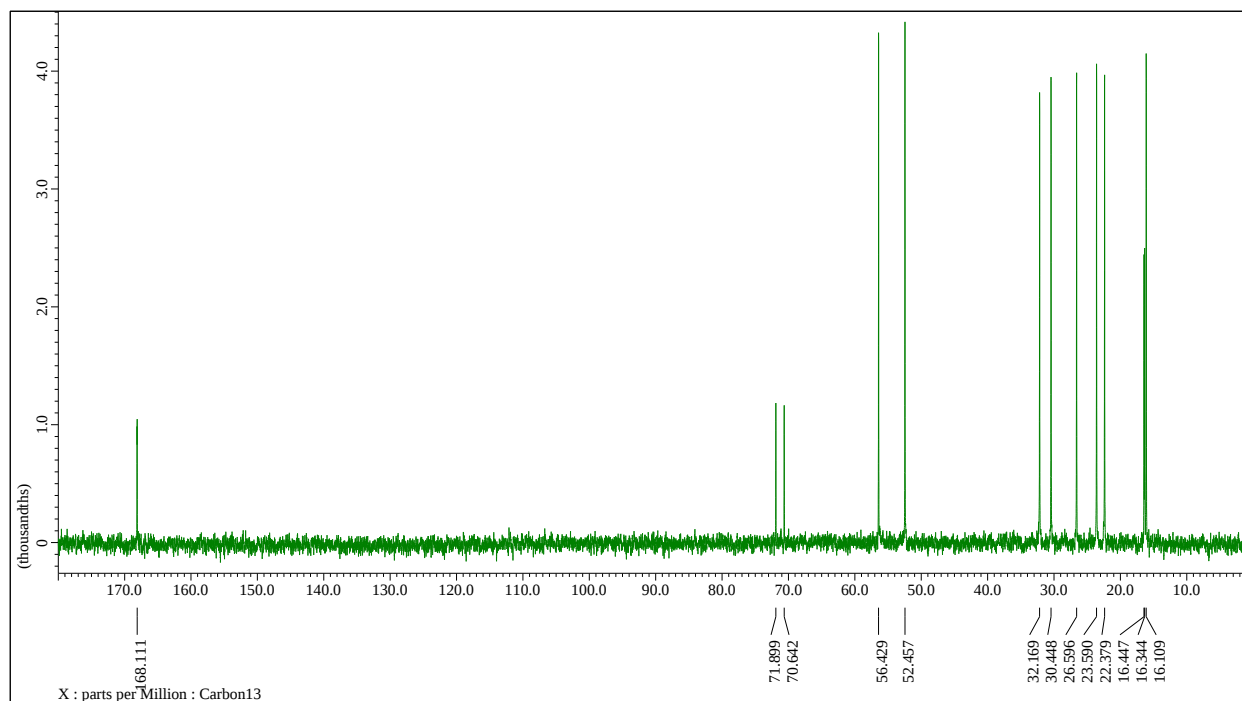


4b [4-isopropyl-(1*R*,4*S*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

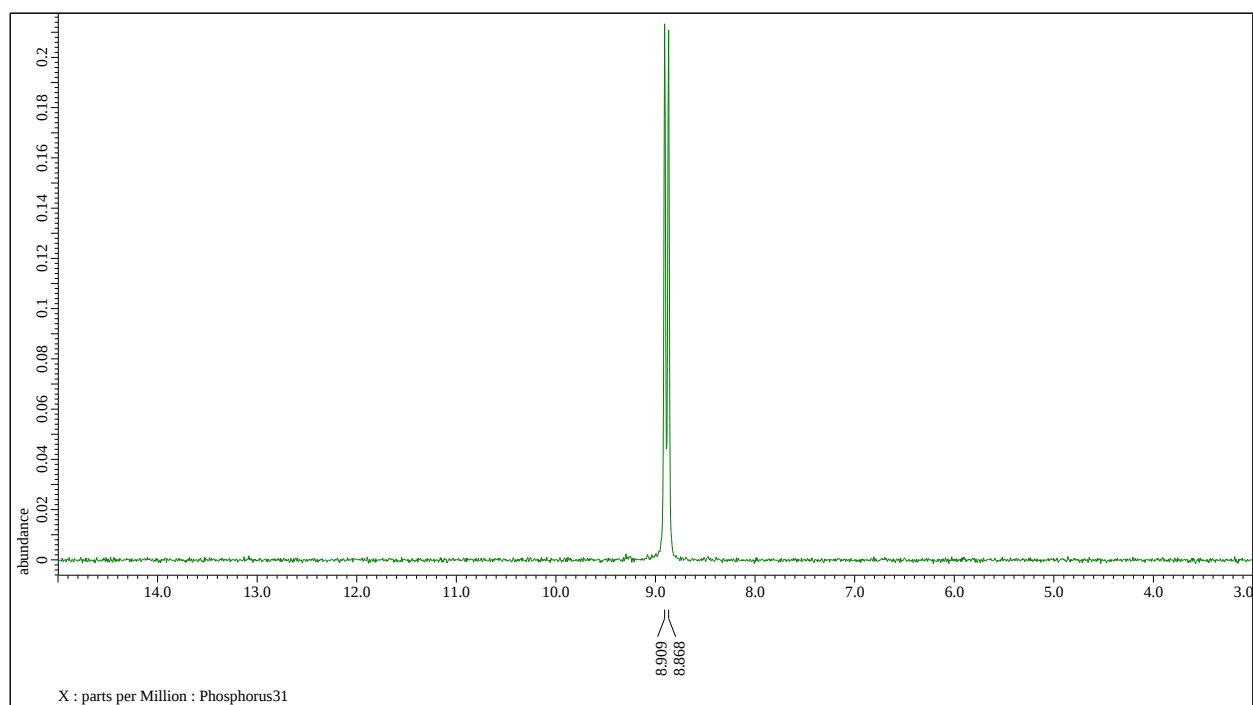
¹H NMR spectrum of **4b**



¹³C NMR spectrum of **4b**

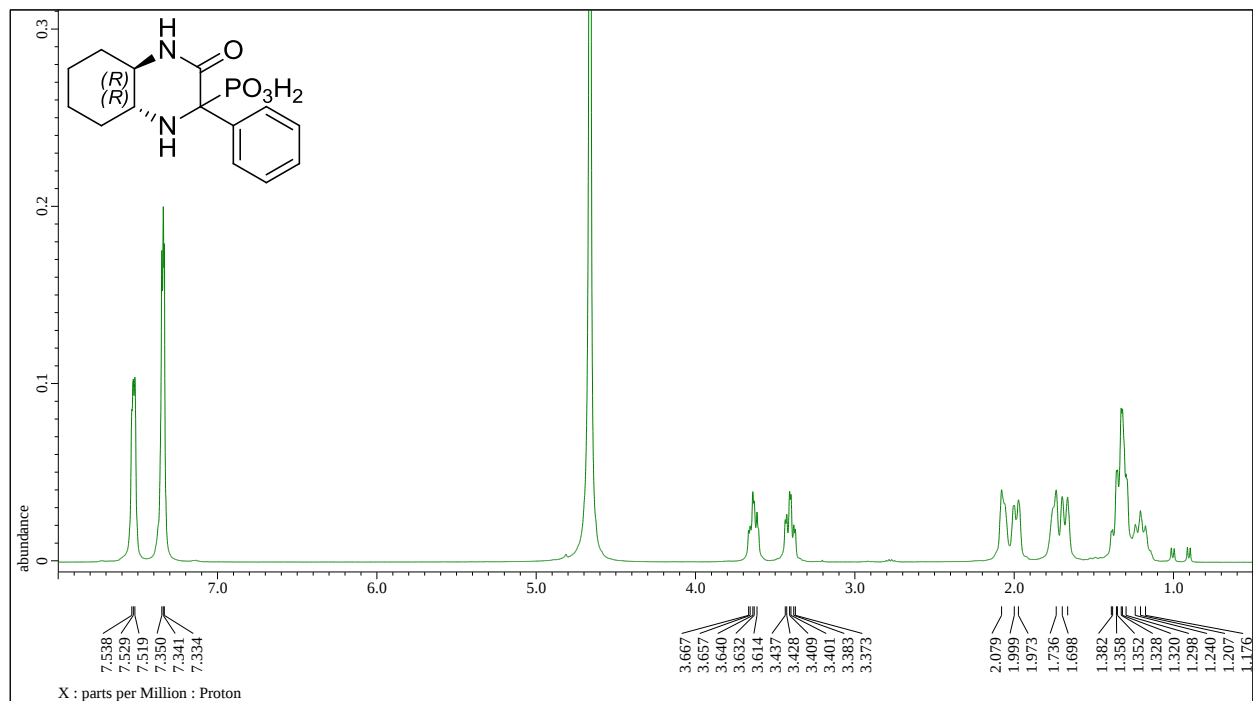


^{31}P NMR spectrum of **4b**

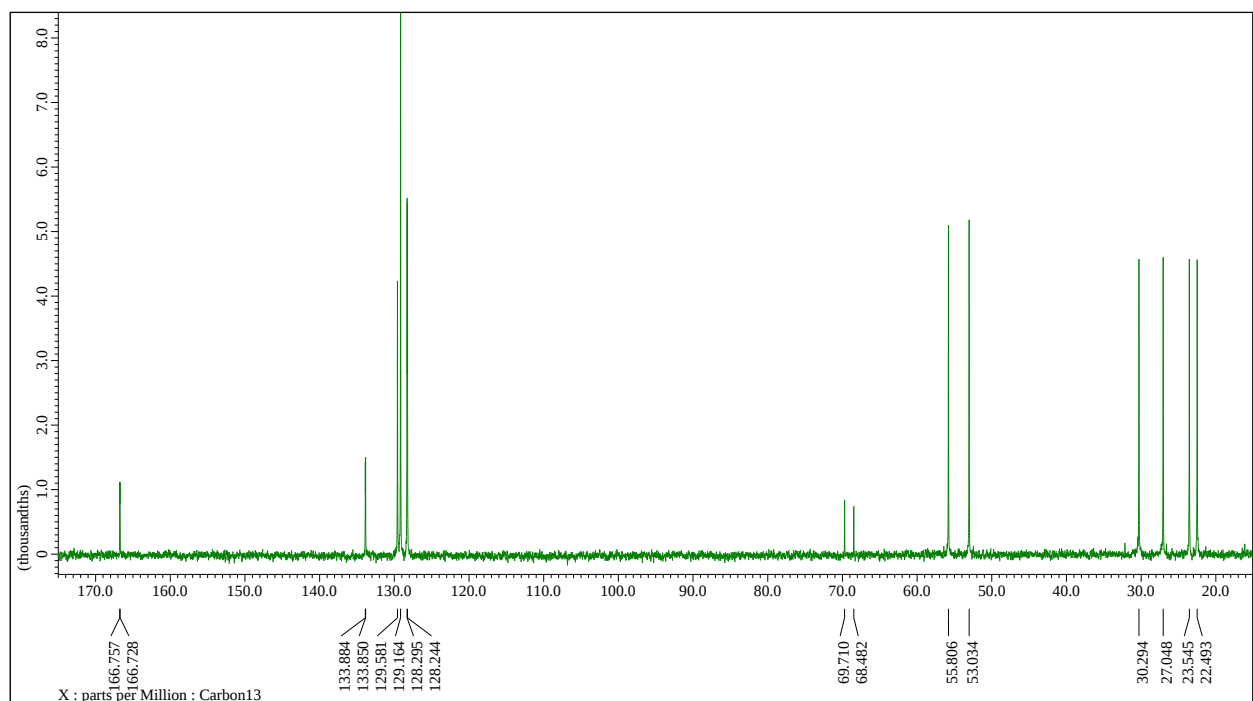


4c [4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

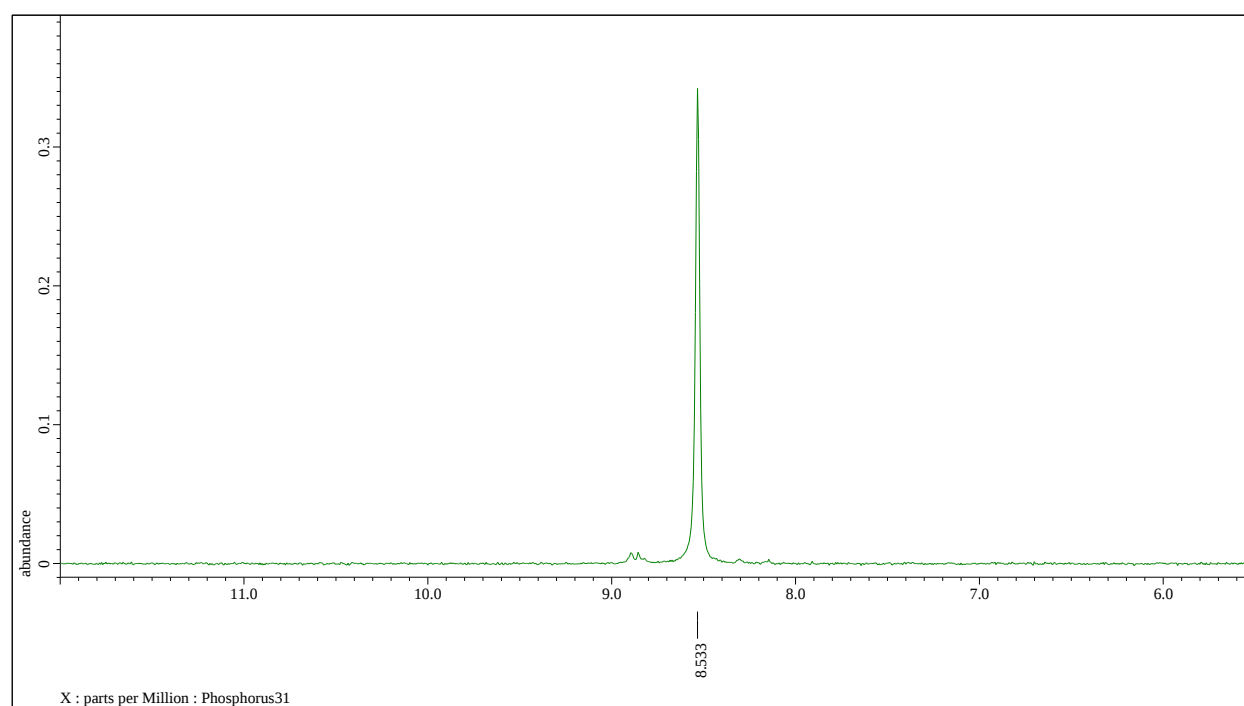
¹H NMR spectrum of 4c



¹³C NMR spectrum of 4c

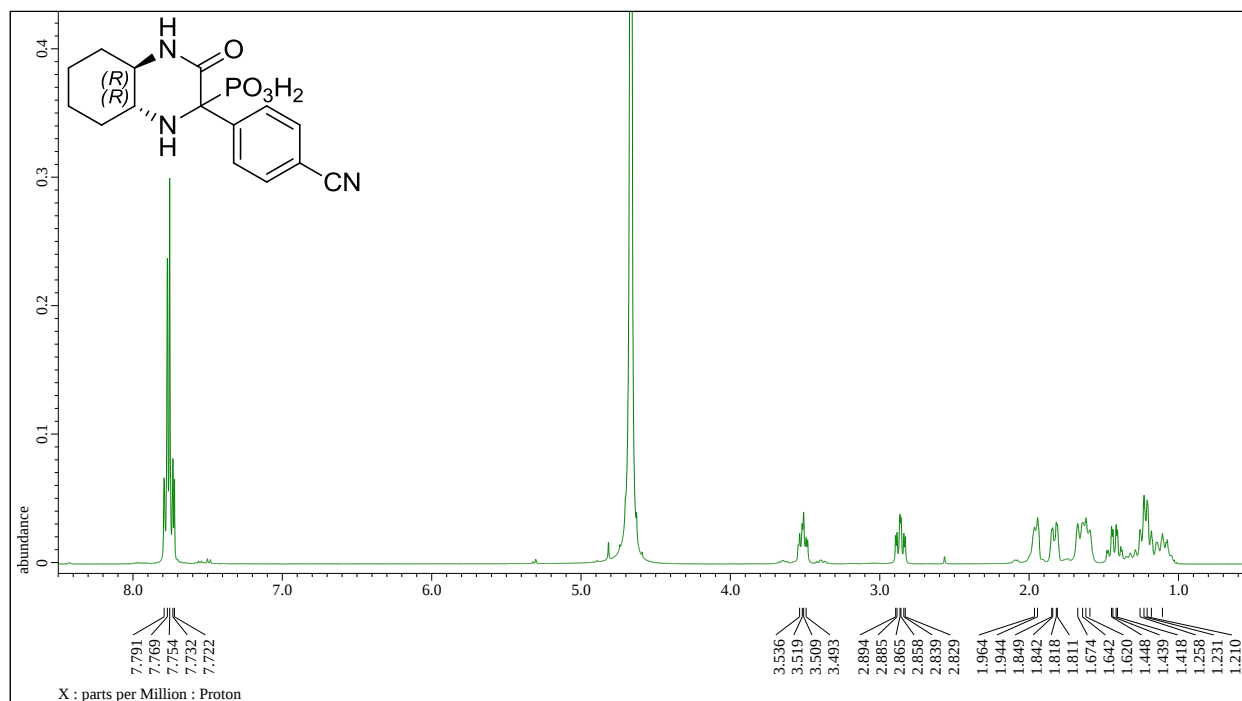


^{31}P NMR spectrum of **4c**

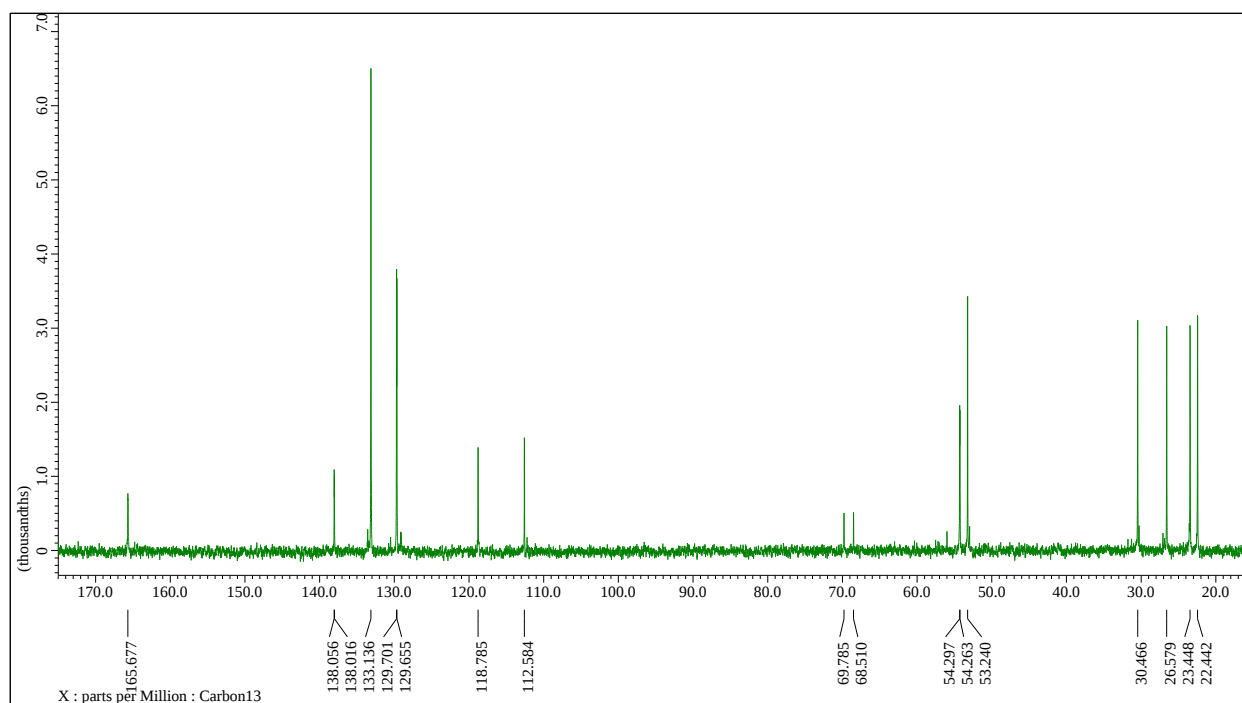


4d [4-(4-cyanophenyl)-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

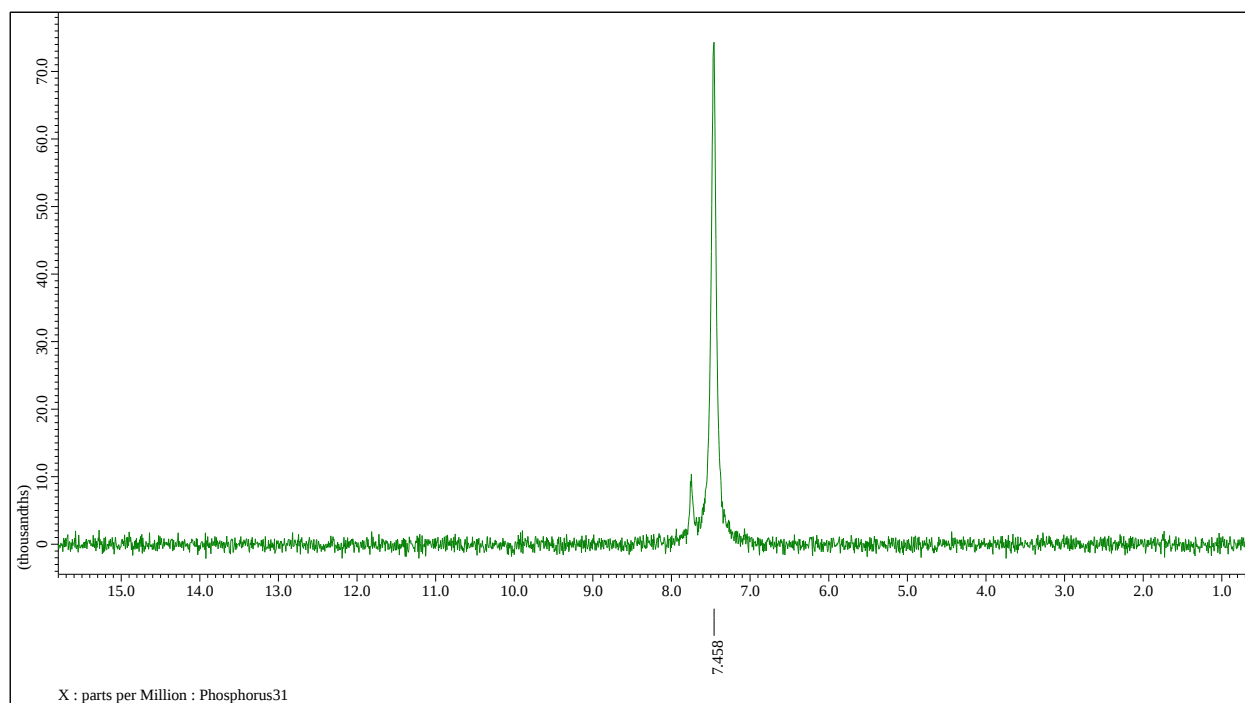
¹H NMR spectrum of **4d**



¹³C NMR spectrum of **4d**

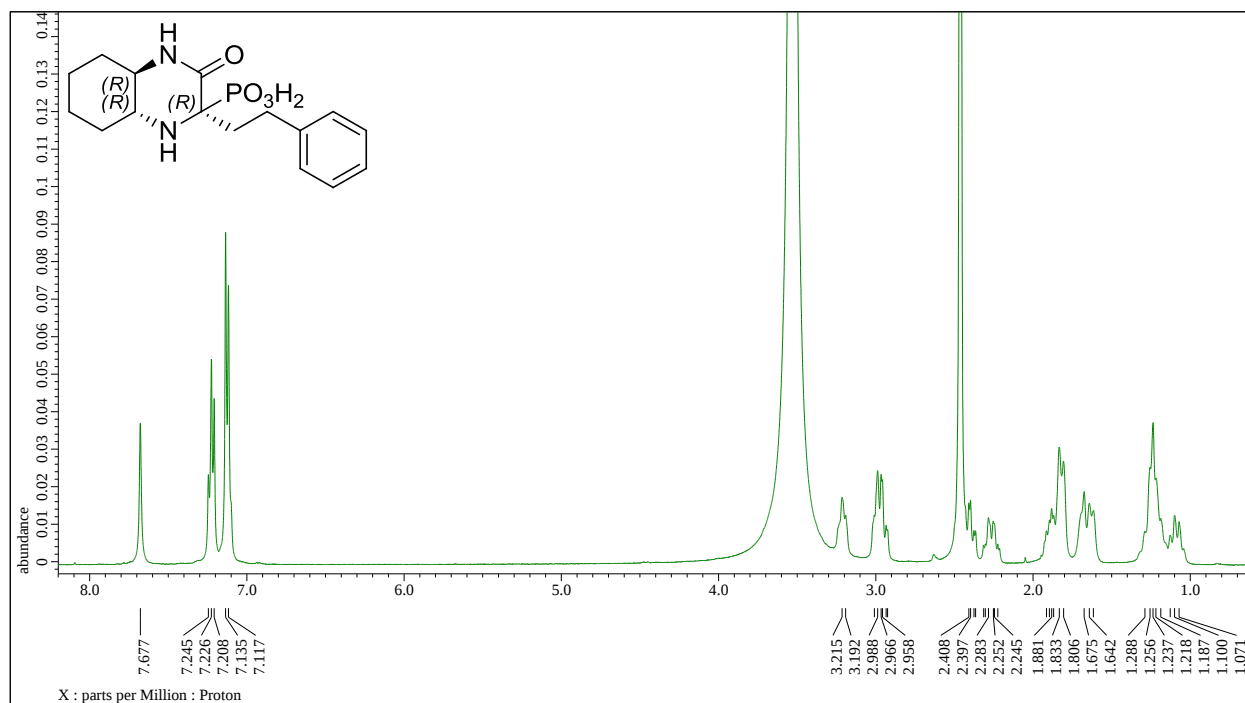


^{31}P NMR spectrum of **4d**

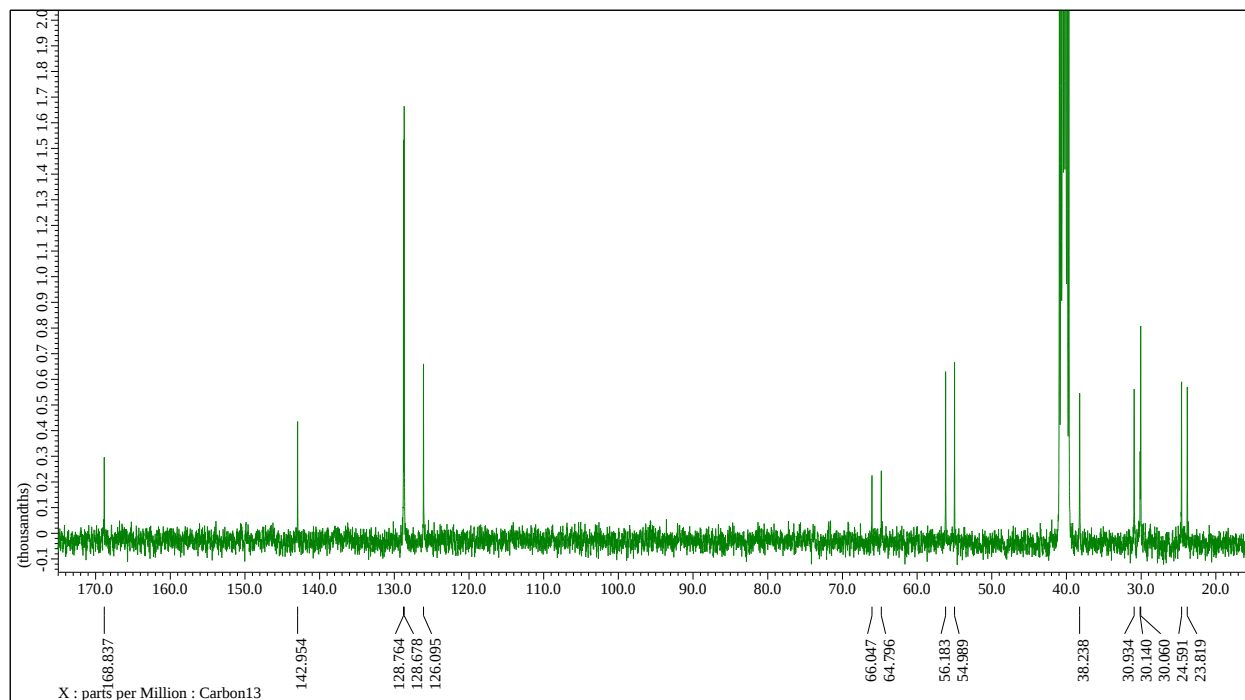


4e [4-phenethyl-(1*R*,4*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

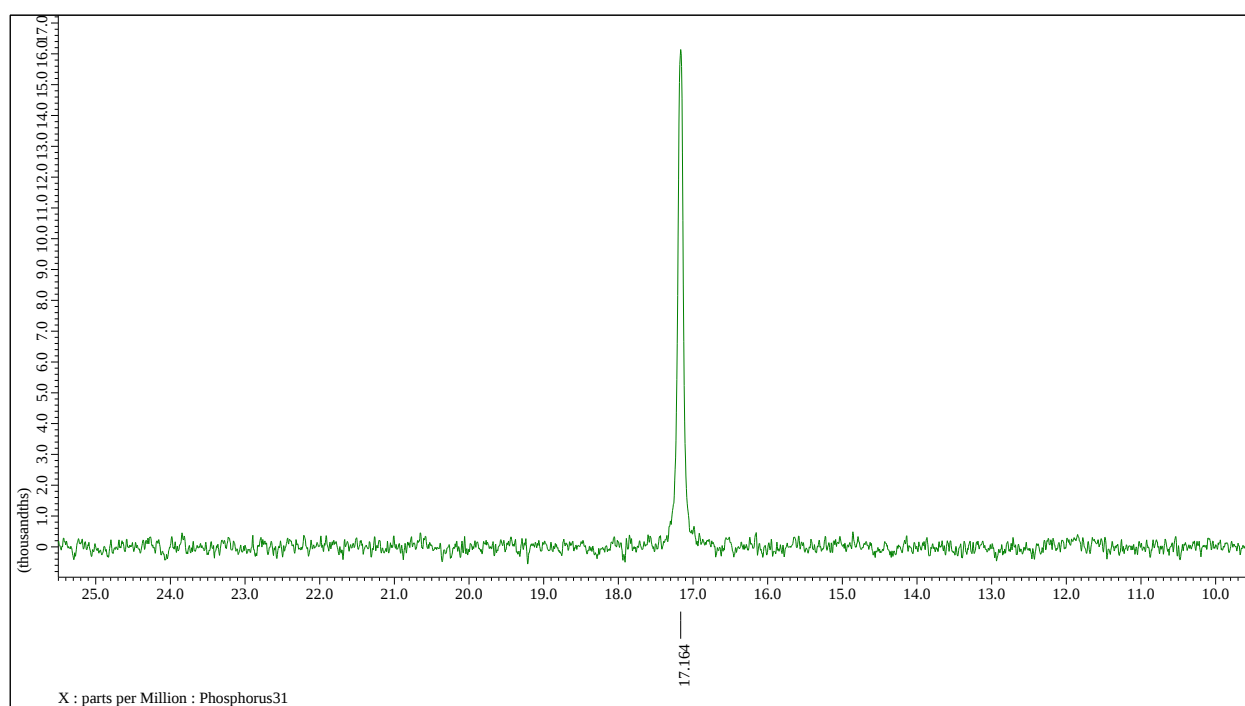
¹H NMR spectrum of 4e



¹³C NMR spectrum of 4e

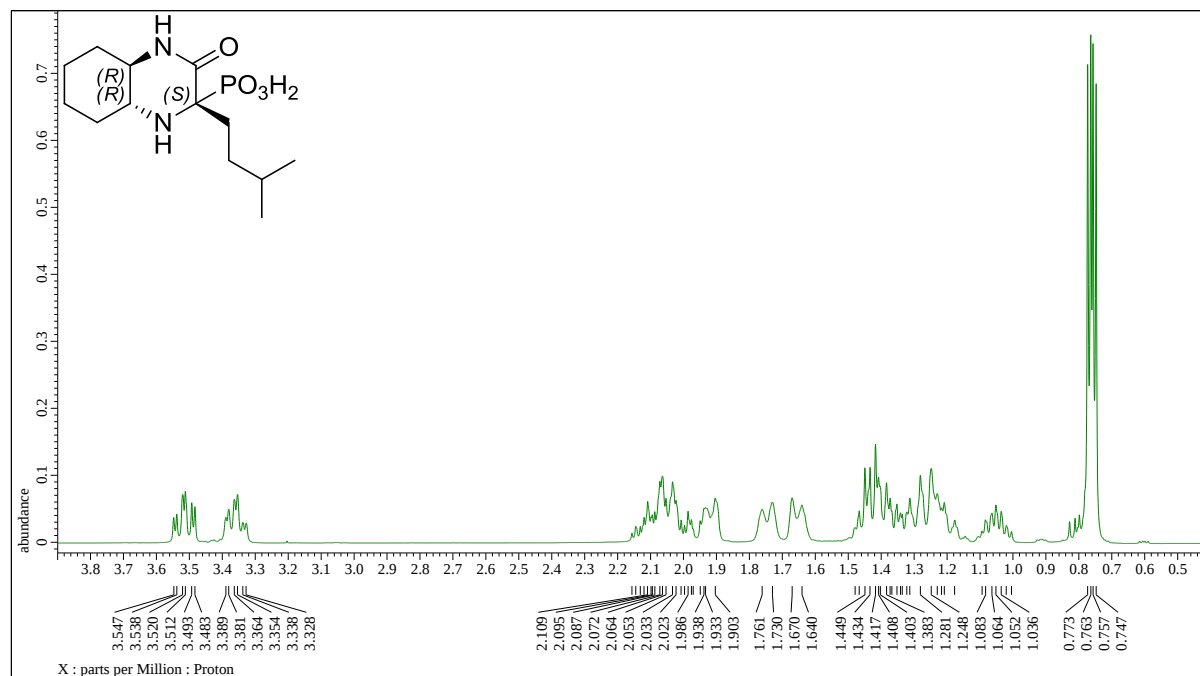


^{31}P NMR spectrum of **4e**

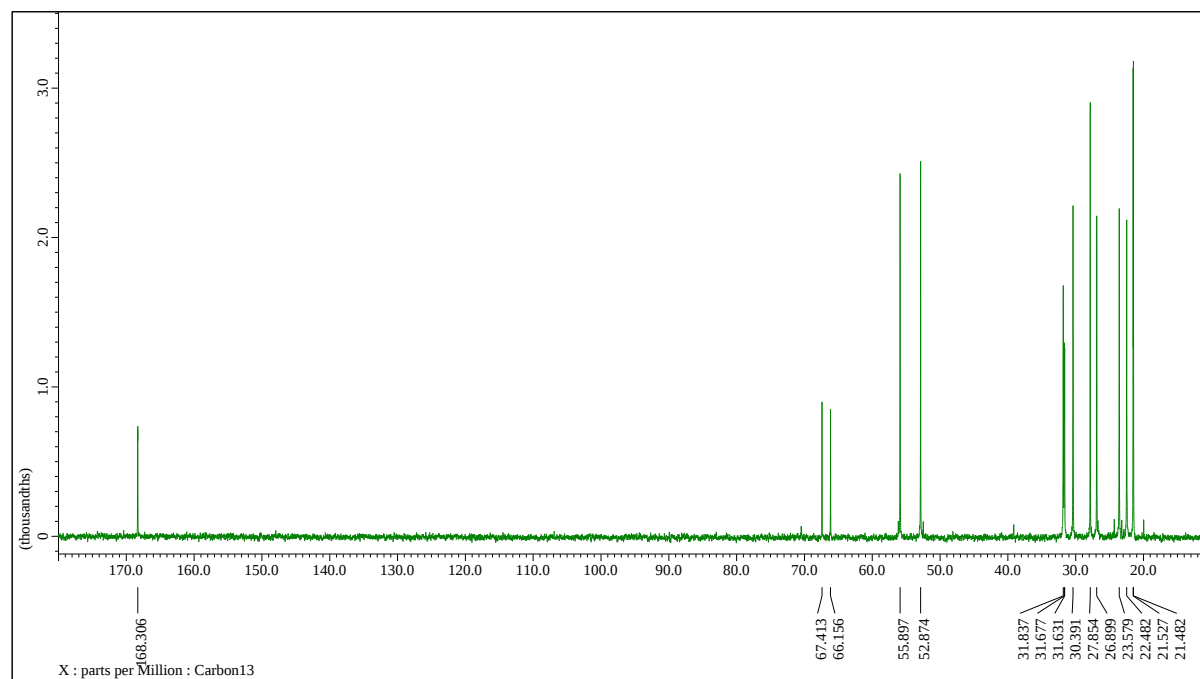


4f [4-isopentyl-(1*R*,4*S*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid

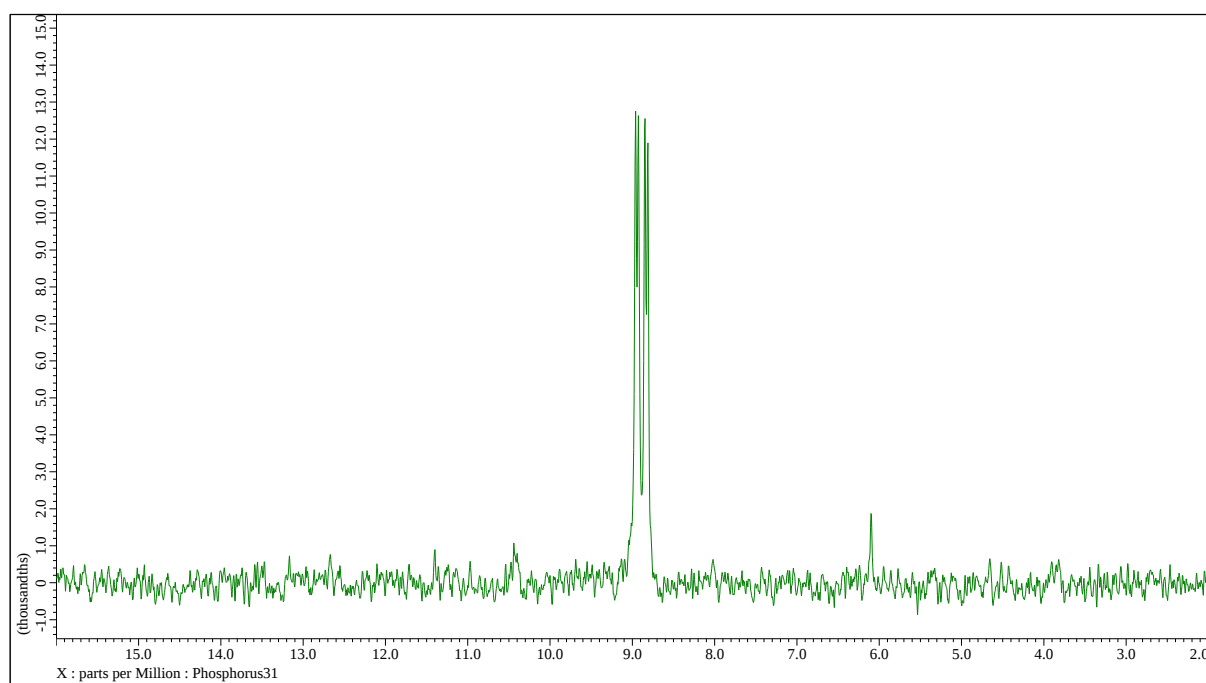
¹H NMR spectrum of 4f



¹³C NMR spectrum of 4f



^{31}P NMR spectrum of **4f**



Computational details

Calculations have been carried out with the ORCA program [1] within the Density Functional Theory (DFT) formalism. The Perdew-Burke-Ernzerhof functional with 25% of exact Hartree-Fock exchange (PBE0) was used [2,3] together with Def2-TZVPP basis set [4,5]. The relaxed scan method was used to evaluate the dissociation energy curves, with the P-C distance varying from 1.8 to 4.5 Å. Each geometry of the scan was relaxed until the maximum gradient reached 0.0003. The dissociation energy graph is shown in Figure 1.

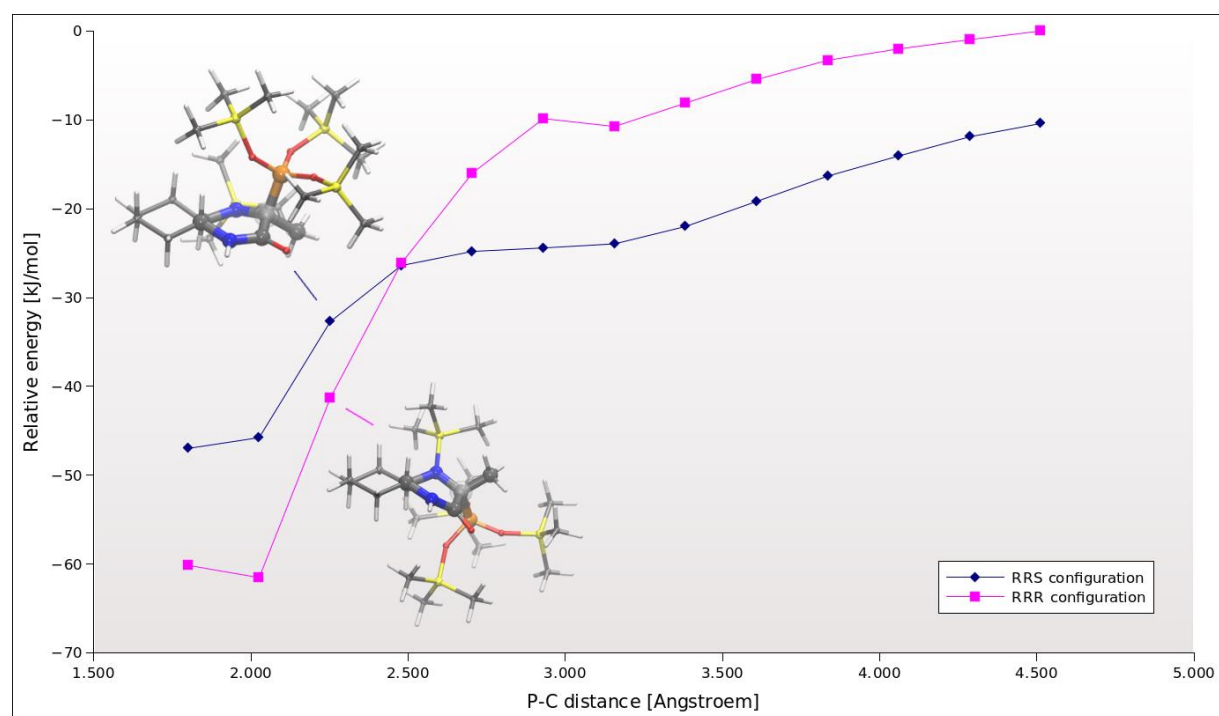


Figure 1. The dissociation energy curve for the *R*- and *S*-epimer of **4a**.

X-ray Crystallographic Measurements

X-ray diffraction data were collected on an Oxford Diffraction four-circle single crystal diffractometer equipped with a CCD detector using graphite-monochromatized MoK α radiation ($\lambda=0.71073$ Å). The raw data were treated with the CrysAlis Data Reduction Program (version 1.171.38.34a). The intensities of the reflection were corrected for Lorentz and polarization effects. The crystal structures were solved by direct methods [6] using SHELXS-2016/4 and refined by full-matrix least-squares method using SHELXL-2016/4 program [6]. Non-hydrogen atoms were refined using anisotropic displacement parameters. H-atoms connected with C atoms from the aromatic rings were visible on the Fourier difference maps, but placed by geometry and allowed to refine “riding on” the parent atom. Visualizations of the structure were made using Diamond 3.2k [7].

Table 1. Crystal data and structure refinement details for **4a**, **4e** and **3fa** compounds.

Compound	4a	4e	3fa
Chemical formula	C ₉ H ₁₇ N ₂ O ₄ P	2(C ₁₆ H ₂₃ N ₂ O ₄ P)·1.282(C ₂ H ₆ O)·0.144(O)	4(C ₁₅ H ₂₉ N ₂ O ₄ P)[+solvent]
Mr	248.21	369.28	332.37
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁	Hexagonal, <i>P</i> 6 ₁
Temperature (K)	295	100	100
a, b, c (Å)	12.0382(2), 9.9050(2), 9.8427(2)	11.1042(5), 11.9889(7), 28.0715(19)	26.6639(8), 26.6639(8), 18.0496(4)
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 120
V (Å ³)	1173.64(4)	3737.1(4)	11113.4(7)
Z	4	8	24
μ (mm ⁻¹)	0.24	0.18	0.17
Crystal size (mm)	0.45 × 0.30 × 0.20	0.58 × 0.40 × 0.03	0.53 × 0.11 × 0.08
Tmin, Tmax	0.928, 0.964	0.909, 0.994	0.950, 0.989
No. of measured, indep. and obs. [I > 2σ(I)] reflections	11526, 2721, 2614	71497, 8806, 8326	93137, 12061, 9097
Rint	0.020	0.071	0.086
(sin θ/λ) _{max} (Å ⁻¹)	0.658	0.658	0.598

R[F ² > 2σ (F ²)], wR(F ²), S	0.025, 0.065, 1.07	0.078, 0.191, 1.15	0.065, 0.131, 1.05
No. of refl./par./restr.	2721/164/0	8806/498/24	12061/852/5
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.22, -0.13	0.99, -0.90	0.44, -0.26
Absolute structure parameter	0.02(2)	0.04 (3)	0.02 (4)

Computer programs: CrysAlis CCD 1.171.33.42 (Oxford Diffraction, 2009), CrysAlis PRO 1.171.38.43 (Rigaku OD, 2015), CrysAlis PRO 1.171.38.34a (Rigaku OD, 2015), SHELXL2016/4 (Sheldrick, 2016), SHELXS2016/4 (Sheldrick, 2016), SHELXS2018/3 (Sheldrick, 2018), SHELXL2018/3 (Sheldrick, 2018).

The compounds **4a**, **e** and **3fa** crystallized at room temperature in non-centrosymmetric space groups **4a** – $P2_12_12$, **4e** – $P2_12_12_1$ and $P6_1$ (Table 1). All the atoms lied in general positions (Figures 2-4). The molecules in **4a** and **4e** are connected to each other by two strong O–H···O hydrogen bonds since the phosphonate group is protonated (Figure 2, 3). Thus, dimeric molecular system is created in these compounds. Besides, the N–H···O interactions exist in the structures and they connect adjacent molecules forming complex network of hydrogen bonds which stabilizes the crystal structure. Geometry data suggest that the N–H···O interactions have medium and weak nature than O–H···O hydrogen bonds of the dimer (Table 2).

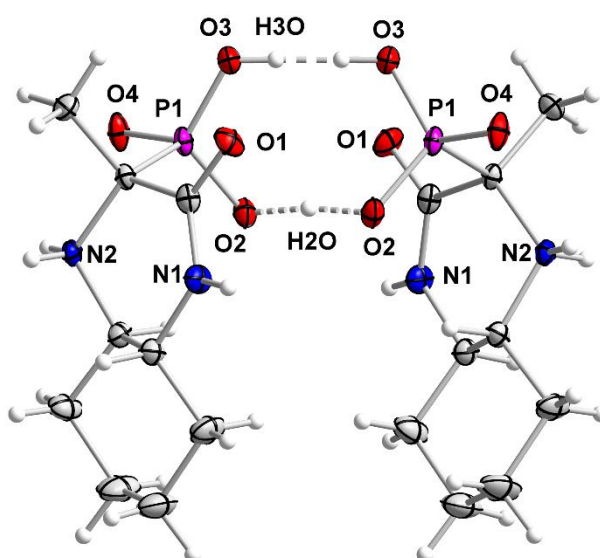


Figure 2. Dimeric structure of **4a** arranged around the 2-fold axis.

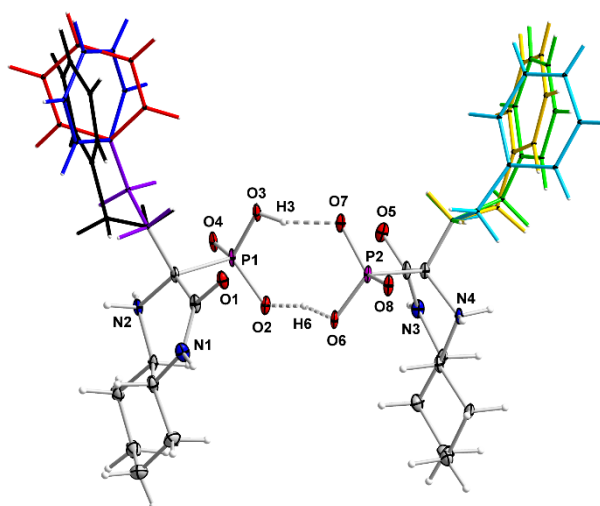


Figure 3. Dimeric structure of **4e**. Each ethylphenyl group is disordered over three positions in both symmetry independent aminophosphonate molecule.

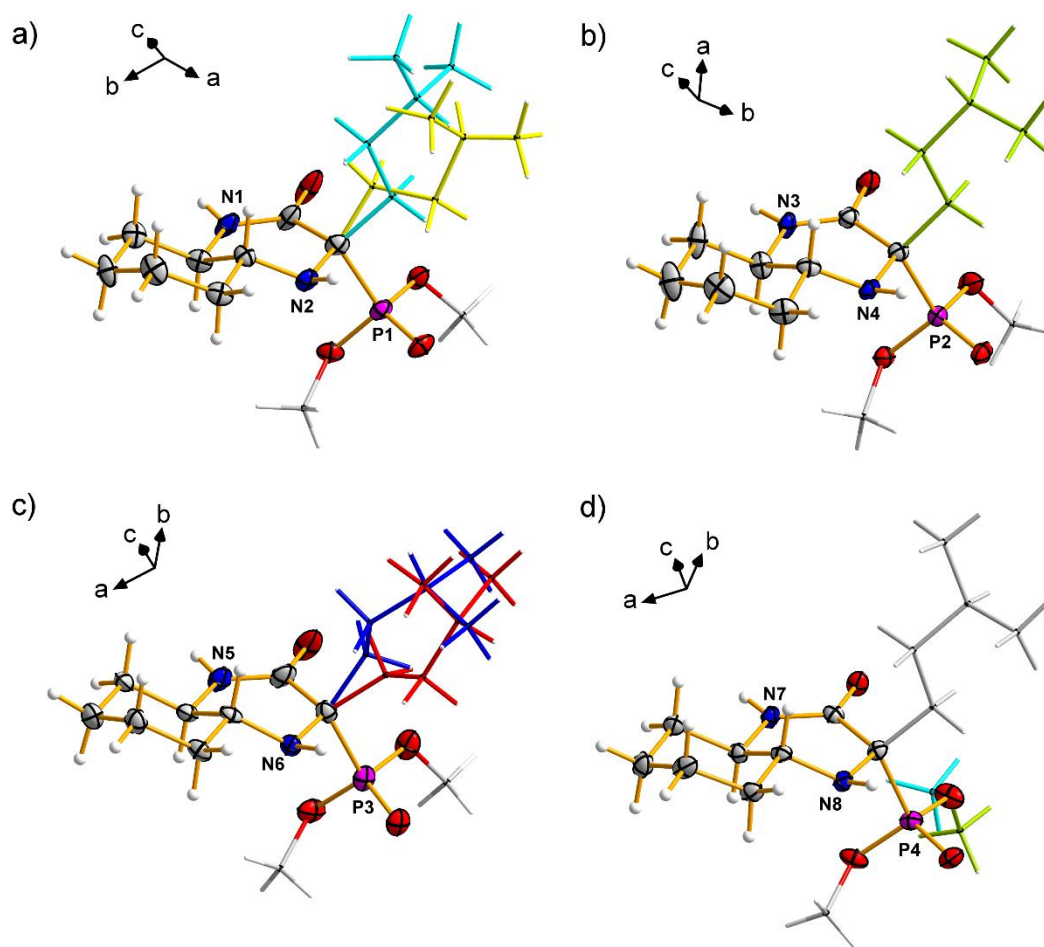


Figure 4. Four symmetry independent molecules of **3fa** that exist in the asymmetric part of the unit cell. Isopenthyl group is disordered over two positions in (a) – depicted in yellow and light blue – and in (c) – coloured in red and blue. All the atoms in (b) are ordered. One methyl group is disordered over two positions in (d) – shown in lime and light blue.

Table 2. Hydrogen bonds for **4a**, **4e** and **3fa**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
4a				
O(2)-H(2O)...O(2)#1	0.74(4)	1.78(4)	2.515(3)	178(6)
O(3)-H(3O)...O(3)#1	0.74(4)	1.78(4)	2.515(3)	178(6)
N(1)-H(1N)...O(4)#2	0.84(3)	1.97(3)	2.7908(19)	166(2)
N(2)-H(2N)...O(1)#3	0.87(3)	2.16(3)	2.986(2)	160(2)
N(2)-H(3N)...O(4)#4	0.92(3)	1.88(3)	2.790(2)	174(2)
4e				
O(3)-H(3)...O(7)	0.82	1.73	2.520(5)	162.8
O(6)-H(6)...O(2)	1.17	1.31	2.451(5)	162.0
N(1)-H(1N1)...O8\$1#1	0.86	2.09	2.836(6)	145.2
N(2)-H(1N2)...O4\$2#2	0.89	2.00	2.881(5)	171.0
N(2)-H(2N2)...O(4)	0.89	2.58	3.071(5)	115.4
N(2)-H(2N2)...O5\$2#2	0.89	1.99	2.827(5)	155.2
N(3)-H(1N3)...O4\$3#3	0.86	2.05	2.847(6)	154.8
N(4)-H(2N4)...O1\$4#4	0.89	1.95	2.787(5)	155.6
N(4)-H(2N4)...O(8)	0.89	2.55	3.031(5)	114.4
N(4)-H(1N4)...O8\$4#4	0.89	2.09	2.942(5)	161.1
O(1E)-H(1E)...O(7)	0.89	2.00	2.880(10)	166.0
O(2E)-H(2E)...O(3)	0.83	2.02	2.74(2)	145.0
3fa				
N1-H1N...O8	0.84(7)	2.07(7)	2.892(7)	165(7)
N2-H2N...O9 ⁱ	0.81(7)	2.20(7)	2.983(7)	163(6)
N3-H3N...O12	0.93(7)	1.98(7)	2.902(6)	171(6)
N4-H4N...O1	0.86(6)	2.14(7)	2.950(6)	157(6)
N5-H5N...O4 ⁱⁱ	0.92(7)	2.01(7)	2.900(7)	161(6)
N6-H6N...O5	1.01(6)	2.03(7)	3.002(6)	163(5)
N7-H7N...O16 ⁱⁱⁱ	0.83(6)	2.09(6)	2.915(6)	172(6)
N8-H8N...O13 ^{iv}	0.96(6)	2.10(7)	3.008(7)	159(5)

Symmetry transformations used to generate equivalent atoms: **4a** – #1 -x, -y, z, #2 x-1/2, -y+1/2, -z+1, #3 x+1/2, -y+1/2, -z+1, #4 -x+1/2, y+1/2, -z+1; **4e** – #1 x-1/2, -y+1/2, -z+1, #2 x-1/2, -y+3/2, -z+1, #3 x+1/2, -y+3/2, -z+1, #4 x+1/2, -y+1/2, -z+1; **3fa** – (i) x, y, z-1; (ii) x, y, z+1; (iii) -y+1, x-y, z+1/3; (iv) -x+y+1, -x+1, z-1/3

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2. John P. Perdew; Matthias Ernzerhof; Kieron Burke. "Rationale for mixing exact exchange with density functional approximations" (PDF). *J. Chem. Phys.* **105** (1996) 9982–9985.
3. Adamo, Carlo; Vincenzo Barone. "Toward reliable density functional methods without adjustable parameters: The PBE0 model". *The Journal of Chemical Physics*. **110** (1999) 6158–6170.
4. F. Weigend and R. Ahlrichs, "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy," *Phys. Chem. Chem. Phys.*, **7** (2005) 3297-305.
5. F. Weigend, "Accurate Coulomb-fitting basis sets for H to Rn," *Phys. Chem. Chem. Phys.*, **8** (2006) 1057-65.
6. Sheldrick, G. M. *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, *64*, 112-122.
7. K. Brandenburg, Diamond 3.2k, Crystal Impact GbR, Bonn, Germany, **1999**.

Cartesian coordinates of the relaxed potential energy scans:

Compound **4a** (S configuration at the stereogenic carbon atom)

82

Coordinates, constrained distance 1.80 Angstrom, absolute energy -2738.44590323079 Ha

C	-1.73038549394793	-5.42491955948135	4.55234747950300
C	-1.84070516114145	-4.67212599745839	5.87915667908580
C	-2.21741158016121	-3.21034600586365	5.63784568709468
C	-3.48042155214947	-3.10365979001454	4.77823546714628
C	-3.28955503060884	-3.77220420858157	3.41361284404492
C	-2.99263691144381	-5.25788930476080	3.69500439587675
N	-4.43215032402120	-3.54706924198413	2.47515297608498
C	-5.26147554656849	-2.33317800737948	2.65603667174201
C	-4.71844796687895	-1.26578041872246	3.68620773997715
N	-3.83154013329670	-1.708754727242471	4.59331564970259
O	-5.10549634386096	-0.09845272732325	3.64418060056250
H	-0.85777283219620	-5.05054851170987	3.98917027440516
H	-1.54637030259906	-6.49465639742056	4.73082911461437
H	-2.60897592657581	-5.15109491004748	6.51110100755644
H	-0.89636006969580	-4.73055095023644	6.43958435210270
H	-2.39079522918826	-2.69180840887898	6.59564452067558
H	-1.39253853038307	-2.68166202511463	5.13059158418539
H	-4.30380784558660	-3.61834236465941	5.30373294248281
H	-2.37578093583503	-3.32220194918200	2.97563481062372
C	-5.49303963623867	-1.51684741468685	1.36335644313564
H	-3.49615294296891	-1.01251765901865	5.25808461484209
H	-3.86247427014931	-5.70387070637184	4.20751423120447
H	-2.86077271072130	-5.81692140300645	2.76272429491236
P	-6.88625611237820	-2.81472664306134	3.26283060473692
O	-7.82751325641327	-1.59507749191065	3.45632827626873
Si	-8.39749390313195	-0.16832524921618	4.28824290847003
C	-10.22829454001051	-0.47639453578377	4.52188189613484
H	-10.43134871254521	-1.35709350073396	5.14775218263074
H	-10.75286491323237	-0.59847696002186	3.56358668206460
H	-10.67642732703574	0.39343876683424	5.02757699376904
C	-8.09028316651572	1.26713405070671	3.14281322037681
H	-8.55775011840529	1.10907024562500	2.16000587467688
H	-7.01571419296176	1.44177656870655	3.00503199881226
H	-8.53527671902905	2.17753768772319	3.57294116330580
C	-7.51122378891822	-0.03693433829011	5.92533860809134
H	-6.44243152333005	0.17037620078802	5.78173227510066
H	-7.62648927726748	-0.94596269755032	6.53299594773619
H	-7.94432524584177	0.79773048388714	6.49869266040496
O	-7.55260833112114	-3.75803831926319	2.20952110175613
Si	-9.02812059600800	-3.87888633004214	1.28359319883293
C	-8.85283220388629	-5.47359667633144	0.33402722616962
H	-9.76339776143821	-5.63682647321593	-0.26384103833290
H	-8.00128422063345	-5.45929954640997	-0.36011875485881
H	-8.73774014370040	-6.33892734403573	1.00199412715974
C	-10.45932243343307	-3.95538282735381	2.48265668974320
H	-10.52071177130257	-3.06097990229946	3.11901341821667
H	-11.40141660227378	-4.02122921694694	1.91649877069556
H	-10.40759196471435	-4.84483276797109	3.12789946291143
C	-9.13229540532210	-2.38512409462522	0.16644093066164
H	-10.08479148386620	-2.41522302921025	-0.38557232989044
H	-9.10421055026391	-1.44243420333304	0.73011551099978
H	-8.32582690411471	-2.36484530805557	-0.58056098545490
O	-6.70789293835766	-3.58049108801534	4.60906349982818
Si	-7.41187051788804	-4.78670540348657	5.64503062196861
C	-9.07975374940671	-4.15799530277117	6.20397274949043
H	-9.54562547057545	-4.90536200854554	6.86575800653291
H	-8.99051050733798	-3.22401727525446	6.77725327203046
H	-9.76619077545444	-3.98888173347059	5.36332848496968
C	-7.52680123847504	-6.37220738699383	4.66605521525061
H	-7.85593079864929	-7.18847197591418	5.32738142049600
H	-8.24781060276657	-6.30202570061468	3.84000616810845
H	-6.55159701766890	-6.65660451952147	4.24596645251206
C	-6.21896122630756	-4.92023948834738	7.07371693532378
H	-6.64097537364579	-5.58592930595401	7.84264869766448
H	-5.25125840249953	-5.34351828837239	6.76970598876713
H	-6.03984978203966	-3.94326917355360	7.54549693319253
H	-5.97457112406508	-0.56617164816452	1.61246570122962
H	-4.51581065081134	-1.29859991558776	0.91359774263251
H	-6.10319184320744	-2.05733930155461	0.63886628646773
Si	-4.28587426520859	-4.51828027135228	0.94704670068269
C	-5.17606530922073	-3.88426012674383	-0.59421951042295
C	-2.47071710502863	-4.54891057081540	0.42424174014054
C	-4.99748116819744	-6.25247583445516	1.18823788190625
H	-4.98745219036185	-4.66184882217402	-1.35350482529295
H	-6.26589072700987	-3.79401193022366	-0.49937412022807
H	-4.77505434567061	-2.94306211775487	-0.98963253305966
H	-2.39857955162148	-5.11885390812620	-0.51477550436080
H	-2.11997358662929	-3.52777976758496	0.20904608402023
H	-1.7668866420407	-5.00185982337814	1.13279394731721

H	-4.53282070474205	-6.84043708865756	1.98811362104804
H	-6.07407004521232	-6.18583710914858	1.40234551766930
H	-4.88368787242472	-6.81890997274456	0.25002182136398

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Coordinates, constrained distance 2.03 Angstrom, absolute energy -2738.445420702846 Ha

C	-1.81117234448792	-5.40322963583427	4.65915279489285
C	-1.93231086053243	-4.57966300908490	5.94233096901443
C	-2.24007810225986	-3.11645759561619	5.62151214225715
C	-3.46593842038290	-3.00358457563913	4.71192903052982
C	-3.23899673929329	-3.73747487303790	3.38724682211516
C	-3.02836770415746	-5.22186100312983	3.74137499213983
N	-4.30956126487595	-3.47814224151400	2.37102318084774
C	-5.15117707456730	-2.32122606588979	2.52785991731878
C	-4.66279232532515	-1.21713741377189	3.51756306728221
N	-3.77446927362436	-1.60959346895193	4.45161909714348
O	-5.07910818693432	-0.06081501615865	3.43284197648560
H	-0.90118132569961	-5.09986336219989	4.11230259565023
H	-1.68532737819117	-6.46959801760999	4.89785908690737
H	-2.73857725809751	-4.99529386608943	6.57149668981261
H	-1.00901967766788	-4.64916049833473	6.53552416073196
H	-2.42475898021092	-2.54793342997079	6.54818688644443
H	-1.37768332929413	-2.64434796308399	5.12080346622757
H	-4.32395144620087	-3.47390439602736	5.22589523669589
H	-2.28578053192701	-3.35110912780116	2.97658069989857
C	-5.53325747497423	-1.59252234412532	1.23703461429546
H	-3.47785564141015	-0.89384331936053	5.11385661713842
H	-3.93919278931834	-5.60531015736481	4.23295677198570
H	-2.88029023910719	-5.82683964490262	2.84028425002061
P	-6.96388940373304	-2.82143072623314	3.28211296635726
O	-7.92150737390828	-1.61532444836527	3.52123014785833
Si	-8.39662207269245	-0.17689357254457	4.39295738314182
C	-10.20244452282925	-0.46919069259038	4.78272850867488
H	-10.35752851257197	-1.34300770274793	5.43139552197266
H	-10.79865654222677	-0.60338247914487	3.86864863257058
H	-10.60872158675751	0.40852156238193	5.30962738149735
C	-8.16196911373238	1.24549962268382	3.21558714750145
H	-8.73105514112973	1.10259215135735	2.28563650467497
H	-7.10020029772418	1.37972701204881	2.97118583340833
H	-8.52694634286774	2.17351436456118	3.68226107842269
C	-7.35367138378561	-0.05334418149234	5.93565250774489
H	-6.30614057309415	0.15695228137555	5.67979497211708
H	-7.40158357110791	-0.96782340451123	6.54420294825578
H	-7.72166542682530	0.77720038651242	6.55836879956473
O	-7.64849791290776	-3.75905571697252	2.22755843551655
Si	-9.10706962059584	-3.85637483977792	1.27739879319886
C	-8.91577720746750	-5.44171255491034	0.31409336736514
H	-9.81824617384467	-5.60981071335974	-0.29429275922480
H	-8.05730926162391	-5.41514326675715	-0.37138039538520
H	-8.79790601791964	-6.31089998248040	0.97682590773047
C	-10.55396262057425	-3.93653611215902	2.45792785230330
H	-10.61135254792079	-3.04809131867806	3.10346749021412
H	-11.49266050548565	-3.98922927873708	1.88513345047947
H	-10.51219840929571	-4.83197538310982	3.09573911989499
C	-9.18746638269828	-2.35032457618475	0.17560079595025
H	-10.10979137484910	-2.39095202822773	-0.42494775101881
H	-9.20880740350171	-1.41561817123232	0.75311449038782
H	-8.34413548743818	-2.30117265138847	-0.52800665028827
O	-6.75307250228625	-3.62368293700715	4.60913560477371
Si	-7.45109557460491	-4.84381129703378	5.63512468355569
C	-9.12597651073979	-4.23454709928615	6.19560310767544
H	-9.58558584609047	-4.98698981671378	6.85595859240957
H	-9.04405533924037	-3.30077421796968	6.77053723420126
H	-9.81364744685179	-4.06882369642681	5.35511075766120
C	-7.55082714077741	-6.42240884677374	4.64287269438284
H	-7.87550086682843	-7.24719403065894	5.29577029999371
H	-8.27047740901555	-6.34983463261928	3.81562639150196
H	-6.57255995633894	-6.69679803109889	4.22299182142677
C	-6.25334840753765	-4.97404418772298	7.05959473205665
H	-6.63789182915162	-5.68973540288464	7.80270115989197
H	-5.26635937517683	-5.33353871736359	6.73629715515942
H	-6.12161790143132	-4.00813532810775	7.56849720329089
H	-6.11035668226458	-0.69475830039523	1.48204867589866
H	-4.61459073994327	-1.26957301541918	0.72837594917566
H	-6.10762380908179	-2.22266902053303	0.55756075030200
Si	-4.16270626570199	-4.52440142314028	0.88927996647573
C	-4.95460396661824	-3.90551324108492	-0.70797580226435
C	-2.33013882941823	-4.66598640771059	0.46417836616131
C	-4.98447956270300	-6.20102379837947	1.17688532841189
H	-4.67996615312133	-4.66685786859638	-1.45708028056365
H	-6.05206372557122	-3.86797529339304	-0.68445497844011
H	-4.57205232503124	-2.94366264267804	-1.06925075384917
H	-2.23198603878214	-5.30994999142562	-0.42341295417187
H	-1.93067660886969	-3.67732632103646	0.19068663618507
H	-1.68190508466247	-5.08484836874098	1.24282838453692
H	-4.55152249059526	-6.79797987028119	1.98796435864744
H	-6.05303581861299	-6.06028285825133	1.39669075162308
H	-4.91551263330195	-6.79598889108396	0.25213461716764

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Coordinates, constrained distance 2.52 Angstrom, absolute energy -2738.440257731519 Ha

C	-2.16075573758281	-5.42628549457839	4.83706183296349
C	-2.23098575480427	-4.44566171628833	6.01443348278544
C	-2.35868118172522	-2.99271339871214	5.54270268973684
C	-3.52163329781873	-2.86218390374424	4.55982898325507
C	-3.25979688590308	-3.73945603270538	3.33020043379430
C	-3.28772270383560	-5.19896489059234	3.81786270522673
N	-4.16591792676022	-3.43478956225075	2.18438458274692
C	-5.08120137469897	-2.391670777682695	2.30843578319958
C	-4.64865063126816	-1.19315920949967	3.18128313482611
N	-3.74484034621523	-1.48775466160480	4.14569471618478
O	-5.07309698336398	-0.05913328852344	2.96244345787474
H	-1.18937040595268	-5.31274942799008	4.32479895953674
H	-2.19297443988528	-6.46245823233019	5.20535543315860
H	-3.10001362365271	-4.69338242677439	6.64706106499617
H	-1.34244170796299	-4.55542340763053	6.65284688949854
H	-2.52616010594598	-2.32647228166191	6.40474062324829
H	-1.42841612615967	-2.65955717449370	5.05247513775565
H	-4.43237338801767	-3.23954900494579	5.05825398839018
H	-2.23264370712607	-3.51595636322813	2.99025377633275
C	-5.72126030918989	-1.88387007249294	1.03124569045619
H	-3.45624044440745	-0.71935995473301	4.74932932535594
H	-4.27080315580031	-5.40858525489779	4.27294690842119
H	-3.17618611600534	-5.89812851968493	2.97947080694065
P	-7.01457632630670	-2.93958139429219	3.32536379565241
O	-7.97176231205513	-1.73044682989724	3.63580924987975
Si	-8.32659586311858	-0.22940549133596	4.43786032403929
C	-10.06249896610793	-0.46149371128957	5.09582144797445
H	-10.12630821572832	-1.27399544933244	5.83355879188542
H	-10.77845359291199	-0.66875742100313	4.28747513732407
H	-10.39164207741898	0.46433740402281	5.59318593662691
C	-8.25255027361063	1.10333369662052	3.13875968469503
H	-8.95091548307955	0.90711925568068	2.31196082462906
H	-7.23705021445960	1.20617187100925	2.73381980956558
H	-8.53964090653645	2.06806508408754	3.58551706463627
C	-7.08117038555379	0.01105603944460	5.80969668131490
H	-6.08346197754459	0.21269887007888	5.39614318281402
H	-7.02651428618708	-0.86051319316280	6.47822349516262
H	-7.36894461377871	0.87970344357624	6.42222320954551
O	-7.81070191458882	-3.87917734862718	2.33463632307942
Si	-9.31152704525832	-3.94803472506837	1.46347280053126
C	-9.18321509044737	-5.52749287727951	0.47742568667980
H	-10.11964729525443	-5.69826888384220	-0.07575066751235
H	-8.36932505974560	-5.48716834510370	-0.26130257375363
H	-9.01529584375530	-6.39982120292649	1.12476731119268
C	-10.70616222986782	-4.01549205683023	2.70815617162157
H	-10.71918059414339	-3.13022095697374	3.36105142693409
H	-11.67081530051723	-4.04854623048975	2.17844793360221
H	-10.65182606315262	-4.91397824762165	3.34053732861685
C	-9.44192775326512	-2.43987175649246	0.36684058057245
H	-10.39602087949614	-2.47377748277708	-0.18194645298590
H	-9.42410955172140	-1.50507734986624	0.94391278275963
H	-8.63747133936651	-2.39868370269238	-0.38161771500412
O	-6.77158497635337	-3.76051016598708	4.65292635303954
Si	-7.49818685489028	-4.92723984814695	5.71437613439285
C	-9.08922738713380	-4.20511755580384	6.37606771774750
H	-9.56407953137975	-4.92805333266071	7.05800708027966
H	-8.90121926672815	-3.28692328732414	6.95168563834899
H	-9.80962910113764	-3.97574942563869	5.57941538693490
C	-7.76232319224664	-6.49954967545115	4.73953109859194
H	-8.11110957995380	-7.29708480473882	5.41361695937190
H	-8.51341909127482	-6.37818548965316	3.94743654995371
H	-6.82798891780000	-6.84436135385048	4.27356826354524
C	-6.24040896305615	-5.16244916250647	7.07438064853121
H	-6.66203267912617	-5.81192237225202	7.85722249039317
H	-5.32433765530905	-5.64524616589927	6.70650437164362
H	-5.96606448144379	-4.20936396253454	7.54793147477090
H	-6.48159406779135	-1.13251827765598	1.26913927922741
H	-4.96392587452338	-1.38647091238267	0.41182055884069
H	-6.17629046578943	-2.69733773596192	0.45688683136601
Si	-3.78555268034275	-4.37338445497227	0.65415061003160
C	-3.90552778478687	-3.39332332849331	-0.95059586441212
C	-1.96882185319695	-4.86477699863282	0.73923156529991
C	-4.92239226654046	-5.86537431864014	0.54435346609696
H	-3.40805072568447	-4.01701571891594	-1.71144821788214
H	-4.92487122909179	-3.20214589745735	-1.30572043099220
H	-3.36061430257708	-2.44018782187179	-0.91450363603666
H	-1.74419137088309	-5.39850758683184	-0.19801504507782
H	-1.32127919745386	-3.97552140539824	0.75990688873544
H	-1.67471788934378	-5.52460939946076	1.56384043200076
H	-4.78913123251941	-6.56245935793746	1.38385952762431
H	-5.97932086490328	-5.56104777157781	0.53260857508431
H	-4.72449670767826	-6.42029136278866	-0.38620668621580

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Coordinates, constrained distance 2.48 Angstrom, absolute energy -2738.437757110195 Ha

C	-2.17049829962512	-5.48542142967137	4.75748209086811
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C	-2.26724301161909	-4.54139496192497	5.96222452673380
C	-2.36111672590032	-3.07255900806054	5.53327084912222
C	-3.49111194134510	-2.89761951208659	4.51913106931819
C	-3.19218880223823	-3.73740860347790	3.27240147957081
C	-3.26042591224368	-5.21138733743334	3.70941572234235
N	-4.06587592805540	-3.39354739496342	2.11030010389131
C	-4.93904611245688	-2.35520183155492	2.22593025148675
C	-4.57580356107341	-1.19545632243423	3.16109331525869
N	-3.69321167443039	-1.50955613056614	4.14105307616816
O	-5.01069509099873	-0.06328530592741	2.95712742897250
H	-1.18141889410983	-5.37052310478548	4.28046036104970
H	-2.23046947071272	-6.53202149354817	5.09084361230237
H	-3.16015411391453	-4.79685296993100	6.55740732957052
H	-1.40218260768200	-4.68416548730066	6.62568023513743
H	-2.54740842975469	-2.43076607367227	6.40966927064703
H	-1.41183664014531	-2.73708578811976	5.08258012463775
H	-4.42109788736710	-3.28515600938315	4.97315214599602
H	-2.15610232920990	-3.51689022369229	2.95985236259901
C	-5.67615521452133	-1.87823383413197	1.00330928587673
H	-3.45008949174172	-0.76388690375904	4.79145328655273
H	-4.26077134182851	-5.41595526800057	4.12783253505509
H	-3.13118041792534	-5.88759763977291	2.85515764475744
P	-7.04779579763471	-2.93984383429717	3.38917804389735
O	-8.07729437222411	-1.76129636109326	3.66746541666963
Si	-8.37479452337210	-0.24228790287389	4.44132771034127
C	-10.11521984165194	-0.40148800080820	5.11003038271990
H	-10.20190132127660	-1.20581609537826	5.85452899749280
H	-10.83981580069480	-0.59483606125843	4.30596432787237
H	-10.41238858044658	0.53899189981206	5.59958124997768
C	-8.25765549672917	1.07582587185843	3.12772951721253
H	-8.95161552743714	0.88618488970065	2.29566566160689
H	-7.23602257392789	1.15248922269488	2.73155523923869
H	-8.52625759735622	2.05249813467477	3.55981967469347
C	-7.11756011302945	-0.01066692954310	5.80662092193886
H	-6.11248835091261	0.13951674655197	5.38805577914118
H	-7.09614071209874	-0.86514460882238	6.49874709254115
H	-7.36816076278722	0.88587172149671	6.39467255984518
O	-7.83505965102241	-3.92038327217746	2.40971853752175
Si	-9.31502389321844	-4.00193096945522	1.52055978189623
C	-9.17406260434736	-5.59813844314024	0.55968510384162
H	-10.10127565966853	-5.78057912140050	-0.00508058174135
H	-8.34881980601581	-5.56895748703525	-0.16721650624935
H	-9.01391525869667	-6.45909440387415	1.22423513025327
C	-10.74152601254246	-4.04816338486771	2.73054145211342
H	-10.76968946516642	-3.14898673343907	3.36338768371165
H	-11.69402281557387	-4.09637866161897	2.18057386542756
H	-10.69777050111757	-4.93199140891905	3.38418085451215
C	-9.42910118740259	-2.51564679520996	0.38974655832010
H	-10.37384259581519	-2.55927073096993	-0.17436755542346
H	-9.42052736014390	-1.57018859069155	0.94958181538919
H	-8.61281267081476	-2.48819097514112	-0.34670300494144
O	-6.84919787785331	-3.74258508973594	4.75018503401411
Si	-7.58305748513865	-4.88254448328097	5.82167804384700
C	-9.19856536514237	-4.17481998981449	6.44149122304257
H	-9.67741125310636	-4.89331539493200	7.12538828890453
H	-9.03546907873742	-3.24454042819148	7.00504005742913
H	-9.90492953919439	-3.96854949839582	5.62609453503328
C	-7.81394726885000	-6.48854200404946	4.89050489868957
H	-8.17658971705210	-7.26829570406147	5.57781633362697
H	-8.54478342593457	-6.39261362633065	4.07597781402179
H	-6.86694269228170	-6.84241942544855	4.45793437053871
C	-6.34581367619500	-5.06511264498392	7.21045493379550
H	-6.75397381324076	-5.72135422214989	7.99436313871032
H	-5.40601535112168	-5.51502225301625	6.86106595521260
H	-6.11375564069241	-4.09658546931808	7.67577872220509
H	-6.44121657386209	-1.15101730090829	1.29271246175611
H	-4.97995021932073	-1.35359483434221	0.33391996842770
H	-6.13931747504252	-2.70774537343701	0.45863160602977
Si	-3.68702814335010	-4.32426446145711	0.55172583221775
C	-3.78613993429811	-3.27877396640503	-1.00826776741898
C	-1.87784641280340	-4.83011513809538	0.65603405277928
C	-4.85334048271280	-5.78678344565938	0.42381672665914
H	-3.27389556263135	-3.86707112550893	-1.78742464527147
H	-4.80044775577832	-3.07512220729691	-1.37018321196554
H	-3.24426088639753	-2.32688836460375	-0.92160894504487
H	-1.64202404319266	-5.34515498643879	-0.28900950667063
H	-1.22363941505156	-3.94713959755797	0.70637157440561
H	-1.60460939755595	-5.51034398005841	1.47106256720732
H	-4.73767713274988	-6.49712887335154	1.25440104367417
H	-5.90370883352536	-5.46186771180975	0.40984249905179
H	-4.65966879516239	-6.33212647993696	-0.51327342264342

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Coordinates, constrained distance 2.70 Angstrom, absolute energy -2738.437128030518 Ha

C	-2.18285070656790	-5.37651895101973	4.81753403360511
C	-2.31865358757236	-4.39944462551031	5.99164103275792
C	-2.38436736877458	-2.94300688907555	5.51775270990068
C	-3.47347162617160	-2.78948199067515	4.45692310941651

C	-3.13244553858633	-3.66587999860413	3.24646950153717
C	-3.23164753716156	-5.12591894007059	3.72297208076795
N	-3.97844365093311	-3.35903318813639	2.05116208738862
C	-4.81716946994645	-2.31383740463021	2.09708051686028
C	-4.51105945800035	-1.13318668486826	3.02042219874797
N	-3.65388983104602	-1.41215168071669	4.03303517748101
O	-4.94134621021871	-0.01341462519888	2.75473077489921
H	-1.17600520820652	-5.28193900997602	4.37467011980455
H	-2.26467620119667	-6.41325109430789	5.17626951129650
H	-3.23531236433240	-4.63174568692582	6.55935113077479
H	-1.47980848058824	-4.52900741713259	6.69048618862187
H	-2.59906269317679	-2.27478780715207	6.36724697964044
H	-1.41590861852293	-2.62702478862881	5.09426547596829
H	-4.42465875242726	-3.16142880968435	4.87972169572621
H	-2.0889608588047	-3.46001344714852	2.94929419562159
C	-5.63042891538826	-1.92726219139372	0.90159267652441
H	-3.43811242020986	-0.64919528311786	4.67293961267628
H	-4.24823282213867	-5.30510425683088	4.11212039655377
H	-3.08021659455285	-5.83023523167043	2.89597840457649
P	-7.08243367403152	-2.93452805942332	3.43753514559719
O	-8.18597370774687	-1.82490841253065	3.78814064978278
Si	-8.40489391253414	-0.28613453929892	4.53067018464545
C	-10.12650978108034	-0.36291222663439	5.25830669427475
H	-10.21952514793097	-1.15539388010311	6.01473425469644
H	-10.88275304116160	-0.53966666977631	4.48001641445151
H	-10.37161620339085	0.59401438592162	5.74437678498539
C	-8.26968292497591	1.00887325521800	3.19365517073315
H	-8.98829077196767	0.83095377675227	2.37991583063401
H	-7.25500065966714	1.04028250032608	2.77213660369190
H	-8.48942431696411	2.00372316160554	3.61157316341200
C	-7.09522057220425	-0.06795499751756	5.85178767869831
H	-6.09313925923035	-0.00014499950806	5.40405069110785
H	-7.10411702800229	-0.89020595417274	6.58228313663345
H	-7.27100669072999	0.86857989552633	6.40320903713357
O	-7.86482242959694	-3.90111612718714	2.42181008547988
Si	-9.33576595424111	-3.95908244517749	1.53009792744742
C	-9.20771617935189	-5.54659021597228	0.54918020177292
H	-10.12473263349128	-5.70275494124320	-0.03963524664262
H	-8.36533029401776	-5.52428761488657	-0.15843926515868
H	-9.08005379823113	-6.42027138415024	1.20419604491627
C	-10.77945327163834	-3.99971411041758	2.72053351247897
H	-10.80328753452427	-3.10238717880936	3.35587126510246
H	-11.72622754736114	-4.03864602626628	2.16021289465372
H	-10.74945419303984	-4.88484652701952	3.37334164134173
C	-9.42967593397111	-2.46590439907432	0.40326785419359
H	-10.37778610268485	-2.48833965804643	-0.15633642789408
H	-9.39935033865081	-1.52236608406443	0.96573593057577
H	-8.61711017374440	-2.45229237521549	-0.33802195612001
O	-6.87968086688158	-3.80828940389044	4.76619675408497
Si	-7.62839630134674	-4.96100682065204	5.80246127512263
C	-9.21650517581259	-4.23964864354175	6.47752839091251
H	-9.70274507062974	-4.96939300465269	7.14390866197985
H	-9.02013413099085	-3.33377374431104	7.06975910514365
H	-9.92962361599070	-3.98513191517625	5.68175687716754
C	-7.91449856213246	-6.53059003214127	4.82354903722219
H	-8.31050525446533	-7.31924556192319	5.48163765333013
H	-8.63421832150068	-6.38047900219137	4.00736980975200
H	-6.97723820871008	-6.90287599284833	4.38497599767547
C	-6.37750507958170	-5.23408242098752	7.16648063074699
H	-6.79380232285043	-5.90716056790099	7.93177199652269
H	-5.45700448748972	-5.69897955216610	6.78597499532487
H	-6.10986545017156	-4.29120571556206	7.66430020940990
H	-6.38963641013488	-1.19743018368938	1.19827146211976
H	-4.98631501252179	-1.42412065457870	0.16508535234105
H	-6.10445389464372	-2.79444632688153	0.42974322674818
Si	-3.61801236955410	-4.38346268388714	0.52701461080749
C	-3.71541523707971	-3.38340559222394	-1.05945674696040
C	-1.81669293098182	-4.90364198507672	0.65722148620579
C	-4.82255730302088	-5.81649430073623	0.48907588774163
H	-3.20031333325006	-3.99194468715962	-1.82107458164335
H	-4.73048724079923	-3.19416186120177	-1.42684209016110
H	-3.17579844349614	-2.42813940264497	-0.99965406217510
H	-1.58935188629003	-5.47228784868654	-0.25891564870527
H	-1.15141450846625	-4.02740735674985	0.65844919604032
H	-1.55182198941135	-5.54284371947740	1.50728230472268
H	-4.67515913843931	-6.52133578203642	1.31884137811020
H	-5.86454609273991	-5.46725819100941	0.53034064316989
H	-4.69315114285391	-6.37417819239485	-0.45178132653002
82			
Coordinates, constrained distance 2.93 Angstrom, absolute energy -2738.436972649999 Ha			
C	-2.16228562979087	-5.19917174445751	4.91887953811495
C	-2.34432524603545	-4.16905865589391	6.03949747241063
C	-2.41431236509623	-2.73885541034223	5.49216631212988
C	-3.47109531084709	-2.65267334476262	4.39133113068183
C	-3.08150606178061	-3.58230097943235	3.23641254795080
C	-3.18173741228311	-5.01719314704837	3.78362451323074
N	-3.90376209996186	-3.35203964277940	2.00489428440081

C	-4.71474935614765	-2.30234885971796	1.95253430525226
C	-4.46773449383726	-1.08044551031449	2.83761965930826
N	-3.65113140724937	-1.29950663531340	3.89596933161897
O	-4.89092764092290	0.01755654724857	2.48655899431273
H	-1.14420953913775	-5.11371444705308	4.50051373745451
H	-2.24357835994189	-6.21838402608498	5.32490139904528
H	-3.27333768157246	-4.38717693842970	6.59238243712696
H	-1.52370672438107	-4.25201597475200	6.76666259208907
H	-2.66689624739988	-2.03316412923758	6.29958128729587
H	-1.43707835892172	-2.42844820005941	5.08488025328422
H	-4.43151377332646	-3.01784375692089	4.80080223938270
H	-2.03413127936346	-3.37873725510491	2.95083799324982
C	-5.56716801023900	-2.01676557337666	0.76257790679666
H	-3.46938298203327	-0.50371352335815	4.50591642219111
H	-4.20813578725686	-5.18218616062580	4.15194147283133
H	-2.99999786029220	-5.76420875127276	3.00211051307818
P	-7.15806402249207	-2.93000545755482	3.44374486377556
O	-8.30994615451716	-1.91946501004557	3.95379650311923
Si	-8.43008525973188	-0.36061967805387	4.66213033102314
C	-10.13852766699519	-0.32965675669277	5.42136719661894
H	-10.26259652485831	-1.11550007651025	6.18035686241669
H	-10.91682705070290	-0.46579667676003	4.65662663746565
H	-10.32031738272524	0.64008455295410	5.90937993747310
C	-8.23396406870975	0.91245790368500	3.30946845947191
H	-8.99571773385043	0.79300764698453	2.52461343830898
H	-7.23802168390979	0.85317685542683	2.84563384132856
H	-8.34737438650428	1.92616188000942	3.72438376223461
C	-7.08321883675299	-0.19421445922575	5.95716482119272
H	-6.08512712863538	-0.21267787736003	5.49414265557018
H	-7.13432969717391	-0.99550894729178	6.70893127774061
H	-7.17962771786479	0.76636518550774	6.48601404677812
O	-7.96680313200292	-3.85819507170231	2.40066330630141
Si	-9.42689406856804	-3.85459160073769	1.50063063198269
C	-9.29565024176832	-5.38041592546979	0.42463400209506
H	-10.20268973319529	-5.49705375781362	-0.18807149711652
H	-8.44026077953199	-5.32041599991411	-0.26512441415239
H	-9.18270171756621	-6.29204359509269	1.02893118046376
C	-10.88323299370293	-3.95971107432678	2.67221266827617
H	-10.91776453034611	-3.09091035739068	3.34549728395407
H	-11.82525052131462	-3.98264162750663	2.10308512542549
H	-10.84942607326080	-4.87134683266747	3.28709088469148
C	-9.50654418554354	-2.29518396476719	0.46412951482147
H	-10.43472708352736	-2.28954977952246	-0.12814327106827
H	-9.50634133938751	-1.39029073176966	1.08779206787147
H	-8.66855778551827	-2.22504638298434	-0.24503683513868
O	-6.87522436489913	-3.91024325254584	4.69061600569567
Si	-7.62715147948082	-5.06085250660107	5.72004045894785
C	-9.18052079366324	-4.32625675860493	6.46127190087381
H	-9.65630659203662	-5.05748365285186	7.13335663310699
H	-8.95186749812470	-3.43040651377160	7.05720847006690
H	-9.91340160747145	-4.04895148630020	5.69146974754088
C	-7.98308999865000	-6.60283350272453	4.71825316477862
H	-8.40059162470534	-7.38985079928323	5.36497023638407
H	-8.70735484640199	-6.40770177083914	3.91533846011936
H	-7.06678340425040	-7.00108499905657	4.25865362840113
C	-6.34490607839001	-5.39606496212810	7.04350827058748
H	-6.73809305461068	-6.10821768503313	7.78515117936248
H	-5.42905873677811	-5.83345077085061	6.62077052424768
H	-6.07248468212704	-4.47547591743436	7.57972373642695
H	-6.32631480517790	-1.27915392759211	1.03788721684851
H	-4.95884221782741	-1.55584671704490	-0.03081908361901
H	-6.04114516720313	-2.92321362867436	0.37027082183303
Si	-3.55576746772868	-4.50529242907535	0.55431628300315
C	-3.66193187731149	-3.61449855580299	-1.09330024474369
C	-1.75366712885632	-5.00956955749855	0.71282966708301
C	-4.78542779549861	-5.91223303436540	0.65468154490090
H	-3.15176609215625	-4.27249303564848	-1.81603177870475
H	-4.67860967228014	-3.44691583584470	-1.46611782319993
H	-3.11884312259254	-2.65928526265298	-1.09791996932722
H	-1.53381291251413	-5.65518471664689	-0.15285541979480
H	-1.09463479257928	-4.13265010152457	0.62671413872714
H	-1.47312933254511	-5.56926357760419	1.61206903536013
H	-4.60597050779301	-6.57777116990834	1.50974135003846
H	-5.81780288670806	-5.53936557821687	0.73133616256733
H	-4.71607433116199	-6.51771755819183	-0.26263794367509
82			
Coordinates, constrained distance 3.16 Angstrom, absolute energy -2738.436791352923 Ha			
C	-2.18022206786695	-4.86926536550222	5.07869857829118
C	-2.47406473406746	-3.75024325249719	6.08437566219504
C	-2.55853421293673	-2.38158873133502	5.39998510322157
C	-3.54477089667819	-2.43751302830260	4.23375684589305
C	-3.06323174735643	-3.46042096137245	3.19825566923575
C	-3.13559748256430	-4.84045124888028	3.87562975913229
N	-3.84857672848137	-3.39111239390737	1.92117200050569
C	-4.66724441860992	-2.37482624456777	1.72260134328383
C	-4.49285490322849	-1.06023650903553	2.48307586876432
N	-3.72597971054659	-1.14492135323652	3.59599476934907

O	-4.92025712294608	-0.02280564758585	1.98611203128766
H	-1.14233478723361	-4.77668763551436	4.71414792376915
H	-2.24725925191230	-5.84983106784725	5.57309816853971
H	-3.42877216056391	-3.95807139094461	6.59562054008099
H	-1.70082973236009	-3.73096431442914	6.86594331823752
H	-2.88815233207949	-1.61461445675082	6.11911656028056
H	-1.56801491818717	-2.07057942455976	5.02646846318665
H	-4.52194996558488	-2.78886737306467	4.61594531320959
H	-2.01376479775910	-3.24200593925941	2.93201561339777
C	-5.55403643971296	-2.270744488087923	0.53247745357096
H	-3.59067909340416	-0.28677120330738	4.12845914617411
H	-4.17517989277271	-5.02044623788641	4.19697252867694
H	-2.87103293457428	-5.64592101113516	3.18068360641676
P	-7.24862773661734	-2.94197490072562	3.44841483971249
O	-8.36704789232226	-1.96331528831658	4.10080604363015
Si	-8.33717432810853	-0.43948437725905	4.88077534253639
C	-10.00132645216961	-0.31049606680624	5.72208536424031
H	-10.16019838040598	-1.13124618590694	6.43653271673886
H	-10.81983467391224	-0.33412412448561	4.98783114895083
H	-10.07970886615729	0.63755329631897	6.27564381350811
C	-8.09798418666802	0.88720554689478	3.58456550767945
H	-8.91567517543927	0.88038166590713	2.84798953827872
H	-7.14756268340351	0.76891070036857	3.04203284441294
H	-8.09105197764307	1.88249324785792	4.05530127627645
C	-6.92869212817154	-0.43827443100510	6.12391742332071
H	-5.95387581364015	-0.55493225238742	5.62551175018021
H	-7.03474578797635	-1.24739970833179	6.86133840694669
H	-6.90346675257299	0.51414914165292	6.67522907875872
O	-8.14450964972278	-3.81555586263384	2.42290399703035
Si	-9.58506712881971	-3.68363958087364	1.51007987285186
C	-9.51174714292675	-5.14317028135772	0.33961664572182
H	-10.40818209829334	-5.17268931665143	-0.29860711302553
H	-8.63676543967968	-5.08649304262948	-0.32551495666439
H	-9.46179399951389	-6.09597396140274	0.88655504589116
C	-11.06200370458382	-3.79424541347182	2.65458466639228
H	-11.07245283123438	-2.96308110135488	3.37477720102070
H	-11.99536230426446	-3.74730361019948	2.07259335647627
H	-11.07285283691321	-4.73886268324876	3.21784239446762
C	-9.57974244152548	-2.05782851335469	0.57614225957621
H	-10.50249314207980	-1.96316272705690	-0.01700508584955
H	-9.53594289476159	-1.19741302418036	1.25866555832802
H	-8.73480352007316	-1.98658840929322	-0.12474771470904
O	-6.90589176124386	-4.00007730961992	4.62099944030272
Si	-7.65042432434365	-5.22116323974101	5.56807733923779
C	-9.24272357765170	-4.57684631974130	6.31109013766827
H	-9.70788017127933	-5.35611277058172	6.93492789106038
H	-9.05822365514565	-3.70329101851929	6.95333350999010
H	-9.96727695121685	-4.28578413739486	5.53828736824962
C	-7.94147282608379	-6.71579055191160	4.47607086544429
H	-8.35907939871101	-7.54683938015688	5.06486809427545
H	-8.64644105956477	-6.48980278250080	3.66383742056568
H	-7.00347679757515	-7.06827887687280	4.02230888522653
C	-6.38719258198803	-5.59304434348695	6.90139518203295
H	-6.76053844863665	-6.37606039315306	7.57918811931439
H	-5.44000888445280	-5.95258168557013	6.47377145860144
H	-6.17475300491431	-4.70188016804306	7.51035254686471
H	-6.35378344666794	-1.55635586212976	0.75130632449832
H	-4.99612130274389	-1.85455504962494	-0.32063314509960
H	-5.97699300591760	-3.24028733489111	0.24812699598156
Si	-3.43770122280020	-4.69432134931303	0.61226485107360
C	-3.56075869626386	-3.98646158706262	-1.11941380500608
C	-1.61841815651553	-5.09584193254487	0.84461488611805
C	-4.61716309800597	-6.12433142583058	0.85992470591350
H	-3.00286553701050	-4.68499431257434	-1.76422450634642
H	-4.57807437564797	-3.91576206854220	-1.52102475878655
H	-3.06988702836285	-3.00792738672691	-1.21673942316788
H	-1.35613091865712	-5.82306744434357	0.05918571555546
H	-0.99798463512043	-4.20430118529238	0.66877003059400
H	-1.32625933270248	-5.53703510191915	1.80416063399350
H	-4.46295295590983	-6.65536830074548	1.80862806667394
H	-5.66496962092017	-5.78978354424871	0.82749021559464
H	-4.47438892291874	-6.84791560118278	0.04172546419656

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Coordinates, constrained distance 3.38 Angstrom, absolute energy -2738.436017352519 Ha

C	-2.18362257679378	-4.88516029803896	5.04762149140544
C	-2.51227029390665	-3.78262529709939	6.06052400057708
C	-2.57334860405333	-2.40358449397844	5.39449310655024
C	-3.52220616814891	-2.44108769971731	4.19685214040239
C	-3.01126428735656	-3.45072966203079	3.16265231356649
C	-3.10445172253579	-4.83998913437781	3.81811859113838
N	-3.76517817318184	-3.36728250733938	1.86608774657103
C	-4.55816947652558	-2.34084807272772	1.64865124929502
C	-4.40609102898848	-1.03740995820491	2.43411007812479
N	-3.67935264448576	-1.13864373737907	3.57101870382690
O	-4.81597827800431	0.00402948833102	1.93170955152724
H	-1.13581064816707	-4.78433571922330	4.71495511883620
H	-2.26291704198242	-5.87352127641698	5.52444161912597

H	-3.48488576295120	-3.99898312334474	6.53247408674838
H	-1.76731605873634	-3.77554679567373	6.86909856627777
H	-2.92589466294682	-1.64723149267317	6.11402212515952
H	-1.57091280952681	-2.08769602813243	5.05826960214740
H	-4.51262568279807	-2.79312584024774	4.54346455130365
H	-1.95544188121567	-3.23032577294956	2.92485156605460
C	-5.45688270580760	-2.23567115940706	0.46989228640156
H	-3.56516178786616	-0.28869267697726	4.12160128181425
H	-4.15276992958006	-5.02279690383664	4.10808650145556
H	-2.81982918559340	-5.63589722803373	3.12020284220769
P	-7.32289065559829	-2.95750339773890	3.49746030697753
O	-8.45108020316852	-1.99684891003199	4.17206365351083
Si	-8.38157115876521	-0.45334690007536	4.90441758385122
C	-10.04731248007604	-0.24550080563135	5.72649560881939
H	-10.23257787880938	-1.03216009810718	6.47202045399660
H	-10.86118707005431	-0.27779461267808	4.98736690361838
H	-10.10425530558457	0.72587928126300	6.24068742662752
C	-8.09283077272527	0.83510022760231	3.57737936315429
H	-8.89810476595868	0.82580962700857	2.82725785568834
H	-7.13617866785583	0.68971170954003	3.05257912929628
H	-8.07530234851810	1.84129599271404	4.02416981061733
C	-6.98387379471078	-0.45283358585468	6.16076951279613
H	-6.01015060260267	-0.62976953472342	5.67810616995896
H	-7.12787183649641	-1.22645271289620	6.92898435514457
H	-6.92617304612885	0.51994234504307	6.67243111936602
O	-8.22867699689125	-3.84885289851439	2.49117030964736
Si	-9.64749671862119	-3.70522161181895	1.55324970289696
C	-9.58141172237899	-5.17790790231993	0.39816469665043
H	-10.46872030156310	-5.20105309488070	-0.25293595041323
H	-8.69532029861345	-5.14254392652252	-0.25353110916243
H	-9.55442913364532	-6.12484273919757	0.95684783442740
C	-11.14564123274157	-3.77904609590650	2.67299935512895
H	-11.15064595390987	-2.94420917576497	3.38886155000755
H	-12.06923031123851	-3.71882432616417	2.07692170833367
H	-11.18149674281116	-4.71965444129742	3.24202612198965
C	-9.59792903272672	-2.09027148219077	0.59983838042468
H	-10.50943013440324	-1.98201723729758	-0.00817362812764
H	-9.54495156469471	-1.22319070257463	1.27327021092455
H	-8.74130409462965	-2.04486610169874	-0.08942312449859
O	-6.95888374634113	-4.01726512361731	4.66666913150654
Si	-7.69790421675905	-5.22760150121977	5.62751894259053
C	-9.27603388898893	-4.57204396179156	6.39178998894894
H	-9.73406596429977	-5.34356636506194	7.03030946703090
H	-9.07930724498061	-3.69229199766798	7.02191557638966
H	-10.01083443291606	-4.28559698917836	5.62690449608545
C	-8.01790153490894	-6.72783041176850	4.55043762872869
H	-8.43511324689806	-7.55067629282312	5.15100510342610
H	-8.73199500951134	-6.49972176861242	3.74682249810089
H	-7.09009740673574	-7.09279562434645	4.08563910285171
C	-6.41685435618279	-5.60538606205052	6.94325226174939
H	-6.78440989437674	-6.38300467624174	7.63025548326732
H	-5.48000422015934	-5.97378754762760	6.50021357060028
H	-6.18713703687655	-4.71342688312830	7.54469792197420
H	-6.27302510951555	-1.54809627911282	0.71668621658076
H	-4.92461895748147	-1.78262131287821	-0.38066726535988
H	-5.85794549138909	-3.20921852628047	0.16908003729841
Si	-3.34644649134456	-4.67525279576890	0.55625738388593
C	-3.45733091910762	-3.95378186047607	-1.16979126232851
C	-1.52986948933118	-5.07450688475319	0.80726381241215
C	-4.53486168772713	-6.09847058281943	0.79584616474869
H	-2.88716179443346	-4.64201254673761	-1.81497430620367
H	-4.47101106904241	-3.88815150941726	-1.58151916732128
H	-2.97346958936799	-2.97050926972054	-1.25362284402784
H	-1.25958062272505	-5.80530065872296	0.02783167726177
H	-0.90939512222711	-4.18278875898203	0.63258947694838
H	-1.24636297536691	-5.51038626543166	1.77181591361070
H	-4.36986214658421	-6.64917177868072	1.73125207159326
H	-5.58023655876332	-5.75500727187239	0.78763729510122
H	-4.41172153858365	-6.80691299301599	-0.03865280962105

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Coordinates, constrained distance 3.61 Angstrom, absolute energy -2738.434899927597 Ha

C	-2.22128190473090	-4.86961926361736	5.02776075239733
C	-2.59882141366541	-3.77210824122018	6.02881941798145
C	-2.62673842940240	-2.39067804492260	5.36555976743935
C	-3.52321063878867	-2.42257269416195	4.12823343495151
C	-2.97519322195342	-3.43251419501233	3.11355303275175
C	-3.09271495340917	-4.82284990796388	3.76251681592387
N	-3.69144302848154	-3.35074257879405	1.79467184748517
C	-4.46611171536986	-2.32048765989871	1.54949029797429
C	-4.32956507569699	-1.01404689159159	2.33485550566218
N	-3.64746903942033	-1.11770779172242	3.49777223810244
O	-4.71571506913071	0.02455584695403	1.80952724455617
H	-1.16110130806960	-4.76351624413214	4.73918180724886
H	-2.31715132966153	-5.86028127630832	5.49694590344331
H	-3.59499078472666	-3.98976830650081	6.44767036475126
H	-1.89601496942183	-3.76865909845548	6.87400935951479
H	-3.00893849725352	-1.63584348745816	6.07139640171469

H	-1.60976869478837	-2.07608254701007	5.07422741425261
H	-4.53105035235614	-2.76861273976746	4.42942240243718
H	-1.91255042417357	-3.21235342357728	2.90816435762697
C	-5.36872299255184	-2.22817998061305	0.37467016521401
H	-3.54865812302154	-0.26843799496142	4.05253360022107
H	-4.15065943348319	-5.00605058514469	4.01380293388865
H	-2.78129099310063	-5.61734744027265	3.07428515181137
P	-7.38475701112947	-2.99650573677187	3.56125402729986
O	-8.49271814129025	-2.01783319762343	4.25201030648525
Si	-8.38717045549930	-0.46574270051936	4.95406651168503
C	-10.03666212014651	-0.21043428329955	5.79554348223164
H	-10.22247697734458	-0.97779728812711	6.56066237277857
H	-10.86198345273551	-0.24713542481063	5.06941991495721
H	-10.07116062046730	0.77276097068548	6.28866856617273
C	-8.09476199099002	0.79911111969079	3.60320118619125
H	-8.90768628794277	0.78941611691802	2.86135785605744
H	-7.14611184147952	0.63413206402497	3.06978296491077
H	-8.05883960013998	1.81189803373770	4.03362397967317
C	-6.97110778460036	-0.46155039373730	6.19038091807539
H	-6.00839325125458	-0.66554326804336	5.69638212576572
H	-7.11561605421959	-1.21709832206316	6.97619086777811
H	-6.88955032373897	0.52042648059064	6.68056303925476
O	-11.34137803460744	-3.90439423791132	2.60423043370015
Si	-9.71294668539939	-3.71933104715187	1.62290733428160
C	-9.68400278529592	-5.21447660936733	0.49480725936496
H	-10.55748668104158	-5.21257817512319	-0.17520237492890
H	-8.78313652194293	-5.22822256341130	-0.13706020631857
H	-9.70877731463273	-6.15125383266967	1.07035072545696
C	-11.24301581698525	-3.70584420481030	2.70100623582501
H	-11.22299111560205	-2.86783425477239	3.41281038231526
H	-12.14648813962688	-3.60248907339765	2.08064871253345
H	-11.34137803460744	-4.63921616176249	3.27455625427361
C	-9.56575552880591	-2.12804859772642	0.63819812068053
H	-10.46045533918622	-1.98282856385426	0.01323621577592
H	-9.47458656679897	-1.25069410108733	1.29399000052120
H	-8.69768582896937	-2.14519618406207	-0.03807832013062
O	-7.00516155844807	-4.04326540488980	4.74007925355822
Si	-7.75342970470876	-5.25962180503436	5.68486024677420
C	-9.36281925943018	-4.62785298250473	6.40356253083479
H	-9.82755945632232	-5.40660473163610	7.02836967114994
H	-9.19622925344286	-3.74559716383619	7.03855680881249
H	-10.07985051441067	-4.35032347330234	5.61880745432105
C	-8.01871449368554	-6.76963814885526	4.60588304250026
H	-8.43908882360808	-7.59758387799907	5.19709920883822
H	-8.71234904351621	-6.55481438740857	3.78096036671564
H	-7.07164308337958	-7.12040613757266	4.16955924067812
C	-6.50510725918746	-5.61406955277163	7.03851802658069
H	-6.88448823169905	-6.38777834972790	7.72358665145358
H	-5.55414521188480	-5.97940099997823	6.62392178323616
H	-6.29824499327112	-4.71442184645572	7.63686155126491
H	-6.22443698674431	-1.60061889827352	0.65196641649902
H	-4.87267291725268	-1.70544334701570	-0.45748809151096
H	-5.71330756652988	-3.20998816731698	0.03648925506349
Si	-3.24638526351799	-4.66409575049627	0.49358644641778
C	-3.31900667038454	-3.92609378984193	-1.22720588594581
C	-1.43732606866855	-5.06628304103337	0.78693894859910
C	-4.44531312139022	-6.08177627738807	0.70729249956496
H	-2.71873995825998	-4.59563836987022	-1.86464373611001
H	-4.32138129094139	-3.87214221458957	-1.66758104788133
H	-2.85034716975909	-2.93351494889367	-1.28490015017354
H	-1.15281849738759	-5.80269021482007	0.01782761122136
H	-0.81092401580084	-4.17733051676223	0.61997919635345
H	-1.17592662496976	-5.49711937239695	1.75995554739196
H	-4.30894496784405	-6.62712288926059	1.65034139824807
H	-5.48922774657049	-5.73673054640102	0.66659794082982
H	-4.29894863288168	-6.79513781105886	-0.11922329530350

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Coordinates, constrained distance 3.83 Angstrom, absolute energy -2738.433772349718 Ha

C	-2.23153448020054	-4.85915720335240	5.01356466977598
C	-2.65635743696700	-3.77287635394527	6.00782417818091
C	-2.68243007457671	-2.38814687399189	5.35168406321858
C	-3.53270733657294	-2.42163234112059	4.08197334790283
C	-2.94049880962023	-3.42200347218743	3.08259121890838
C	-3.06314495587633	-4.81607806157779	3.72145497722336
N	-3.61973826014184	-3.34278269688729	1.74264861323630
C	-4.37694157504951	-2.30837425398674	1.47137635070141
C	-4.25798277932725	-1.00187364826942	2.26059015025033
N	-3.63625063369538	-1.11256048861255	3.45482170619715
O	-4.60934433080862	0.03775694903115	1.71398202379930
H	-1.16418102392063	-4.73808285684704	4.75978850774615
H	-2.33009111730851	-5.85395528380634	5.47345120546604
H	-3.66091149613782	-4.00811320748834	6.39580141623276
H	-1.97996411815530	-3.76360665590182	6.87416155336225
H	-3.10150602539954	-1.64373480518234	6.04748160082516
H	-1.66054363865598	-2.05605804044975	5.09938734296348
H	-4.54959943579182	-2.77525848077471	4.34249697070871
H	-1.87492007101042	-3.18912360959540	2.90855082532799

C	-5.27055087551567	-2.22087377143937	0.29017630227233
H	-3.55696763092755	-0.26559886624784	4.01630742265611
H	-4.12586396265648	-5.01198460065812	3.94011417443640
H	-2.72184790673226	-5.60410224639902	3.03998912626937
P	-7.49595552087250	-3.02807172651538	3.58309257776811
O	-8.56182775335639	-2.03844304102371	4.32788086003922
Si	-8.41275272592036	-0.48318464617820	5.00644521333094
C	-10.03598696786006	-0.18496158183590	5.88465135617499
H	-10.21440978089188	-0.93628619865828	6.66716571568355
H	-10.87991573533505	-0.22197966250904	5.18026806508021
H	-10.04303514857953	0.80699297917810	6.36096983572559
C	-8.12782319731511	0.76430369919289	3.63608165224776
H	-8.95503352225436	0.76155806916931	2.91029804949570
H	-7.19311917980967	0.57718596307012	3.08561350169896
H	-8.06479450502394	1.78034926351293	4.05550834706798
C	-6.96743095217246	-0.48519487755648	6.20954945662061
H	-6.01634932414423	-0.68436245629982	5.69152215570800
H	-7.09289137198465	-1.24604080171755	6.99355956280817
H	-6.87538120546948	0.49377085320621	6.70403158618496
O	-8.51204052252998	-3.95616016020467	2.71468053980550
Si	-9.83178287700560	-3.71914947042557	1.66627498359807
C	-9.86189378059342	-5.25237278996608	0.59080172455931
H	-10.70711022164970	-5.21792483734976	-0.11361677747214
H	-8.93994518745077	-5.35201023079686	-0.00120468647078
H	-9.97333155003403	-6.16158262975729	1.19940851588088
C	-11.39592431046639	-3.56738698673145	2.68288612059496
H	-11.33668912477153	-2.72015201487394	3.38120477748699
H	-12.26795599035394	-3.41082933409334	2.02982664235160
H	-11.58062158005128	-4.47927722354434	3.26956151263076
C	-9.53281290569245	-2.17722880592209	0.63574877820429
H	-10.36000782444639	-2.02135255470636	-0.07352354488816
H	-9.45824861107849	-1.27548433475209	1.26035368062043
H	-8.60772641208546	-2.26098153960398	0.04565267055280
O	-7.05388850833089	-4.06151607135204	4.75449514823302
Si	-7.77770221343376	-5.27996400221249	5.71434045835368
C	-9.39915536492625	-4.67475554254783	6.42965494661623
H	-9.85068729385711	-5.45952428451041	7.05661968039809
H	-9.24981831253140	-3.78656810002013	7.06037181073925
H	-10.11941638656285	-4.41315643164069	5.64229118946308
C	-8.01413565121476	-6.80813975960015	4.65435636421041
H	-8.42732844104126	-7.63499476755402	5.25203310847277
H	-8.70465504108918	-6.60965131754179	3.82284560656720
H	-7.05943742502969	-7.15116887877565	4.22845870161918
C	-6.51960961192873	-5.59439635795291	7.06946020969988
H	-6.88157044917034	-6.36796135221501	7.76406333835273
H	-5.56310555181594	-5.94612325485487	6.65568866485497
H	-6.32857729688907	-4.68433181422866	7.65723127186187
H	-6.14868198388763	-1.62979183504532	0.58162226868273
H	-4.79207918218577	-1.65870182848611	-0.52605564447968
H	-5.58195087962151	-3.20479490851623	-0.07178159041643
Si	-3.14074875801170	-4.65781734106135	0.45086580372442
C	-3.18776052180438	-3.91689701928839	-1.26917328897996
C	-1.33474697619286	-5.04258197774601	0.78173064917025
C	-4.33427145299481	-6.08280527659504	0.64257803427466
H	-2.56294765131335	-4.57499676401360	-1.89488210885480
H	-4.18085830202347	-3.87762038488712	-1.73161227537344
H	-2.73367968621370	-2.91686725020875	-1.31443738831488
H	-1.02985311583499	-5.78254587198512	0.02388835809084
H	-0.71356152254259	-4.14918438084984	0.61910597453956
H	-1.08721956431108	-5.46324170738885	1.76273213418062
H	-4.21741516058558	-6.62388413200987	1.59061142173145
H	-5.37918953801565	-5.74510720077713	0.57486409504551
H	-4.16314039239235	-6.79774523875162	-0.17773956321389
82			
Coordinates, constrained distance 4.06 Angstrom, absolute energy -2738.432875002369 Ha			
C	-2.48412333585073	-4.58811242499547	5.17486050635546
C	-2.93913099198830	-3.40181426598036	6.03051005450462
C	-2.84238226450518	-2.08393456863713	5.25445635961470
C	-3.60278858124789	-2.20371637331147	3.93481848147923
C	-2.98801083713320	-3.30855619391614	3.06962898141504
C	-3.20421274121447	-4.63644876683655	3.81764715342753
N	-3.59283501982601	-3.33346280509559	1.69208769087973
C	-4.30387748695108	-2.30998465812288	1.29096499038582
C	-4.16593421521039	-0.93528531878870	1.95458488991256
N	-3.61868034964664	-0.95396607121241	3.18854764775538
O	-4.43869215499004	0.05482727697008	1.28579945040973
H	-1.39522578841739	-4.52956411302647	5.00615240497738
H	-2.66408774146541	-5.53289052076991	5.70980595270946
H	-3.98484597428162	-3.55698527954780	6.34321212905402
H	-2.33928021993318	-3.34227039051184	6.94918879468750
H	-3.27374580519830	-1.26002848549970	5.84506055508672
H	-1.78911021424741	-1.82392867191648	5.05154032397831
H	-4.64743726144406	-2.49928174501060	4.15548188504879
H	-1.90695938064739	-3.12490366871664	2.93719162076106
C	-5.16116779785720	-2.31799858854842	0.08141418348385
H	-3.51898414938504	-0.06119661024665	3.67017852545950
H	-4.28728431331750	-4.78321192198035	3.96246127402653

H	-2.83247150113905	-5.49018630210310	3.23821920211286
P	-7.55619531025808	-3.06401176074503	3.60278979000767
O	-8.50697660924146	-2.13250292431773	4.55173879168904
Si	-8.33652346765655	-0.57312351080180	5.20342707088616
C	-9.87838298829409	-0.29815462474503	6.22290435209692
H	-9.96115664482589	-1.03601419207957	7.03389269170207
H	-10.78352729309946	-0.37472923439410	5.60297851474051
H	-9.86951816604780	0.70338339123661	6.67852160848371
C	-8.19418864339578	0.66561834395475	3.80152423720585
H	-9.08092000805655	0.63953998275047	3.15038401021561
H	-7.30942668989697	0.47468913098115	3.17498575777995
H	-8.10638426549980	1.68990913702374	4.19517313844632
C	-6.78768402547268	-0.53049378435310	6.27089141004723
H	-5.88648242124996	-0.66782992941487	5.65337173457696
H	-6.80155307863008	-1.32019560170159	7.03651511678452
H	-6.69403052366958	0.43716300199189	6.78649860382498
O	-8.69143078189061	-3.92048799109631	2.80672293310118
Si	-9.96788729735039	-3.57958696932349	1.73709834799343
C	-10.27151946699101	-5.18842850261077	0.82846113930738
H	-11.09097806646664	-5.07479050772339	0.10263024880016
H	-9.37827775423261	-5.51713845523665	0.27711622493096
H	-10.55312823021841	-5.99057467019883	1.52615684349840
C	-11.47174773423900	-3.05486774978550	2.72088429996257
H	-11.27569073743543	-2.14092765076003	3.29944564022481
H	-12.32098767799947	-2.85620652470029	2.04931443464495
H	-11.77969338108168	-3.83973029788405	3.42658851298800
C	-9.43494193996601	-2.22252939895250	0.55018327749345
H	-10.25280116685336	-1.98504611882797	-0.14706739472009
H	-9.17276947524511	-1.29318649880162	1.07735546966689
H	-8.56937200361339	-2.53144659725100	-0.05522522084875
O	-7.01055215768446	-4.19285681013098	4.63811401246813
Si	-7.68198202906033	-5.50547048714665	5.50949483406956
C	-9.34742183317592	-5.04795753156925	6.23203420888857
H	-9.75207624285179	-5.89430719524938	6.80884124241303
H	-9.26436109601661	-4.18675701879820	6.91031204639567
H	-10.07401403397873	-4.79282553440936	5.44875852036742
C	-7.80669315996660	-6.96920250857633	4.34345015165007
H	-8.19402519345830	-7.85478365014480	4.86999216842532
H	-8.48253647065032	-6.75038038986953	3.50484789455716
H	-6.82276102686600	-7.23560140983005	3.92928324193531
C	-6.43119960515978	-5.84063222310418	6.86737072392833
H	-6.75759713471381	-6.68403546208026	7.49528669640181
H	-5.44545046954094	-6.10180196248165	6.45454825588897
H	-6.30861171118613	-4.96708706161156	7.52479202744901
H	-6.06977404011632	-1.74533331019955	0.31774600089515
H	-4.68232353691486	-1.77709644600845	-0.74828255639517
H	-5.43159999978643	-3.32868526192243	-0.23492179067363
Si	-3.07046412289806	-4.75705558302921	0.53416939811847
C	-2.98988480907657	-4.12990563026943	-1.22916743218578
C	-1.30380467603852	-5.15467245196612	1.02049352548488
C	-4.30358882294534	-6.14310864729908	0.74974281163827
H	-2.33063696303569	-4.82969066517031	-1.76813841365755
H	-3.94883654041943	-4.11407562875996	-1.75978777366905
H	-2.52458099554115	-3.13683656301678	-1.30554731006478
H	-0.96005530485319	-5.94165740273753	0.32963644223529
H	-0.64807649498318	-4.28566939058788	0.86236974921347
H	-1.14985432240157	-5.52839233441964	2.03918445817454
H	-4.25430074631572	-6.61701341336176	1.73870018357036
H	-5.33589939788348	-5.79732250693945	0.59316350821072
H	-4.09546108770549	-6.91649754373904	-0.00642346879035
82			
Coordinates, constrained distance 4.29 Angstrom, absolute energy -2738.432020190716 Ha			
C	-2.52759101552616	-4.48551759445656	5.18349712389270
C	-3.00750625715442	-3.26941362162156	5.98151771579479
C	-2.89008695369752	-1.98066409414827	5.16074495093754
C	-3.60362311540863	-2.14621029336251	3.81977310507120
C	-2.96426582440415	-3.28520260163291	3.01836400460673
C	-3.20969618743872	-4.58252950963909	3.80962588566964
N	-3.52886489477382	-3.36290072737486	1.62519715912568
C	-4.20680058306655	-2.34492399579566	1.15984185302758
C	-4.05778126251811	-0.94611772630254	1.76716372486589
N	-3.58213403596089	-0.92378148270134	3.02926187133675
O	-4.26407816701508	0.01748059700054	1.03871130904669
H	-1.43442369378271	-4.43246668386784	5.04260080220688
H	-2.72317609407904	-5.41007705869852	5.74722121822268
H	-4.06021778789240	-3.41686320422364	6.27366495323149
H	-2.43145609661319	-3.17373915328448	6.91235822659274
H	-3.34275361382318	-1.13783024776564	5.70676636787382
H	-1.83099463705899	-1.72460008843969	4.98525633512909
H	-4.65811987460996	-2.42973620921392	4.01128231303842
H	-1.87886996679615	-3.11011146372748	2.91213620607411
C	-5.04954743429380	-2.39456533249218	-0.05876724457636
H	-3.47501139454053	-0.01471902063030	3.47749134216194
H	-4.29739451831359	-4.71783595803613	3.93123475350366
H	-2.82725619914260	-5.45836391654351	3.27200382489044
P	-7.61989274629787	-3.01580423063849	3.66557890695395
O	-8.56768362527797	-2.13012728874392	4.66114738659990

Si	-8.40490710474915	-0.59489603954215	5.36655674340472
C	-9.88791935739652	-0.41234078933339	6.48891620429156
H	-9.89811280602470	-1.18712757287112	7.26943073139615
H	-10.82711686444358	-0.49177006053300	5.92230203085166
H	-9.88043364102798	0.56807333843316	6.98868128093879
C	-8.39218669183974	0.70210349353468	4.01113100295065
H	-9.31697036102971	0.66780158971677	3.41594812884496
H	-7.54323852568506	0.56574110485375	3.32376715645170
H	-8.31449373541747	1.71329636346380	4.43925336783977
C	-6.79697796568973	-0.54125456014114	6.34236701660677
H	-5.92773218064998	-0.65396201107645	5.67638396909643
H	-6.75725179748862	-1.34341490853170	7.09444496260620
H	-6.69195539614978	0.41884737704247	6.87002922457918
O	-8.76108480320694	-3.85670668882620	2.85853627331928
Si	-9.99662541739355	-3.50776408119614	1.74738736399883
C	-10.35065302960168	-5.13925468784670	0.89885033273660
H	-11.15312118190896	-5.02384650954457	0.15458198760241
H	-9.46163766762353	-5.52354693274779	0.37739517132410
H	-10.67403373673475	-5.90130475434482	1.62291043752577
C	-11.49581138667162	-2.87424679115367	2.67225090908791
H	-11.27441967724987	-1.93855771752916	3.20510330479392
H	-12.32444873674959	-2.67908590305747	1.97453018857086
H	-11.84594762654595	-3.60783814236049	3.41292327656458
C	-9.37870352940398	-2.23013551820393	0.51370167667834
H	-10.16437976820013	-2.00100142240838	-0.22221293467752
H	-9.099263344495775	-1.28474583435078	1.00170016309353
H	-8.50568961025888	-2.60206051410718	-0.04410727437224
O	-7.05379056983353	-4.17662230655560	4.65521713397343
Si	-7.70473877327395	-5.52742399367656	5.47895459303048
C	-9.38149169472476	-5.12858114981092	6.20954026149003
H	-9.77799367511240	-6.00656292694180	6.74297735703665
H	-9.31899363084684	-4.29809720276788	6.92732068740189
H	-10.10409791586616	-4.84921738733808	5.43077515702145
C	-7.80185126453952	-6.95286545857037	4.26282585839054
H	-8.17258512354144	-7.86351258995154	4.75748027567078
H	-8.48169965700861	-6.71738337258732	3.43203824361118
H	-6.81288201033940	-7.18568235745394	3.84042986849639
C	-6.44674043938416	-5.88671528527606	6.82466665628713
H	-6.75097750870129	-6.75895102505459	7.42325379263129
H	-5.45762017253041	-6.10964874440893	6.39730314620786
H	-6.33964403399875	-5.03333405003704	7.51059982049166
H	-5.96980134902903	-1.83175100924355	0.16156215455345
H	-4.57520719956013	-1.86259657756897	-0.89605647550523
H	-5.30419653213669	-3.41587882722335	-0.35269548602843
Si	-2.99156523721129	-4.83843428796352	0.53809194461701
C	-2.86034895804698	-4.27240959896390	-1.24296116964821
C	-1.24324034901707	-5.23276313296007	1.08863369133937
C	-4.24349805193318	-6.20422444113619	0.77170449554798
H	-2.18756222648367	-4.98968005558339	-1.74053651909295
H	-3.80454340822978	-4.27438916067121	-1.79954080548405
H	-2.39269628002761	-3.28219806822251	-1.34024179355547
H	-0.88042252077381	-6.03185016479615	0.42189757941933
H	-0.57811254686539	-4.36936734567516	0.93927595742004
H	-1.12718582730265	-5.59146762430291	2.11762891283134
H	-4.23378041747094	-6.63327655964104	1.78184907742720
H	-5.26625980504870	-5.85839223353592	0.56180688074274
H	-4.01599889757675	-7.01241698307937	0.05889991229198
82			
Coordinates, constrained distance 4.51 Angstrom, absolute energy -2738.431429189658 Ha			
C	-2.65853045246051	-4.47751462834379	5.13583217261891
C	-3.14366738794948	-3.24682832329524	5.90796168818001
C	-2.96131326641873	-1.96696121302754	5.08515987181896
C	-3.62278784280140	-2.12162088132447	3.71615175978895
C	-2.98809633830997	-3.28672416008919	2.94918029119214
C	-3.29669237008960	-4.56979370843398	3.74066320181279
N	-3.50261749184102	-3.35841194301365	1.53469511002882
C	-4.11227882917013	-2.31595694817685	1.03151487708527
C	-3.92759164560482	-0.91981153119104	1.63498712629223
N	-3.52235488905872	-0.90595708703010	2.92005516037471
O	-4.04928079985016	0.04309397384680	0.88636018079308
H	-1.56042832928101	-4.44558417982593	5.03091749824378
H	-2.89070780777700	-5.39396073334910	5.69883923870391
H	-4.21067366433873	-3.37147528264403	6.15482287094262
H	-2.60486294429846	-3.15839090359032	6.86148386933359
H	-3.41483278873805	-1.10904170475285	5.60664029005125
H	-1.88988231974770	-1.73860344565561	4.95214198819599
H	-4.69382599021752	-2.36662958735603	3.86550386957764
H	-1.89489583160513	-3.14332791613005	2.87982792674330
C	-4.89870088441932	-2.33630469943739	-0.22540058226103
H	-3.39404021618819	0.00125957055828	3.36644020106699
H	-4.39057897003543	-4.67600766190806	3.82859810703656
H	-2.91846494787846	-5.45951227471950	3.22354720075265
P	-7.63109204634132	-3.00101087293078	3.77308675266162
O	-8.60170525851393	-2.14679320101309	4.77449222310801
Si	-8.48996413206813	-0.61466296641174	5.49423312682932
C	-9.1442990416525	-0.53689280507095	6.70168880208376
H	-9.82944163014340	-1.31551729305233	7.47379313365549

H	-10.87696910737013	-0.67547448657918	6.18781016141691
H	-9.94435691424082	0.43874450394526	7.21000509209927
C	-8.64010067889596	0.69604478726379	4.16027559756704
H	-9.59832506691921	0.61252133941132	3.62604027647252
H	-7.83089828443346	0.61724339945784	3.41805237882022
H	-8.59366415544421	1.70563691297341	4.59654091945378
C	-6.83616179316654	-0.46728194079403	6.38000647642926
H	-5.99753742987747	-0.45498009257776	5.66683895410394
H	-6.68059082409792	-1.30127416391374	7.08034180506703
H	-6.79149393579374	0.46789717466690	6.95898131335697
O	-8.75678448173632	-3.85018375202743	2.94979259352625
Si	-9.90752989952380	-3.49676663996437	1.75426224877549
C	-10.24431201905839	-5.13370190158042	0.90944556571201
H	-10.98748171782681	-5.01140551061040	0.10702197561493
H	-9.33071346197793	-5.55078008231820	0.46089868331259
H	-10.63991600510511	-5.87353547216856	1.62089719062951
C	-11.44817600672393	-2.80947531521701	2.56611632058257
H	-11.23287339736651	-1.87265479051623	3.09962109418447
H	-12.22291265257171	-2.60008226615064	1.81301934848875
H	-11.86717948626022	-3.52133374278806	3.29225999208561
C	-9.17502663104275	-2.25414657277222	0.54593852885044
H	-9.88381518992876	-2.04670266736731	-0.26974946313792
H	-8.94138217622587	-1.29556152724206	1.03232051244488
H	-8.25084660503578	-2.64292484132015	0.09212843029576
O	-7.05679624283989	-4.16787672541350	4.75131997044580
Si	-7.70149533920414	-5.52272608752371	5.57346239987111
C	-9.37685047951332	-5.13046600830762	6.31072200541003
H	-9.77149143044040	-6.01144336304567	6.84054468938763
H	-9.31411515741308	-4.30332791462432	7.03228514525216
H	-10.10065438569900	-4.84822406825833	5.53399130694533
C	-7.80229062881765	-6.94542780821771	4.35441369693058
H	-8.16058474425882	-7.85988374046164	4.85131269831560
H	-8.49454489781244	-6.71209054840202	3.53328556666234
H	-6.81761414704613	-7.17114979750596	3.91828473875361
C	-6.43553687230441	-5.88101513263694	6.91136729627826
H	-6.73999112474278	-6.74769795887517	7.51793866614571
H	-5.45129113509610	-6.11284936102306	6.47754940654091
H	-6.31796070714321	-5.02432099272953	7.59136010554163
H	-5.77968070481885	-1.69410002799766	-0.07522203129602
H	-4.34037723385877	-1.87257295227609	-1.05180178374981
H	-5.21561536442017	-3.34432326970596	-0.50596367419279
Si	-2.98951608093413	-4.87239276821321	0.48749144079522
C	-2.77707144385460	-4.34523785318965	-1.29706946211093
C	-1.27420238383932	-5.32643127614359	1.09502383149690
C	-4.30675043049431	-6.17884120758231	0.70061258077346
H	-2.14322299137432	-5.11621986898200	-1.76498937655118
H	-3.70308877379113	-4.29017695419339	-1.88022877340165
H	-2.23742051134050	-3.39240743057043	-1.39549876890667
H	-0.91829941386068	-6.13614497372875	0.43743961581289
H	-0.57578166682262	-4.48612347617702	0.96755963918607
H	-1.20147975291525	-5.69043999335057	2.12576079561631
H	-4.36437806196863	-6.57399033627432	1.72263668118713
H	-5.30175435789957	-5.79649911928574	0.42950049100607
H	-4.08122463554086	-7.01779192974628	0.02396514899044

Compound **4a** (R configuration at the stereogenic carbon atom)

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Coordinates, constrained distance 1.80, absolute energy -2738.451111157345 Ha

C	-7.03790121192123	-1.21671898156394	-7.39047090931526
C	-6.37240331786073	-0.24199149631877	-6.41812733377001
C	-5.60118801435979	-1.00471363795424	-5.34049394225308
C	-4.58723191514887	-1.97015331968200	-5.96413299901649
C	-5.22595941340061	-2.93515482163139	-6.97152277410420
C	-6.01643882257239	-2.16455820187269	-8.03059813185320
N	-4.19728609881568	-3.87271135146552	-7.48923805526983
C	-3.69006069406752	-4.74083124797911	-6.41680357113205
C	-3.79502847807270	-4.12202173440265	-4.98473114316641
N	-3.97314588480454	-2.78637769233576	-4.91389067541803
O	-3.62436077641811	-4.84622621766728	-4.00014072703533
H	-7.80280181616352	-1.80513627003476	-6.85383092282530
H	-7.56923500453403	-0.66805304308320	-8.18186430276058
H	-5.68594797309167	0.42332964376142	-6.96989889252063
H	-7.12372181692532	0.40898083802188	-5.94777850438685
H	-5.07476784909739	-0.30848259551448	-4.66658263090438
H	-6.30749435322936	-1.58060937958415	-4.71692122482149
H	-3.80759888602882	-1.38725456755013	-6.48850340607013
H	-5.96785807006411	-3.53219552866810	-6.40420628401168
C	-2.17613396643515	-5.07099171197592	-6.51034439921524
H	-3.93693053686596	-2.40460825943369	-3.96815131972859
H	-5.33541572438028	-1.57104399570623	-8.66054234725199
H	-6.52758143101911	-2.87646330050874	-8.69277181412042
P	-4.60622059165950	-6.28890067318171	-6.35252289234226
O	-4.86032185138518	-6.71700042384798	-7.83131159374656
Si	-6.02581884276614	-7.59171866247887	-8.77633369092398
C	-7.54599402123708	-6.51666618975127	-8.92333218124844
H	-8.28865565449102	-7.00701685154108	-9.57148579188300
H	-8.01631134089329	-6.34329021036257	-7.94590190292761
H	-7.30972266917747	-5.54083706951777	-9.37063310281600
C	-5.16934791854001	-7.86338042080335	-10.41032906277972
H	-4.23503923469678	-8.43065166963873	-10.29077345293195
H	-5.82373834986039	-8.43906193919971	-11.08307404249257
H	-4.93286019756432	-6.91328425280543	-10.90983936272641
C	-6.38694932024476	-9.20345672081093	-7.89758808260864
H	-5.49136706599003	-9.83652401641879	-7.82060477643819
H	-6.78787958454442	-9.04466370573364	-6.88652937142059
H	-7.14177051100617	-9.76880502987995	-8.46582057143579
O	-3.83895737094644	-7.42412718602349	-5.62748752923278
Si	-2.71174162338089	-8.73139194392328	-5.49704219695523
C	-3.68984038892113	-10.15457815225324	-4.78726843996423
H	-4.04271677078565	-9.93073990194067	-3.77088653171475
H	-3.04977174373195	-11.04822197210502	-4.72358271386288
H	-4.55982437322277	-10.41361277595126	-5.40744628343942
C	-1.37429203836896	-8.15676740987367	-4.33229351830150
H	-1.80638410197788	-7.71103193232723	-3.42553085775746
H	-0.70304072665710	-7.41827204955552	-4.79219156374625
H	-0.75861008053884	-9.01642623681576	-4.02622885918160
C	-2.06784209825175	-9.10656782168726	-7.21277393080392
H	-2.86574000897082	-9.42103452991758	-7.89978424549139
H	-1.34132740775121	-9.93207987812694	-7.15053867158744
H	-1.54560182518759	-8.24764907698863	-7.65886183062507
O	-5.99025035506066	-6.08754553255873	-5.66463232704218
Si	-6.88931179058730	-6.24290821024529	-4.17644665602163
C	-5.90036403798933	-7.24497245789019	-2.95696608123789
H	-6.43950543085303	-7.27551936990120	-1.99740158386714
H	-5.76048859580338	-8.28229422117847	-3.29061332978619
H	-4.91770399807341	-6.78522953359120	-2.78318820378025
C	-7.19860071770613	-4.50307947799494	-3.57496869360850
H	-7.85722231819364	-4.53411873363786	-2.69326763158557
H	-6.25935569991461	-4.01860512673555	-3.27357731608801
H	-7.69457374387578	-3.88509535891953	-4.33758024676961
C	-8.47454281758195	-7.08645504015531	-4.69359405849361
H	-9.00739201793940	-6.51706000620825	-5.46935275627990
H	-8.29909088371996	-8.10490898770215	-5.06764421333228
H	-9.14692048524890	-7.16819187458139	-3.82527718789930
Si	-3.44653886116328	-3.63148020260843	-9.11369336488376
C	-4.72084722668669	-3.66056095363881	-10.51194125489143
C	-2.50228048363830	-1.99944437230438	-9.17689746667020
C	-2.23390081654351	-4.99763108765662	-9.59746394477353
H	-5.30155115606010	-2.73762644687019	-10.62539400795416
H	-4.16631601204852	-3.80937922008221	-11.45202697535925
H	-5.42988555588605	-4.49510487804936	-10.41736214864315
H	-2.02447587321455	-1.89202687482752	-10.16343314542957
H	-3.14424578287300	-1.11889712751608	-9.03207599617951
H	-1.70412912727894	-1.95927325957333	-8.42041340943931
H	-2.08299508396054	-4.88409697697817	-10.68241340759317
H	-1.24650487824650	-4.91441202658306	-9.12776890606930
H	-2.62532245030522	-6.01115876579577	-9.43273702654862
H	-1.94547621442380	-5.76655695472417	-7.32103112475378
H	-1.62399296957785	-4.13744003547283	-6.68274418567632

H	-1.84669984751915	-5.50525030940795	-5.56075998700577
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Coordinates, constrained distance 2.03, absolute energy -2738.451658941593 Ha

C	-7.02456178727947	-1.19120841460608	-7.51569736072327
C	-6.44124763600229	-0.21963438354033	-6.48969094978736
C	-5.71381295480007	-0.98723250813163	-5.38654905512464
C	-4.63767287867627	-1.90966492416991	-5.96955055877831
C	-5.19540101968172	-2.87555102578880	-7.02636893814889
C	-5.94531117487639	-2.10329797661626	-8.11285487839402
N	-4.10491551268318	-3.77477029635474	-7.49580896459699
C	-3.63268579761541	-4.60713090975509	-6.42735378966275
C	-3.83011791114320	-4.04690635860289	-4.99760480599611
N	-4.05776590789049	-2.72034999623316	-4.89680569032532
O	-3.69299809973340	-4.79878934792383	-4.02698177836562
H	-7.80544429659528	-1.80708830606184	-7.03586138168160
H	-7.52142786125848	-0.64120477681538	-8.32816607165044
H	-5.74229223625871	0.47391746331628	-6.98887591353021
H	-7.23500928745751	0.40219996542777	-6.05103498850832
H	-5.24828255998411	-0.29527567508241	-4.66519490684263
H	-6.43849247276659	-1.60055054974220	-4.82265397070102
H	-3.85021017163026	-1.29387566718021	-6.44267896752083
H	-5.94660173968613	-3.50764335991159	-6.50892716346876
C	-2.15288549663867	-5.02036310300873	-6.47615866334275
H	-4.09411537825013	-2.35757176057921	-3.94395715536768
H	-5.24172620458118	-1.48136954808816	-8.68957922209153
H	-6.40587695368970	-2.81013457919630	-8.81522482409153
P	-4.65801727506547	-6.35086036548454	-6.31276190908632
O	-4.94611220501978	-6.72143068042439	-7.80643997337836
Si	-6.10995271841687	-7.58526852156892	-8.76095883325555
C	-7.61507378928732	-6.48879118229194	-8.90789503028502
H	-8.36880749835932	-6.96258906856383	-9.55526940474124
H	-8.07860021745203	-6.30863697055694	-7.92810106930875
H	-7.36125440429168	-5.51606373177773	-9.35341479491784
C	-5.24563899811262	-7.85423927009307	-10.39201009558487
H	-4.32116054607357	-8.43691935596693	-10.26957023866726
H	-5.90241559164555	-8.41279253606702	-11.07670422456712
H	-4.98927943660654	-6.90293541737772	-10.87939838891838
C	-6.49182376174543	-9.19872907616027	-7.89445146736458
H	-5.60098100613085	-9.83794777062520	-7.81220344854419
H	-6.90054471484082	-9.04033514162336	-6.88653220967751
H	-7.24517985192382	-9.75649143347614	-8.47202226151994
O	-3.88616438382088	-7.51933023255206	-5.63681264973345
Si	-2.71779989946458	-8.79113518159322	-5.53561395237637
C	-3.6739750341307	-10.24980626236257	-4.84531079272046
H	-4.01861349644408	-10.04598534650987	-3.82758717959913
H	-2.99604940753620	-11.12831268602235	-4.79033374030003
H	-4.51996871732944	-10.52155084710813	-5.47048571843520
C	-1.38792865093807	-8.20128456742948	-4.36932630920673
H	-1.82298463622587	-7.80375099868796	-3.44177275306908
H	-0.75510521038367	-7.42097221915531	-4.81446898056506
H	-0.73255004324775	-9.04383620639082	-4.10013904262903
C	-2.07451897020782	-9.11683158661885	-7.26140605182345
H	-2.86971389940025	-9.43654919518666	-7.94921302851623
H	-1.32777551034710	-9.92550870138007	-7.22118059480825
H	-1.57650940887161	-8.23626755378211	-7.69290445061475
O	-6.03699759722511	-6.17676882078816	-5.59790947621044
Si	-6.87962573971511	-6.31195852657994	-4.07694945619530
C	-5.82885918906088	-7.25516926371919	-2.86109531373137
H	-6.34244469150444	-7.28190888457013	-1.88732088112601
H	-5.66468515331504	-8.29463841045162	-3.17665881257793
H	-4.85690931976124	-6.76256607364065	-2.72145197334304
C	-7.21742931196276	-4.56288651189838	-3.51854603198456
H	-7.88294671914845	-4.57733768697055	-2.64176396757746
H	-6.28480269639057	-4.06201295126294	-3.22489831689123
H	-7.71284524257852	-3.97135021478361	-4.30249433989222
C	-8.45411270539402	-7.21396456018358	-4.52650508015574
H	-9.02061633687832	-6.68272082429483	-5.30554811842947
H	-8.25650748928688	-8.23678165826053	-4.87729156942792
H	-9.10376450898629	-7.29098429918967	-3.64075101198169
Si	-3.34193482201856	-3.58059626208467	-9.12736071696403
C	-4.61018408759157	-3.61767006124978	-10.52983695439852
C	-2.37267989639927	-1.96641175637720	-9.20075823967819
C	-2.15834971214522	-4.98430202203292	-9.56856253187635
H	-5.15717514222372	-2.67899093797613	-10.67667374005383
H	-4.05727159724674	-3.81808251141570	-11.46116872650332
H	-5.34739170052150	-4.42437772080642	-10.40826420522079
H	-1.88252571285585	-1.87667680693230	-10.18287487220019
H	-3.00418243883846	-1.07593165773587	-9.07175726955772
H	-1.58313515398031	-1.93070737008519	-8.43519704029162
H	-1.98663922377536	-4.89342724705276	-10.65250871506408
H	-1.17750769632989	-4.92402432848259	-9.08232428625721
H	-2.58576503830616	-5.98221547430720	-9.39477706327929
H	-1.93510613878516	-5.72726487840380	-7.28041928406040
H	-1.53478837954064	-4.12338866130335	-6.62545561442953
H	-1.88088446645318	-5.47430447167791	-5.51721779772551

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Coordinates, constrained distance 2.52, absolute energy -2738.443664651167 Ha

C	-7.04474082351434	-1.28862562974428	-7.82244522664222
C	-6.64325654786168	-0.29315062080314	-6.73346208105149
C	-5.97858832122257	-1.02517769346963	-5.56852570306197
C	-4.78156045468168	-1.85732540596063	-6.04408794159104
C	-5.16619586160498	-2.85123743175705	-7.15063026680676
C	-5.84637728825807	-2.11698661680973	-8.30568822606226
N	-3.97285949376882	-3.67934293332993	-7.50237278947529
C	-3.55094827670041	-4.44565191210447	-6.41347190916728
C	-3.88126059354850	-3.92133648163850	-5.00066232830137
N	-4.24392564124294	-2.62246477151628	-4.92196471534948
O	-3.73089945735048	-4.65074573383376	-4.01697970624395
H	-7.82511605463751	-1.96592667868623	-7.43330018055604
H	-7.48905865565486	-0.76488590374501	-8.68131793417197
H	-5.94916273210599	0.45700281306792	-7.15129065545484
H	-7.52124244075326	0.26253986334391	-6.37391520602106
H	-5.64199256304961	-0.31365264259957	-4.79670490672075
H	-6.70845489804253	-1.69904739552247	-5.08652281390013
H	-4.00635979526279	-1.17382268071293	-6.44027582447426
H	-5.91964580116556	-3.54114085149389	-6.71523284430580
C	-2.11732962874361	-4.95527337506059	-6.37711886868453
H	-4.37041416832184	-2.25665052552805	-3.97848294311896
H	-5.12720217046954	-1.44128454745935	-8.79853038557451
H	-6.17840935783308	-2.84324955031385	-9.05758284866468
P	-4.70572196644277	-6.37204695723008	-6.24677701920101
O	-5.06650766442344	-6.69721268305413	-7.74758259855944
Si	-6.28800381522310	-7.49113941073418	-8.68190324821087
C	-7.74910058266956	-6.32768263854489	-8.76724737600728
H	-8.54389887609878	-6.75765475338695	-9.39569254071422
H	-8.17261312684474	-6.14304520277202	-7.77000233072002
H	-7.46747409504124	-5.35982821871991	-9.20709167042642
C	-5.48547994623534	-7.75736260563958	-10.34677864457694
H	-4.57895622759184	-8.37432941598775	-10.26449283987486
H	-6.18192604452127	-8.27692159595424	-11.02272876144344
H	-5.20917259439269	-6.80605043098460	-10.82316984839272
C	-6.72390331781666	-9.10877306845418	-7.84962926529092
H	-5.85254910983118	-9.77512268265228	-7.77223833857023
H	-7.13475574076198	-8.95430528415306	-6.84245885852570
H	-7.48863888227490	-9.63375564705258	-8.44276334069574
O	-3.93034661651068	-7.59405987186517	-5.64534809847662
Si	-2.75410218547232	-8.85442453052383	-5.63716059706699
C	-3.66110232136741	-10.35596642120772	-4.99481467062699
H	-4.02166273736893	-10.19620980052522	-3.96879752409295
H	-2.98326609746787	-11.22339327555691	-4.97536755416363
H	-4.52224104370309	-10.62016342210104	-5.62513366390686
C	-1.39515192542203	-8.31289803722296	-4.47908289125147
H	-1.80601725557216	-7.99376918308287	-3.51081691933763
H	-0.80221101267231	-7.48361037202460	-4.89017027875761
H	-0.70571312162953	-9.15034720469797	-4.29122076448380
C	-2.15185897057811	-9.09552327759242	-7.39227644760589
H	-2.97056365556328	-9.35385092278672	-8.07830570839887
H	-1.42425154581147	-9.92189636540891	-7.41785889726301
H	-1.64264336853669	-8.20203984564950	-7.78264452309815
O	-6.07029415767494	-6.26134423592861	-5.47011825047668
Si	-6.80380371909290	-6.41530488719560	-3.90128764051667
C	-5.61483511006680	-7.23754082469905	-2.72346725932029
H	-6.06212722729187	-7.26580378008288	-1.71749488966353
H	-5.39327341556993	-8.27264236967842	-3.01670797811953
H	-4.67555103084358	-6.67135735341666	-2.66323255868305
C	-7.23989220000518	-4.67832079873507	-3.36989752512405
H	-7.82602257402121	-4.70813011636027	-2.43882377046812
H	-6.32977161164248	-4.09416744781513	-3.17720139563573
H	-7.84568574995413	-4.16052604374716	-4.12819992260002
C	-8.33164365330506	-7.44561568883802	-4.22067733618146
H	-8.97783129893547	-6.99153138973423	-4.98660877534240
H	-8.07873502958423	-8.46613996234124	-4.54157885226727
H	-8.92392505928509	-7.52939994218940	-3.29619139617062
Si	-3.10502966109334	-3.52187439010859	-9.10601423985012
C	-4.27837471974331	-3.54014942086809	-10.58574605345693
C	-2.11667102405826	-1.92341131197178	-9.07689813496722
C	-1.94315109842754	-4.96270206568760	-9.46450704691467
H	-4.80068385687140	-2.59495537871457	-10.77305183756829
H	-3.65921860189478	-3.75086597494600	-11.47186696375956
H	-5.02956938187891	-4.34070759452927	-10.51882236890217
H	-1.54906409375744	-1.81823199760720	-10.01472584852076
H	-2.75246891668121	-1.03254306225467	-8.97624278380461
H	-1.39174741687269	-1.91433245354237	-8.24914279155696
H	-1.69649527603101	-4.87787986148367	-10.53440619803465
H	-0.99657647569075	-4.94403608677273	-8.91286244501668
H	-2.42433244525031	-5.94209017419332	-9.32563198199673
H	-1.90150659826176	-5.68766238348910	-7.15790470832002
H	-1.42431708960629	-4.10769214799404	-6.49559115005449
H	-1.93741163296802	-5.41029002383123	-5.39718637156549

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Coordinates, constrained distance 2.48, absolute energy -2738.437661937449 Ha

C	-6.95125963107700	-1.78038510845263	-8.55284441452571
C	-6.92679059671248	-0.66893857492972	-7.50242773288914
C	-6.40949890972458	-1.21110650203689	-6.17049603111697

C	-5.02714487353530	-1.85647405928047	-6.33039487830588
C	-5.03507684059923	-2.95568694127670	-7.39764948128939
C	-5.57181751969462	-2.43137568309798	-8.72868608763564
N	-3.69192850852915	-3.61962528674074	-7.43062602862766
C	-3.43246072412425	-4.26012269024388	-6.25053899074126
C	-4.02516902123953	-3.68015400974725	-4.95389841863302
N	-4.61694419912087	-2.46716535320145	-5.07101643234557
O	-3.87367073890569	-4.25518256868048	-3.87509869054757
H	-7.68524792831298	-2.54823149994603	-8.25254260051576
H	-7.29054006004910	-1.38944138315038	-9.52325675758003
H	-6.28399287813820	0.15849175662469	-7.84882645368288
H	-7.93205737713625	-0.24482873755667	-7.36712322452085
H	-6.34870409339540	-0.41197617775194	-5.41394459230082
H	-7.10701691344192	-1.97239165954946	-5.77965459693314
H	-4.29890491554672	-1.07776894156705	-6.62788029563274
H	-5.74190832176022	-3.73537107159829	-7.04616162163672
C	-2.09547895112623	-4.88832974366995	-5.96055291532107
H	-4.91394111737666	-2.03777124383452	-4.19565982370406
H	-4.88226833322069	-1.68643722824104	-9.15689737063052
H	-5.64211400760283	-3.25906739640234	-9.44507043288619
P	-4.81516002868542	-6.31299513712710	-6.12550186565450
O	-5.35065962414747	-6.54777926061090	-7.60510750816919
Si	-6.73150260167350	-7.20671125013998	-8.40735213495529
C	-8.17152577609313	-6.04737524801186	-8.11579813188457
H	-9.07200300839527	-6.43643985550518	-8.61466290498913
H	-8.39751799691182	-5.94409972086608	-7.04549536704881
H	-7.97573207338368	-5.04655789892579	-8.52798131987241
C	-6.23026329503403	-7.25717768719495	-10.20675974363940
H	-5.32770973235273	-7.86636330134509	-10.35800536754584
H	-7.03597567412537	-7.69906995194921	-10.81261066145907
H	-6.03505840945898	-6.25028642827137	-10.60352131592231
C	-7.07137766017011	-8.91728522391887	-7.73023285100629
H	-6.22736728332254	-9.60037337108932	-7.90440674890109
H	-7.28610955098426	-8.89452187162835	-6.65270508623067
H	-7.94966765762823	-9.34601384681032	-8.23678767445564
O	-3.98012693456481	-7.58868449514389	-5.70605322790536
Si	-2.93542859305930	-8.913048883037297	-6.02552296532230
C	-3.87596475280587	-10.44127667044531	-5.50314220811891
H	-4.12853067124243	-10.40848857073786	-4.43338435963312
H	-3.26182137763320	-11.33954909460517	-5.67060339128926
H	-4.80821612307822	-10.56269275185972	-6.07143457459559
C	-1.41915053117050	-8.64875809240940	-4.96803252824358
H	-1.69451956656703	-8.49671595716465	-3.91411112792929
H	-0.82150707731565	-7.78530144471376	-5.29369275640595
H	-0.76962699676185	-9.53678717133359	-5.01642160943370
C	-2.53672885227212	-8.92040175946183	-7.85544504417336
H	-3.43546302203273	-9.06239678011956	-8.47193606833220
H	-1.84423589140648	-9.74587825875074	-8.08220161071848
H	-2.04901397386761	-7.98749532809179	-8.17490354347138
O	-6.10606159183894	-6.32439352900745	-5.20607370934898
Si	-6.61416069742924	-6.53604135182508	-3.56075007867432
C	-5.19433526888655	-7.19335496777187	-2.54335862356932
H	-5.50861060981921	-7.28119969961079	-1.49184063883475
H	-4.87325408138295	-8.18802486966820	-2.88063085016152
H	-4.33706023811464	-6.50675859125660	-2.58455479760930
C	-7.18346083798719	-4.85466540751836	-2.97901937366492
H	-7.63208071531206	-4.93465079589544	-1.97737249626929
H	-6.32803482749078	-4.16745780355008	-2.91264359617022
H	-7.94215843333981	-4.42667347661788	-3.65079899340795
C	-8.03548718383878	-7.74811693692795	-3.67711925620744
H	-8.82630976663096	-7.38374537864191	-4.34922646223465
H	-7.70669394868454	-8.73459752403381	-4.03422970888984
H	-8.48682309422960	-7.89186339587096	-2.68356956486601
Si	-2.56179661812944	-3.42068141391013	-8.87935319287377
C	-3.38441038134654	-3.99082828987701	-10.47424035051850
C	-2.05583581970799	-1.61043967872218	-8.92474421498301
C	-0.97733604604363	-4.42735112704500	-8.78160240421233
H	-4.05047386461517	-3.25077375633008	-10.93383456775620
H	-2.58336815365573	-4.20860064191751	-11.19798023535542
H	-3.94827396509794	-4.92371694055595	-10.32443032245286
H	-1.37951452055441	-1.45405424881239	-9.78013205192247
H	-2.89051600142897	-0.90627901170634	-9.03779564890435
H	-1.50174467220955	-1.33628239057359	-8.01441121009199
H	-0.44518323547047	-4.17274936011463	-9.71377436488572
H	-0.30924353281571	-4.17632582754194	-7.95016402496435
H	-1.14141860487132	-5.51321912077041	-8.79854005957471
H	-1.78867023994132	-5.60824346997449	-6.72268350928892
H	-1.32430001402834	-4.10494428570002	-5.88697875679308
H	-2.15632683858392	-5.38217034531595	-4.98529536620416

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Coordinates, constrained distance 2.70, absolute energy -2738.433639940959 Ha

C	-6.89833451987797	-1.81705548486651	-8.61335742568134
C	-6.94994023195076	-0.71450676691942	-7.55538428285913
C	-6.45268742873810	-1.24861910383050	-6.21307452683278
C	-5.03946261402913	-1.83444815777332	-6.33315999896132
C	-4.97109984542631	-2.92045391089847	-7.40909002071971
C	-5.48926577040374	-2.41239305837887	-8.75316563055178

N	-3.59861659010581	-3.53623650377911	-7.41018462683391
C	-3.31823659616862	-4.13136339527799	-6.23409914876209
C	-3.96589381828823	-3.60817145039653	-4.94337724268041
N	-4.64535785862883	-2.44122444910088	-5.06898139094202
O	-3.76775424345314	-4.15848351365565	-3.86098455433245
H	-7.60925584790138	-2.61629788849013	-8.34164196147075
H	-7.22253939227640	-1.43280416417245	-9.59156481836837
H	-6.33048291444156	0.14077017446547	-7.87554834552995
H	-7.97475692222660	-0.33169243083762	-7.44773869386155
H	-6.44718084652115	-0.45605369856211	-5.44729095889485
H	-7.12951206106330	-2.04168482159851	-5.85041607912118
H	-4.33665150210648	-1.02075287475781	-6.59881828802363
H	-5.64393854067360	-3.73964583700704	-7.08241349236455
C	-2.03428937843182	-4.84202563604590	-5.94326435907893
H	-4.96491118221979	-2.02227389030912	-4.19674932466173
H	-4.81771944942015	-1.64096580475964	-9.16229119288433
H	-5.51434359138771	-3.24065964145696	-9.47122237704895
P	-4.87908872662587	-6.33673715886451	-6.11763404169482
O	-5.43795850830515	-6.57617198093471	-7.59916872601012
Si	-6.81978645798387	-7.23911718732894	-8.38365016266938
C	-8.27461085315666	-6.10855747018305	-8.04869719572041
H	-9.18077659491816	-6.50591912961914	-8.53008245476350
H	-8.47401585497156	-6.02083830720696	-6.97169572869393
H	-8.10393081541448	-5.09991541922962	-8.45311257852171
C	-6.35174074142022	-7.24467277785561	-10.19466262716755
H	-5.44984771490604	-7.84670887635912	-10.37642546017239
H	-7.16534844681780	-7.67334324056754	-10.79935828912958
H	-6.16558084302696	-6.22695721625242	-10.56849821429770
C	-7.12888699944061	-8.96921412742692	-7.74051699804876
H	-6.27787312285550	-9.63630281192497	-7.94096175954879
H	-7.32508597385329	-8.97093159650217	-6.65908981902740
H	-8.00903568896324	-9.40038541853045	-8.24169943251007
O	-4.05027335793479	-7.63786643761151	-5.72212485385885
Si	-2.99013622022276	-8.93304779243435	-6.06527918896121
C	-3.89505248486033	-10.49073081164911	-5.56443833920420
H	-4.14774105087889	-10.47619779420160	-4.49423154293137
H	-3.26260424546114	-11.37369949044833	-5.74405634232242
H	-4.82579397263748	-10.62364951962094	-6.13278271763437
C	-1.46807798557211	-8.66832402250460	-5.01262161325473
H	-1.73855574376384	-8.54085174463771	-3.95408604020483
H	-0.88596172784597	-7.78892706712915	-5.32424559754038
H	-0.80423416767872	-9.54420358645528	-5.08236894332045
C	-2.59051389773368	-8.91038293207128	-7.89644344894888
H	-3.48816011078984	-9.05257812329050	-8.51454459383726
H	-1.88796723706275	-9.72327420427327	-8.13692375330856
H	-2.11523870368436	-7.96598760914406	-8.20148089872889
O	-6.17871324958221	-6.40572121631451	-5.19273581169850
Si	-6.63481176436668	-6.56359948340202	-3.53520365291404
C	-5.17563621338044	-7.15499313427929	-2.53103163147891
H	-5.46152800814878	-7.22273393912408	-1.46992447852058
H	-4.83453100579064	-8.14901045349637	-2.85045381680812
H	-4.33699623435231	-6.44799547986847	-2.60983834835791
C	-7.21078302997905	-4.87019958133401	-2.98877009999422
H	-7.62612112397263	-4.92007520735879	-1.97097662058340
H	-6.36379675531738	-4.16886894869607	-2.97036082015880
H	-7.99508549526964	-4.47352408204543	-3.65007672096673
C	-8.03950978552508	-7.80006603760740	-3.55933649953104
H	-8.85784230373647	-7.47010718097402	-4.21592483677200
H	-7.70452112924712	-8.79056784575840	-3.89966771263585
H	-8.45436720165342	-7.92134288121983	-2.54728122737813
Si	-2.46031577873990	-3.36285297754572	-8.87847143782646
C	-3.27610286244895	-4.00901756292050	-10.44408105527091
C	-2.00404543872076	-1.54201258794682	-8.95232595134094
C	-0.85308531054038	-4.32101818087361	-8.72893743913877
H	-3.92453732117193	-3.28200195508630	-10.94754475337451
H	-2.46996587204716	-4.27463178145931	-11.14583425762777
H	-3.85525392469829	-4.92517919843012	-10.25384070779601
H	-1.32340760067048	-1.38982341290981	-9.80519549674586
H	-2.85136419791193	-0.85750887818719	-9.08539013681046
H	-1.46169085125913	-1.23992215654329	-8.04374971271343
H	-0.30504207115346	-4.05761880403120	-9.64975381895898
H	-0.21368971823369	-4.04257756768625	-7.88358826938576
H	-0.98463459608067	-5.41093421004542	-8.73970090219706
H	-1.75409537215846	-5.55270091764738	-6.72343807327607
H	-1.21823754008335	-4.11080007194145	-5.82008338743556
H	-2.14902384923290	-5.35812710259977	-4.98399221980462

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Coordinates, constrained distance 2.93, absolute energy -2738.431214859277 Ha

C	-6.86148240804080	-1.85589254087951	-8.59294949611352
C	-6.94454187233762	-0.77274598720231	-7.51773366152929
C	-6.43495581595227	-1.31625229648912	-6.18416408342097
C	-5.00576202436992	-1.86137547039338	-6.31004376360707
C	-4.90638461247836	-2.92437605665676	-7.40454928241169
C	-5.43610516924410	-2.40942396000017	-8.74116226389568
N	-3.51000481720428	-3.50208130945389	-7.41765875072989
C	-3.17686179269816	-4.06108814238074	-6.25371595065160
C	-3.85086857425024	-3.60516273707096	-4.95077325072056

N	-4.59956470015921	-2.47955991485146	-5.05638611391219
O	-3.59904054284286	-4.15110161301479	-3.87903215861981
H	-7.54906346349231	-2.67985028002183	-8.33640503939331
H	-7.19412267440338	-1.46517909472652	-9.56571394255795
H	-6.34820020183083	0.10446112710395	-7.82215176540443
H	-7.97944605381895	-0.42009398540413	-7.40507078220393
H	-6.45018084126079	-0.53693970933769	-5.40505759139602
H	-7.09069007422727	-2.13259169472251	-5.83503241645853
H	-4.32541987097716	-1.02252412434742	-6.55802178472124
H	-5.54752383975402	-3.77375141805556	-7.09631871887275
C	-1.90347814412765	-4.78840753351912	-5.98722323902252
H	-4.92507187464902	-2.08239655060444	-4.17623866334576
H	-4.78563700475950	-1.61434142609687	-9.13862784853934
H	-5.44191096938158	-3.22771879919831	-9.47033287761582
P	-4.92425147862322	-6.41006426084685	-6.12569934670881
O	-5.55172032546363	-6.54853821011465	-7.60150923148590
Si	-6.92723529832133	-7.25780864802085	-8.35114019055475
C	-8.35487831810578	-6.06056146689468	-8.14918655479495
H	-9.26492727318784	-6.46623267353199	-8.61603142075345
H	-8.57306145956055	-5.87716429968790	-7.08765818737197
H	-8.14157644967824	-5.09471362634064	-8.63053816754138
C	-6.42864119181941	-7.43517785885286	-10.14674112319075
H	-5.55689718124027	-8.09629466651810	-10.25832706253255
H	-7.25205368462058	-7.86768869399245	-10.73519866579556
H	-6.17874871422534	-6.46200894348516	-10.59426860391570
C	-7.31176668479479	-8.91483582468325	-7.57222794929189
H	-6.47404757843508	-9.61939300511973	-7.67506774420057
H	-7.54985274518636	-8.81667843436096	-6.50423872888517
H	-8.18429307963018	-9.36225515801281	-8.07273142449009
O	-4.32942593343288	-7.86510494469079	-5.77615003761619
Si	-3.06695843790864	-8.96764024569055	-6.09055792041336
C	-3.81595109386341	-10.66027622218591	-5.82836629237939
H	-4.20899911729805	-10.76391574293023	-4.80652416482899
H	-3.05493913548407	-11.44194379639529	-5.97380062068050
H	-4.63854462404100	-10.85707288657911	-6.52995457448560
C	-1.69182298123163	-8.64842224064176	-4.86179893036394
H	-2.06657931676968	-8.69447013679979	-3.82854326400437
H	-1.21358178625673	-7.66882554423192	-5.00327726528802
H	-0.90880739315535	-9.41592416175710	-4.96468362805085
C	-2.48767655447053	-8.73283788876344	-7.86053925392874
H	-3.31149034744125	-8.86912422933688	-8.57574828155071
H	-1.70574974497027	-9.46779093657255	-8.10461924933337
H	-2.06004662214606	-7.73222154086905	-8.02466064501197
O	-6.21870620040063	-6.33794670697566	-5.18044109877702
Si	-6.65319985368245	-6.53971189527373	-3.52873392101601
C	-5.16291227048815	-7.05754972416943	-2.52771221275685
H	-5.43956645800278	-7.13300403028076	-1.46465226214078
H	-4.78348987805585	-8.03839185073595	-2.84521889201308
H	-4.35312790858582	-6.31792875582490	-2.61318935708948
C	-7.30702965330706	-4.87395036837600	-2.97811390172564
H	-7.70604055098065	-4.93696248530784	-1.95474860368866
H	-6.49973413081805	-4.12685562389824	-2.97501294198581
H	-8.11788102983716	-4.52107166254212	-3.63204570594188
C	-7.99595004150238	-7.84402202050914	-3.52152722740741
H	-8.84052371475175	-7.56193551842844	-4.16708697062272
H	-7.61405855656245	-8.81740862795651	-3.86219377235127
H	-8.38797168580064	-7.98079218225248	-2.50244407947931
Si	-2.39657853176932	-3.32144133204715	-8.92356570592093
C	-3.23913632443763	-4.00084869461192	-10.45834676950075
C	-1.98235864128255	-1.49184833637617	-8.99720970747358
C	-0.77068982254156	-4.24657572138150	-8.78951316600739
H	-3.89272757987148	-3.28240804342502	-10.96734339185771
H	-2.44332853689809	-4.28419587193831	-11.16487166268165
H	-3.81722014182663	-4.91123664869302	-10.23943921074360
H	-1.30393373868240	-1.32943144399552	-9.85000406607871
H	-2.84231416711543	-0.82434288401198	-9.13193487849157
H	-1.44490447462380	-1.17850971847051	-8.08951109958260
H	-0.23984315661526	-3.97336949144723	-9.71780178250236
H	-0.12599541363044	-3.95316208058595	-7.95328121329085
H	-0.88043148883758	-5.33888494326622	-8.79810077425332
H	-1.63377311963446	-5.48742047778883	-6.78081752778110
H	-1.07762506183105	-4.06986609946867	-5.85001583621170
H	-2.02295097400399	-5.31361595472971	-5.03318028603258
82			
Coordinates, constrained distance 3.16, absolute energy -2738.431565045413 Ha			
C	-6.76115652358300	-1.72856752275605	-7.99945299923270
C	-6.76155237283270	-0.83481326631249	-6.75797239720469
C	-6.06009179032204	-1.53751845460333	-5.59569961303080
C	-4.63756526008333	-1.97819737826382	-5.97128049784536
C	-4.65298547008252	-2.85134482848272	-7.22651172169582
C	-5.33050265298632	-2.12975147529605	-8.38583210248528
N	-3.27234094697153	-3.39753648489463	-7.49395050731677
C	-2.77664879009516	-4.08210724554205	-6.47443313281936
C	-3.24793614456239	-3.82839556738045	-5.04005067793973
N	-4.05455489549377	-2.75069670396483	-4.88304737937349
O	-2.79601339623183	-4.48871718530416	-4.10790644573878
H	-7.36501983327812	-2.63229882354079	-7.80813902140980

H	-7.23031606067189	-1.21116612405345	-8.84902592355714
H	-6.25110140158321	0.11660918135436	-6.98603146169915
H	-7.78912703466800	-0.57458851707090	-6.46783258441987
H	-6.00646971392361	-0.88037603096023	-4.71304949332533
H	-6.63108141172562	-2.43319587260391	-5.29817313390116
H	-4.02225340679559	-1.07658714599882	-6.16785751952349
H	-5.25162436856289	-3.75453875483405	-6.99280565535894
C	-1.55363977557084	-4.92291519944872	-6.53681666402228
H	-4.24944882307231	-2.48143137592994	-3.91980377445225
H	-4.77298235361082	-1.22084402628469	-8.65348299673000
H	-5.35309916787576	-2.78207907939383	-9.27057311546439
P	-4.93400890148834	-6.37823111579045	-6.28145080148682
O	-5.58513951663314	-6.50762792326677	-7.75218878875022
Si	-6.94939148110712	-7.19682476428722	-8.53145058611961
C	-8.46415749606059	-6.19382189158420	-8.07012509203740
H	-9.35163026910666	-6.59045856085333	-8.58582667431387
H	-8.65703198643898	-6.22526940820167	-6.98883075525687
H	-8.35349644654845	-5.14013585432186	-8.36580895931724
C	-6.56552020030509	-7.03122948766152	-10.35712899401950
H	-5.63763613149488	-7.55804064854427	-10.62360485455962
H	-7.37733990180731	-7.46303418632889	-10.96183499245176
H	-6.45918331085666	-5.97733576488079	-10.65484741909094
C	-7.12895155238103	-8.99286938840428	-8.03493907337365
H	-6.24436599720416	-9.57966592140152	-8.32289170399320
H	-7.27748829159960	-9.10719897980201	-6.95213154255548
H	-7.99862423755853	-9.43601131339305	-8.54413738865633
O	-4.63249332343998	-7.90491225898518	-5.83024198489858
Si	-3.32121627189563	-8.99924255391127	-5.81057450365200
C	-4.10605660226623	-10.68119857515013	-5.59234929735281
H	-4.68312459259286	-10.73262896558544	-4.65764566513836
H	-3.33091401717290	-11.46132187408910	-5.54790531901481
H	-4.78298684110060	-10.92534453805867	-6.42329511008714
C	-2.20891924807185	-8.56975356444219	-4.36653570966098
H	-2.71559799065636	-8.75581778162609	-3.40828639374837
H	-1.90011250433635	-7.51463869151195	-4.37185885085776
H	-1.30020204333574	-9.18983398198630	-4.38484396300496
C	-2.41057599567583	-8.87737713077587	-7.44851215674623
H	-3.08691801468727	-9.06047175580951	-8.29580947935311
H	-1.60617976356178	-9.62731037390790	-7.49480973989676
H	-1.94587345851612	-7.89059611274072	-7.58794190434990
O	-6.20267856239124	-6.01040481944595	-5.35490460555540
Si	-6.82876206478956	-6.38516915118003	-3.80450909003050
C	-5.42584415819488	-6.55150001396035	-2.57833385261853
H	-5.82706556835309	-6.60392892068120	-1.55439479049218
H	-4.84482614200240	-7.46797440581443	-2.75291629796193
H	-4.72956420188961	-5.70051948998143	-2.62597684558697
C	-7.93135655584364	-4.92622259200175	-3.39577644795445
H	-8.45143000954701	-5.09433241276407	-2.44054883027475
H	-7.34982692894295	-3.99792886946700	-3.29364100676542
H	-8.69825000748107	-4.76933288853685	-4.16817415610399
C	-7.81977676310880	-7.96857403734496	-3.94096934079022
H	-8.61827637435162	-7.88668496849306	-4.69299662103963
H	-7.17540449117394	-8.81681552387164	-4.21225246881050
H	-8.29628110172275	-8.20502856967364	-2.97720927940811
Si	-2.38165754583417	-3.35186795939004	-9.16795956576499
C	-2.86728871762220	-4.92529913101120	-10.05557080711620
C	-2.82728257727604	-1.83592113178779	-10.17981912914841
C	-0.53617715972051	-3.17834164619308	-8.85294675895486
H	-3.95385627247245	-4.98297976207881	-10.21044487489572
H	-2.38371303918742	-4.93599604497557	-11.04404064894278
H	-2.56029822778971	-5.83548779815884	-9.52247491993880
H	-2.09116102254228	-1.82313203469438	-11.00055559706483
H	-3.82241817408499	-1.84915085439194	-10.63537810223736
H	-2.69893815739020	-0.89437230411124	-9.62711539717628
H	-0.11227255117912	-2.71107403875937	-9.75551464098565
H	-0.31453598614765	-2.50098599313281	-8.01507960747264
H	0.00020018645286	-4.11969994660094	-8.69187817896313
H	-1.43784546128111	-5.43777352541272	-7.49429549310782
H	-0.65745930253852	-4.30990313273789	-6.34770972913858
H	-1.60815007911065	-5.64240578447903	-5.71128639340803

82

Coordinates, constrained distance 3.38, absolute energy -2738.430521192111 Ha

C	-6.71234820854245	-1.79178361928307	-7.97635506551791
C	-6.73027133925680	-0.90246813090146	-6.73172939262027
C	-6.00247131880241	-1.58951844358184	-5.57625205310633
C	-4.56975512093419	-1.98576204659395	-5.96180256597023
C	-4.57007307867993	-2.85866730404454	-7.21715877231896
C	-5.27385741075683	-2.15478727052568	-8.37136002160394
N	-3.17617704632330	-3.36764964254469	-7.49861371673336
C	-2.63229286215100	-4.00743916785096	-6.48164082856464
C	-3.11279108863930	-3.78659125453858	-5.04401883955871
N	-3.95578985069691	-2.73942885512846	-4.87740941271399
O	-2.6356377736835	-4.44277578078373	-4.12239785486012
H	-7.29140446177106	-2.71166164588187	-7.78574641583039
H	-7.19846989191885	-1.28371707781629	-8.82193364428435
H	-6.24861875286736	0.06404960106434	-6.95881798028902
H	-7.76316057866305	-0.67289958917795	-6.43455271074835

H	-5.96297552808725	-0.93468791132691	-4.69118000206380
H	-6.54489825066938	-2.50335973172618	-5.28062524300377
H	-3.98418836057941	-1.06526574613393	-6.16252326512397
H	-5.13565405288995	-3.78224253169633	-6.97976482857877
C	-1.40713124179558	-4.84060426401276	-6.55556672538534
H	-4.16211280386502	-2.48470194994792	-3.91253728613874
H	-4.74085618076788	-1.23160352227484	-8.64088989271503
H	-5.28557250625562	-2.80701819509184	-9.25613184394966
P	-5.01864321302103	-6.39421239699498	-6.25650327883564
O	-5.66321839671466	-6.51662488857705	-7.73401163629104
Si	-7.01242450815131	-7.21476275866341	-8.52598249947554
C	-8.54545793888241	-6.23848104749136	-8.06653725053959
H	-9.41771525192051	-6.62191436939872	-8.61702820662283
H	-8.76326990520104	-6.31094012810417	-6.99192335785272
H	-8.43607602987089	-5.17348442504508	-8.31968037956003
C	-6.61591220451795	-7.02229203176597	-10.34755201729602
H	-5.67957242181756	-7.53572606358355	-10.61098937167077
H	-7.41629338876342	-7.45297957212822	-10.96778415921931
H	-6.51653244090742	-5.96272170714685	-10.62745885454132
C	-7.17738295395984	-9.01892415076200	-8.05328251253594
H	-6.28248437801791	-9.59287991408633	-8.33523104419196
H	-7.33846297130704	-9.14592137000910	-6.97364162189832
H	-8.03541955607579	-9.46605909748931	-8.57846531066187
O	-4.72605848898260	-7.93213214530583	-5.81773773311487
Si	-3.37050405689085	-8.96871436837855	-5.80639404417877
C	-4.08247600411755	-10.68772942463702	-5.63189706493307
H	-4.66907347243590	-10.78170912479118	-4.70632260980465
H	-3.27637174517683	-11.43589371970474	-5.59297421477649
H	-4.73949060965306	-10.94199666486843	-6.47591741484059
C	-2.28572916439413	-8.52094311701985	-4.34606349395123
H	-2.78876752599743	-8.74735519970402	-3.39447465819003
H	-2.02543276195924	-7.45237769596678	-4.33157441665828
H	-1.35029833493704	-9.09957108899040	-4.36904926288036
C	-2.44605575731172	-8.76956367526482	-7.43037573132647
H	-3.10739696869154	-8.94314794746421	-8.29149083268641
H	-1.61737890124947	-9.49098485347258	-7.49277359372826
H	-2.01322385277526	-7.76322950412847	-7.52592648811545
O	-6.30623890793119	-6.04403777226766	-5.34289850459711
Si	-6.91596603827716	-6.40844000975834	-3.78743371878714
C	-5.50448210749432	-6.51312231052046	-2.56183452870279
H	-5.89999603412912	-6.56516526783784	-1.53563454706697
H	-4.89545578211206	-7.41303485622442	-2.72696213907242
H	-4.83424573959717	-5.64218197590302	-2.61954444577474
C	-8.06174422030357	-4.97735732461985	-3.39791370641441
H	-8.56973139690501	-5.14270875999901	-2.43572704035136
H	-7.51195537205212	-4.02763299460018	-3.31971346525219
H	-8.83882471158720	-4.86156997915296	-4.16767151863437
C	-7.85782461279211	-8.02410539369356	-3.88912074782417
H	-8.66085162211173	-7.97840967606999	-4.63960091523854
H	-7.18764228933843	-8.85495951841216	-4.15153199535632
H	-8.32312308631645	-8.26039981296507	-2.91994936982582
Si	-2.33029454773486	-3.33677195380433	-9.20532947739177
C	-2.84279571236756	-4.92462067714243	-10.04915119499840
C	-2.81239267243346	-1.83107198948663	-10.21501259070699
C	-0.47811747094694	-3.15195321030218	-8.94410342170327
H	-3.9335796659787	-4.98266210815421	-10.17395377310373
H	-2.38664639510593	-4.95220827708512	-11.05044221228350
H	-2.52242305083094	-5.82706659282552	-9.51040100237950
H	-2.09430175707914	-1.81504911819117	-11.05135036139893
H	-3.81720192298196	-1.85693569102320	-10.64806367579735
H	-2.68186253425085	-0.88542600443095	-9.66968935140087
H	-0.08312088140577	-2.69671822786759	-9.86573741702508
H	-0.23474878429146	-2.46073003184285	-8.12388442715195
H	0.06771516182325	-4.08808753022224	-8.78454682297133
H	-1.28845492605843	-5.34374065851705	-7.51851409394844
H	-0.51101325171571	-4.23133406960810	-6.35391586428847
H	-1.46411545109146	-5.56671067672938	-5.73452624849407
82			
Coordinates, constrained distance 3.61, absolute energy -2738.429473338979 Ha			
C	-6.67483286308585	-1.84586425647103	-7.91505316288940
C	-6.68994868373542	-0.94694079229663	-6.67754447700846
C	-5.92341554446110	-1.60806048713156	-5.53188334967051
C	-4.48972798729750	-1.97333133600714	-5.94390012309327
C	-4.49461313735057	-2.85626491233946	-7.19225430516083
C	-5.23624070676941	-2.17719527965059	-8.33730373007395
N	-3.09203514338049	-3.33168367674135	-7.50050365672516
C	-2.49346386717948	-3.92293464405622	-6.48978480224643
C	-2.96501772521678	-3.72257062581901	-5.04436435996592
N	-3.83610787018623	-2.70207646932592	-4.86519078090568
O	-2.46076259061358	-4.37505391823214	-4.13557928569340
H	-7.22298762454579	-2.77999479090562	-7.70458837264759
H	-7.19118047198073	-1.35868335676359	-8.75485723745944
H	-6.23582639959316	0.02891269948986	-6.92060744655793
H	-7.72207887394489	-0.73972471879056	-6.36186622340876
H	-5.88069559337257	-0.94602719139985	-4.65232576526710
H	-6.43958122943861	-2.53147814055860	-5.21958010147412
H	-3.93116291214341	-1.04049873840990	-6.16353210151455

H	-5.03089519141889	-3.79376884995583	-6.93868178532886
C	-1.25847326510242	-4.73735917628349	-6.58187082976269
H	-4.04457547236726	-2.45753808099326	-3.89811805147602
H	-4.72824469393877	-1.24545119807757	-8.62503276213967
H	-5.25283133370509	-2.83773947515791	-9.21568893560416
P	-5.08793086087948	-6.41832163373070	-6.23587681611302
O	-5.70668442007067	-6.52080538560806	-7.72983266523608
Si	-7.05426384920066	-7.20707610029321	-8.53208560574342
C	-8.58146795905172	-6.20806489226971	-8.10012694886806
H	-9.45908779405613	-6.60877281466133	-8.62934074196319
H	-8.78936307323927	-6.24142194080021	-7.02163330835113
H	-8.47169837376408	-5.15326893365098	-8.39246960884431
C	-6.63449448986013	-7.03688415289376	-10.35113250877614
H	-5.71081238848901	-7.57897285610386	-10.60175184027042
H	-7.44112432879164	-7.44821485587778	-10.97645871960374
H	-6.50115004091181	-5.98273711656272	-10.63740803961085
C	-7.25261960408745	-9.00594150316126	-8.05076605915668
H	-6.36013025220634	-9.59314249745006	-8.31264750606750
H	-7.43324753108247	-9.12463153610267	-6.97329978093856
H	-8.10702373482887	-9.44524264512006	-8.58835793838328
O	-4.79933487114112	-7.96698907052375	-5.82220981924209
Si	-3.42633614123301	-8.97665945512094	-5.80848013427462
C	-4.10244559531145	-10.71563692839244	-5.69787113240703
H	-4.70600560330448	-10.84959472533655	-4.78818412899072
H	-3.28017561093914	-11.44614488257322	-5.66336238235952
H	-4.73621348146217	-10.96055093881991	-6.56232840258409
C	-2.37795468936789	-8.55160741281306	-4.31459023017505
H	-2.91010817122601	-8.77749003587967	-3.37870047543672
H	-2.09957428074205	-7.48765025633676	-4.28726799628120
H	-1.45132017343148	-9.14480302931755	-4.31580516666020
C	-2.46370607911141	-8.71149956464403	-7.40138765050918
H	-3.09580326261845	-8.87867983266975	-8.28558815980035
H	-1.61272540797101	-9.40643193924235	-7.45902597515534
H	-2.06081222508164	-7.68958132995285	-7.45470282015204
O	-6.40766713088301	-6.10282436139489	-5.34853239379227
Si	-6.99977529943041	-6.44623651209015	-3.78445545910074
C	-5.58848089308435	-6.38414576539623	-2.55352987143516
H	-5.97705201976680	-6.45513382826007	-1.52581970957501
H	-4.88503557946923	-7.21649663142831	-2.69892509601146
H	-5.01507900785147	-5.44806774655433	-2.62986369496314
C	-8.25171313638593	-5.08989541278250	-3.45921434059633
H	-8.74052170490387	-5.24158761163707	-2.48490036636923
H	-7.77793604765997	-4.09702018705372	-3.43934465983741
H	-9.03990846096051	-5.07626743972745	-4.22666515429530
C	-7.81672652212667	-8.13126349024286	-3.81225151211305
H	-8.63772021293035	-8.16942189895762	-4.54360732393455
H	-7.09144614223390	-8.91661762204226	-4.06771176734569
H	-8.24043549812681	-8.37024861885245	-2.82484047680316
Si	-2.30046881246694	-3.32297102185265	-9.23957529697492
H	-3.820309788189165	-4.94804238630900	-10.01345424937724
C	-2.84662098060325	-1.85621169723747	-10.27322803467854
C	-0.44675327903290	-3.08609410839139	-9.03869022241614
H	-3.89420839642652	-5.02488577126682	-10.12316360878683
H	-2.35827729727938	-5.01034287216418	-11.01840371262029
H	-2.46379876243044	-5.82283542876785	-9.44174574460182
H	-2.15356716810966	-1.85050250981640	-11.13051208999332
H	-3.86325661714188	-1.91220651611177	-10.67436144733636
H	-2.71763298283229	-0.89324290932938	-9.75848929796156
H	-0.09198020736839	-2.64912852975052	-9.98516885659940
H	-0.19596680509306	-2.36446525056415	-8.24745270331841
H	0.12796735800873	-4.00297112339948	-8.86925825035042
H	-1.15006293615878	-5.24436018658166	-7.54394454643148
H	-0.36558379608357	-4.11782490024898	-6.39828981823141
H	-1.29372530498771	-5.45861098000170	-5.75400608612068

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Coordinates, constrained distance 3.83, absolute energy -2738.428614688944 Ha

C	-6.64724404329743	-1.92196500010846	-7.69520168804485
C	-6.60007638273065	-1.00940738773875	-6.46858652997409
C	-5.75482428211846	-1.64542041359503	-5.36537461801944
C	-4.34400752982026	-1.99653633061434	-5.86124616322090
C	-4.40923748963769	-2.88863911878015	-7.10157239533713
C	-5.23310724012479	-2.23724233239775	-8.20502863289074
N	-3.01562432099089	-3.33554305295228	-7.49095118784348
C	-2.33906874220163	-3.89532457862968	-6.51513296040645
C	-2.75365198611224	-3.72603089490035	-5.04793127872481
N	-3.61924136932793	-2.71145986587585	-4.81795296544096
O	-2.21544125676053	-4.39960423336997	-4.17521846776452
H	-7.16747253479405	-2.86062407662049	-7.44089651059279
H	-7.22293129042994	-1.45134150590770	-8.50538566561443
H	-6.17759222798191	-0.02926338756641	-6.74793844056962
H	-7.61426088600644	-0.81476903101818	-6.09229737593270
H	-5.66532782109374	-0.97143012734358	-4.49841339572503
H	-6.23761990130095	-2.57044447550146	-5.00824361911266
H	-3.81237946525615	-1.05757862939521	-6.11704994954627
H	-4.90411929937486	-3.83874812444227	-6.80965080681792
C	-1.08636211221327	-4.67231094734525	-6.66899605313351
H	-3.79711122031347	-2.48614525128995	-3.83989965507260

H	-4.76019052346635	-1.30249963260772	-8.53890303120323
H	-5.29712675103715	-2.91204294197900	-9.07025877336111
P	-5.19468013947896	-6.44100794461445	-6.24954378597974
O	-5.74397767560533	-6.54040652150536	-7.77167525453155
Si	-7.06542089674730	-7.23499506855455	-8.61010491087502
C	-8.59384041896062	-6.19889613503244	-8.28246973051110
H	-9.44662903585366	-6.58637029101101	-8.86008735519414
H	-8.86801957350471	-6.21469708000566	-7.21856001175975
H	-8.44193492947254	-5.15067760343103	-8.57941544519174
C	-6.56401525562747	-7.12954462432364	-10.41425869098762
H	-5.62694075940268	-7.67326181582768	-10.60367136446855
H	-7.33976098608512	-7.57138727416802	-11.05767917320583
H	-6.42762487544455	-6.08600054473609	-10.73638400406036
C	-7.31624254075107	-9.01443925244935	-8.08250583881854
H	-6.42417427037489	-9.62491932520189	-8.28551000989534
H	-7.54529900678264	-9.09539397396405	-7.01088740431734
H	-8.15516025277746	-9.45515894885728	-8.64295923611950
O	-4.88072350828056	-7.98916365240854	-5.84602154179723
Si	-3.46393642972363	-8.93238342232386	-5.79245566754406
C	-4.06097754059225	-10.69879042085307	-5.66392611381430
H	-4.68170328513788	-10.84198253929473	-4.76722434157671
H	-3.20771141543834	-11.39001472581126	-5.59390634750340
H	-4.66056748959563	-10.98962013202783	-6.53871177341817
C	-2.4569628915285	-8.43672226096539	-4.29139659620993
H	-2.97532087996191	-8.70389704922678	-3.35846402874901
H	-2.25297663632464	-7.35561602131229	-4.26044042939238
H	-1.49152453786733	-8.96470105848521	-4.29013324939353
C	-2.49162462785944	-8.65130502502362	-7.37763075722650
H	-3.10902766249041	-8.85685796680717	-8.26420507374571
H	-1.61299509701116	-9.31189870979245	-7.41720698786747
H	-2.13102957312459	-7.61418167657681	-7.44565192888256
O	-6.57435422802360	-6.19142856047019	-5.42948366770062
Si	-7.14433753189159	-6.44407010990097	-3.84267705261994
C	-5.72694966528517	-6.24642181758821	-2.63024404452304
H	-6.10816547508200	-6.22918953542536	-1.59760614313815
H	-5.01165042924879	-7.07863562612821	-2.70382725611422
H	-5.16546835891024	-5.31388923716477	-2.79355093275440
C	-8.44659827868254	-5.11829463834926	-3.60010424987556
H	-8.91933202662535	-5.21351608258904	-2.61086326539110
H	-8.01456929670001	-4.10812354917055	-3.66408079847816
H	-9.24144032694724	-5.19521008039554	-4.35678688523412
C	-7.88915556734551	-8.15881806889487	-3.74501896680022
H	-8.72614161901791	-8.27303611758179	-4.44934224615664
H	-7.13844868887597	-8.92756443370296	-3.97669033261007
H	-8.27631331905696	-8.35698383574791	-2.73386710962010
Si	-2.31820484633250	-3.32594343175950	-9.27686351229833
C	-2.79078439902588	-4.99222746316573	-9.97806334686173
C	-2.98938115101580	-1.91745831827259	-10.31613374528690
C	-0.47172853214195	-2.99389830484351	-9.16844924494355
H	-3.88223787666037	-5.12395428301469	-9.99538930409757
H	-2.42496350101647	-5.05765356899497	-11.01428297488180
H	-2.36479980025099	-5.83605527558278	-9.41807527832005
H	-2.34706307755930	-1.91189379808580	-11.21200262992432
H	-4.02367172850858	-2.03102386248520	-10.65537807411172
H	-2.87345287200046	-0.93332247063112	-9.84004048286972
H	-0.18366071719065	-2.55243707676350	-10.13517433438563
H	-0.22133157594278	-2.25119843045044	-8.39688787301771
H	0.15499297095673	-3.87889119167080	-9.01582698934192
H	-0.99957661323028	-5.16635757775475	-7.63967006276566
H	-0.20543813567321	-4.02856455864617	-6.51224797000941
H	-1.06579106689419	-5.40334529019743	-5.84836400848094

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Coordinates, constrained distance 4.06, absolute energy -2738.428106040667 Ha

C	-6.59417881901011	-2.05455641365111	-7.38671226600966
C	-6.45762704821440	-1.14465002911744	-6.16516101337083
C	-5.48845568455933	-1.75528045925482	-5.15316710821143
C	-4.12037256574110	-2.05746592876994	-5.78373488347571
C	-4.27760856100025	-2.94231188752583	-7.02063124171378
C	-5.22751285163175	-2.31960481090800	-8.03513921022233
N	-2.91415323334929	-3.34328954287755	-7.54557552561673
C	-2.12824209363557	-3.88026479309838	-6.64414927695704
C	-2.42813099181076	-3.76126487033830	-5.14475622879892
N	-3.27973137254444	-2.76134589360785	-4.82024072402182
O	-1.82104935802659	-4.46047298008279	-4.34022891476275
H	-7.05151726547746	-3.01235766996068	-7.08836050156992
H	-7.26344549899003	-1.60285858920184	-8.13325716234383
H	-6.09826646768476	-0.14950713445377	-6.47707060588350
H	-7.43619661576319	-0.98699281646859	-5.68972117260944
H	-5.33923237880459	-1.08278119558551	-4.29329536784114
H	-5.90493906724914	-2.69743011084905	-4.75875417825635
H	-3.64301393099242	-1.10027052449789	-6.07437191668217
H	-4.71123067949768	-3.91056043446248	-6.68796383436775
C	-0.86554814222963	-4.60510714962192	-6.91892556579307
H	-3.39568688320185	-2.57564377557228	-3.82457500624148
H	-4.82358028140484	-1.37077334708050	-8.41732819096215
H	-5.35371630947420	-2.99990203837479	-8.88899639562127
P	-5.27258414777066	-6.41736912566391	-6.23564410327786

O	-5.75072878662326	-6.54511305724759	-7.78157536602899
Si	-7.02788257784252	-7.26353742166433	-8.66664647052934
C	-8.57895486066019	-6.23957647481328	-8.41807628749000
H	-9.39632721889826	-6.62559718212952	-9.04582689652067
H	-8.91202916192785	-6.26524350164544	-7.37123906556238
H	-8.41419257147563	-5.18815657893566	-8.69650838998974
C	-6.45113523720734	-7.17584663008114	-10.44933788508089
H	-5.49995234812401	-7.71086732951155	-10.58637752215837
H	-7.19201624720299	-7.63852224654073	-11.11846599677557
H	-6.31268478324473	-6.13627472357397	-10.78292672609296
C	-7.28185803603779	-9.04020461264981	-8.13114683077443
H	-6.37390505311164	-9.64133069690922	-8.28450535366253
H	-7.55917093080988	-9.11114755840171	-7.07040025713151
H	-8.0885932409381	-9.49744741073554	-8.72433094682055
O	-4.96187225809744	-7.95818316060545	-5.79775820042951
Si	-3.51742995816688	-8.85265382970743	-5.66294889668985
C	-4.06605780915397	-10.62906216526647	-5.47123207454119
H	-4.69707795597419	-10.75520000505307	-4.57912617806512
H	-3.19555265827785	-11.29306640561802	-5.36188569722670
H	-4.64262991850852	-10.97010694942326	-6.34348612137763
C	-2.56153488856730	-8.25515119443690	-4.16580858686396
H	-3.12487662236150	-8.42972823074512	-3.23705488586423
H	-2.32719732567067	-7.18112577037454	-4.21914623404619
H	-1.61137862866416	-8.80330343336654	-4.07823896826663
C	-2.51597985332808	-8.60450658244201	-7.23570793893541
H	-3.07149537080886	-8.93779579222848	-8.12452068987792
H	-1.57509281630929	-9.17241643769749	-7.19369849671833
H	-2.26399435615629	-7.54172727367499	-7.37256769412059
O	-6.69410540646105	-6.17201633563631	-5.48553795594228
Si	-7.35983104132520	-6.43554314264073	-3.93942341858270
C	-6.01797682225867	-6.25473672433984	-2.64006888631365
H	-6.45654767781102	-6.29530368061045	-1.63116125088353
H	-5.27285959292961	-7.06037055887964	-2.70986199397606
H	-5.48462040368827	-5.29627508731223	-2.73033844111960
C	-8.66449672947009	-5.10288097171536	-3.75765969321844
H	-9.19626775462949	-5.20587335039123	-2.79950134674536
H	-8.22135032533149	-4.09577330864802	-3.78370767244739
H	-9.41335271499231	-5.16443299682619	-4.56130640207126
C	-8.11621677873401	-8.14763873640664	-3.90002194393240
H	-8.90998238881234	-8.25405997669074	-4.65426531638561
H	-7.35562051374635	-8.91737607305902	-4.09216635995173
H	-8.56465238243940	-8.35102656988178	-2.91549486790157
Si	-2.36847697483836	-3.29014939438247	-9.38801410477269
C	-2.76691995521676	-4.99478105173905	-10.04283611517420
C	-3.23291481764669	-1.95624091410985	-10.37816583710867
C	-0.55153057277532	-2.80894606772770	-9.40609675777330
H	-3.82350272550899	-5.25076798461063	-9.87578916953734
H	-2.58279459896038	-5.00786494168716	-11.12861940065047
H	-2.15732881407675	-5.78981404509802	-9.59265616977636
H	-2.68513808984756	-1.93887131761336	-11.33506222774096
H	-4.28648794468384	-2.14416043077928	-10.60765392705619
H	-3.13286172250165	-0.95322386412002	-9.93999583112472
H	-0.37247611492112	-2.28835103103727	-10.35926355100457
H	-0.29625828342810	-2.09890497597068	-8.60587977137881
H	0.14790921818233	-3.65101838299276	-9.35592658510958
H	-0.81223466799969	-5.02486007518469	-7.92569327347253
H	0.00328177734541	-3.94686528042952	-6.75314352800757
H	-0.78134237512427	-5.39498755297473	-6.15859314858795

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Coordinates, constrained distance 4.29, absolute energy -2738.427695741647 Ha

C	-6.53118344077516	-2.14361594395389	-7.35363072082873
C	-6.40535362480486	-1.23130588873491	-6.13286986454866
C	-5.41076626984677	-1.81673072682070	-5.13082732338034
C	-4.04225887123732	-2.08308476555491	-5.77572595052957
C	-4.18867565194919	-2.97344612501835	-7.01011237675033
C	-5.16479912828576	-2.37651570031527	-8.01502725828628
N	-2.81844393575692	-3.33164341410978	-7.55209140057098
C	-1.99541710242342	-3.82580815788451	-6.66078124892052
C	-2.29226644857766	-3.73229108384318	-5.15823981090737
N	-3.17298983312191	-2.76362213326081	-4.82014888591000
O	-1.66747004754843	-4.42956534582295	-4.36572052702707
H	-6.96378371715038	-3.11226262711771	-7.05351682537311
H	-7.21704251950553	-1.70716296214874	-8.09416161344941
H	-6.07483543637945	-0.22699930110119	-6.44760062756290
H	-7.38280123422189	-1.09911520322978	-5.64736607791889
H	-5.26998041966469	-1.14043595091097	-4.27250339335411
H	-5.79837630223899	-2.76944809297857	-4.73229557663031
H	-3.59320741461121	-1.11375288335366	-6.07101665740790
H	-4.59279854188829	-3.95394195671430	-6.67312328117694
C	-0.70761515744535	-4.50047378789072	-6.94777490495304
H	-3.29944790033136	-2.60046425285858	-3.82173762346983
H	-4.78761817669155	-1.41905100755528	-8.40342753346492
H	-5.28448713321205	-3.06189129826681	-8.86563377990466
P	-5.38962732613074	-6.40572524139664	-6.21204901881121
O	-5.84331655291535	-6.50146783513885	-7.76757623895492
Si	-7.10732979951250	-7.22260119391922	-8.67019968889716
C	-8.64452688449462	-6.16577813824043	-8.48292176007062

H	-9.45548646422138	-6.55150324430565	-9.11910948001973
H	-8.99939710624975	-6.16252285828497	-7.44285003870989
H	-8.45465602178951	-5.12418208925510	-8.78140931591584
C	-6.47881225425199	-7.18588933540236	-10.43748877510951
H	-5.53663794469150	-7.74469861908924	-10.53533433048927
H	-7.21079487216365	-7.64669645667528	-11.11775999744373
H	-6.30910963936289	-6.15660214994310	-10.78767159577734
C	-7.40766149786089	-8.98135350136072	-8.10081179344010
H	-6.50678840971642	-9.60142265876697	-8.21411597951722
H	-7.71481977871245	-9.01966683017910	-7.04670262561161
H	-8.20709030518431	-9.43802222156640	-8.70467037063169
O	-5.03870909786777	-7.95095329932030	-5.81922094979908
Si	-3.57726630832193	-8.81319760154588	-5.67969247262601
C	-4.08967973732630	-10.60047483364200	-5.48751620498776
H	-4.72475572294572	-10.73706732705662	-4.59974774270967
H	-3.20672211511904	-11.24635131287858	-5.37009384119114
H	-4.65345326662338	-10.95552781312645	-6.36255495111078
C	-2.63810231745607	-8.19733168741511	-4.17981485783224
H	-3.20967957547271	-8.36747274341926	-3.25516042479075
H	-2.40526095227302	-7.12353578141085	-4.24162380519676
H	-1.68619679558773	-8.74027723403234	-4.07854850310226
C	-2.57812721457862	-8.55017991247698	-7.25179762218524
H	-3.14937466792219	-8.85400922817834	-8.14130969355053
H	-1.64991663048843	-9.13972052224141	-7.22978965076257
H	-2.30132694783148	-7.49161207561571	-7.37221734603479
O	-6.83242811416030	-6.23333570098470	-5.47945216161339
Si	-7.45403115426628	-6.49446685440816	-3.91434815123037
C	-6.11736830519827	-6.11442905643183	-2.65141018966182
H	-6.50608467292327	-6.24211572750467	-1.62934297921252
H	-5.24890081658674	-6.77971341686642	-2.76223010921709
H	-5.76332065248261	-5.07621079731825	-2.74082790445888
C	-8.88261505819847	-5.29284491341506	-3.76421081303471
H	-9.39307088624790	-5.41233299835712	-2.79621357971033
H	-8.53986274658909	-4.24914511529364	-3.83119591353816
H	-9.62938757272970	-5.45601114180494	-4.55535977408094
C	-8.02848976163213	-8.27148132041386	-3.78814357487053
H	-8.81521967282439	-8.48991443055942	-4.52515701183433
H	-7.19614371205762	-8.96802125181491	-3.96095497278809
H	-8.44267485006815	-8.47628640517782	-2.78892352690596
Si	-2.30992449479015	-3.28141556180265	-9.40792137977759
C	-2.66722414439411	-5.00821593869122	-10.02720939531554
C	-3.23234519758432	-1.99178447090804	-10.40437840573144
C	-0.51020660397232	-2.74076880706212	-9.46720739953906
H	-3.72257252743798	-5.27782395949088	-9.87304653553284
H	-2.46620007504895	-5.04150210074295	-11.10960158898517
H	-2.05151634324719	-5.78238169797753	-9.55000732216484
H	-2.70429202222837	-1.97742901976356	-11.37240042758887
H	-4.28434541869224	-2.21445763689819	-10.60844783590245
H	-3.15236631111235	-0.97842166960688	-9.98668960480694
H	-0.37079886004516	-2.21151397399858	-10.42211864779429
H	-0.25888249178477	-2.02597162598770	-8.67007923947605
H	0.21749303966918	-3.55981201740466	-9.43678466045097
H	-0.64870576136802	-4.92371289893052	-7.95282547302955
H	0.13613044860735	-3.80671749254618	-6.79702175994406
H	-0.58324574586505	-5.28135864250810	-6.18360732419756

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Coordinates, constrained distance 4.51, absolute energy -2738.427311006843 Ha

C	-6.44559324812403	-2.19225935974441	-7.30140979283905
C	-6.30711069444724	-1.28211480748805	-6.08057248118876
C	-5.29204740874235	-1.86214662688103	-5.09642567327184
C	-3.93283299158571	-2.11455758879252	-5.76479618190065
C	-4.08962892343976	-3.00467474252343	-6.99801876097806
C	-5.08887096900112	-2.41625502368826	-7.98508385441383
N	-2.72107220780438	-3.33464437183443	-7.56729323579068
C	-1.86203492969265	-3.79617628803273	-6.69335622237046
C	-2.14233065882353	-3.72863008987869	-5.18534692290451
N	-3.04030017015944	-2.78600325466652	-4.82397891472334
O	-1.50039752326522	-4.43221405888312	-4.41211776667305
H	-6.86932945959798	-3.16403925344701	-6.99854401252160
H	-7.14475437504170	-1.75744327341805	-8.03041421581660
H	-5.98957551863887	-0.27436452478314	-6.39791988856089
H	-7.27764232153277	-1.15842636738618	-5.57920503378659
H	-5.14201132838315	-1.18674362157809	-4.23896059167228
H	-5.66606880127051	-2.81891934838463	-4.69445624172516
H	-3.49815161916155	-1.14078333981717	-6.06673947558884
H	-4.47779397513287	-3.99086713098341	-6.65980510326196
C	-0.55933298403125	-4.43018428786518	-7.00459525304285
H	-3.17059497911356	-2.64883043864514	-3.82205536627494
H	-4.72427174743483	-1.45726154707864	-8.38196475893979
H	-5.21910213131140	-3.10473504073069	-8.83138445587806
P	-5.50441017507419	-6.41933958056974	-6.22465742259971
O	-5.95683282531092	-6.46692526633202	-7.78253620489907
Si	-7.22467465005779	-7.16974938534482	-8.69458928419113
C	-8.74916818672084	-6.09447732858974	-8.50653522262880
H	-9.57109440068568	-6.48040609098206	-9.12830158585587
H	-9.09218226461102	-6.07297688207157	-7.46267696189841
H	-8.55175470890574	-5.05939555187474	-8.82207525202430

C	-6.58900815570814	-7.12783809751106	-10.45972103046101
H	-5.65483956294511	-7.69958433825146	-10.55965983268003
H	-7.32479676006588	-7.56950789062200	-11.14840304236225
H	-6.40148916495776	-6.09719139849769	-10.79692884940048
C	-7.54779068143465	-8.92662352872497	-8.13268312694682
H	-6.65016237503923	-9.55368079030148	-8.23114537469927
H	-7.86927294041964	-8.95933283313881	-7.08276247863102
H	-8.34306856696194	-9.37674620837321	-8.74677318586565
O	-5.10999863668788	-7.97160874659095	-5.90265551391748
Si	-3.63002692064134	-8.77789692671387	-5.67540521501456
C	-4.07783690022345	-10.59014696370050	-5.58035775434141
H	-4.76706325911228	-10.78587506502351	-4.74562217666073
H	-3.17943958293331	-11.20609431921176	-5.42514709873570
H	-4.56425801499151	-10.93266359022208	-6.50542949064368
C	-2.83710448503323	-8.17299820991116	-4.08829989179285
H	-3.48818729266989	-8.36507523812796	-3.22248789732961
H	-2.61558610985792	-7.09552121850906	-4.11881306607416
H	-1.88865074088336	-8.70120674204203	-3.90771272640929
C	-2.52066455511439	-8.42383000951146	-7.15351245068477
H	-3.00270712698892	-8.72794965058552	-8.09431627413422
H	-1.56990541792649	-8.97069788352293	-7.07116452129017
H	-2.28765185142591	-7.35001793490212	-7.22042289019773
O	-6.95498850796904	-6.32399749866686	-5.48933479867942
Si	-7.53133376907321	-6.55811641230476	-3.90397800027938
C	-6.27942010278163	-5.85735502130309	-2.68977231789874
H	-6.62308688914419	-6.00995439916525	-1.65484689299619
H	-5.29657234878305	-6.34152262029289	-2.78587539890267
H	-6.14245013018268	-4.77468776909327	-2.83342325565707
C	-9.14211082413951	-5.60608444405240	-3.83615073499111
H	-9.60580821856801	-5.69675691133964	-2.84170046752518
H	-8.98474306381681	-4.53580613982791	-4.03521836151538
H	-9.86328840233678	-5.98759950079296	-4.57384122231624
C	-7.79864200302629	-8.38847684272993	-3.61713624870541
H	-8.53268572760499	-8.80124120256401	-4.32458528513439
H	-6.86209042560822	-8.95130784257804	-3.73477842771327
H	-8.17846927605744	-8.56817378077126	-2.59957666942075
Si	-2.26268996857131	-3.29485901118078	-9.43919813522851
C	-2.59662435688938	-5.04159744398116	-10.01467346126617
C	-3.23966562051732	-2.04817095900233	-10.43826796379810
C	-0.47974541974452	-2.70935357217814	-9.55291051009898
H	-3.64799573529497	-5.31864818804643	-9.84531341551281
H	-2.40225807381086	-5.10344854203742	-11.09679629222961
H	-1.96922725851385	-5.79357326875390	-9.51778307444672
H	-2.73503217831840	-2.04577048850502	-11.41905971304176
H	-4.29117021677446	-2.29756709881737	-10.61212710075493
H	-3.17122209027119	-1.02387507374931	-10.04633688397394
H	-0.38011351111013	-2.18779461502517	-10.51697273171278
H	-0.22513469311132	-1.97948825448378	-8.77065903468184
H	0.26913557828105	-3.50951143892700	-9.53348161083600
H	-0.50966820167349	-4.86512852179142	-8.00514509771699
H	0.26317595214721	-3.70517984835170	-6.88485321221945
H	-0.39044423761078	-5.19539023339606	-6.23317365425186