```
(
 tag: "CDXML",
 attrs: (
   CreationProgram: "ChemDraw 18.2.0.48",
   Name: "test-reaction.cdxml",
   BoundingBox: "94.39 138.98 186.30 160.69",
   WindowPosition: "0 0",
   WindowSize: "0 1073741824",
   WindowIsZoomed: "yes",
   FractionalWidths: "yes",
   InterpretChemically: "yes",
   ShowAtomQuery: "yes",
   ShowAtomStereo: "no",
   ShowAtomEnhancedStereo: "yes",
   ShowAtomNumber: "no",
   ShowResidueID: "no",
   ShowBondQuery: "yes",
   ShowBondRxn: "yes",
   ShowBondStereo: "no",
   ShowTerminalCarbonLabels: "no",
   ShowNonTerminalCarbonLabels: "no",
   HideImplicitHydrogens: "no",
   Magnification: "166",
   LabelFont: "3",
   LabelSize: "7",
   LabelFace: "96",
   CaptionFont: "3",
   CaptionSize: "7",
   HashSpacing: "1.75",
   MarginWidth: "1.25",
   LineWidth: "0.45",
   BoldWidth: "1.60",
   BondLength: "12.20",
   BondSpacing: "20",
   ChainAngle: "120",
   LabelJustification: "Auto",
   CaptionJustification: "Left",
   AminoAcidTermini: "HOH",
   ShowSequenceTermini: "yes",
   ShowSequenceBonds: "yes",
   ShowSequenceUnlinkedBranches: "no",
   ResidueWrapCount: "40",
   ResidueBlockCount: "10",
   .. (31 pairs omitted),
 ),
 children: (
   "\n ",
     tag: "colortable",
     attrs: (:),
     children: (
        "\n
        (
          tag: "color",
          attrs: (r: "1", g: "1", b: "1"),
          children: (),
```

```
),
   "\n ",
    tag: "color",
    attrs: (r: "0", g: "0", b: "0"),
    children: (),
   ),
   "\n ",
    tag: "color",
    attrs: (r: "1", g: "0", b: "0"),
    children: (),
   ),
   "\n ",
    tag: "color",
    attrs: (r: "1", g: "1", b: "0"),
    children: (),
   ),
   "\n ",
   (
    tag: "color",
     attrs: (r: "0", g: "1", b: "0"),
    children: (),
   ),
   "\n ",
    tag: "color",
    attrs: (r: "0", g: "1", b: "1"),
    children: (),
   ),
   "\n ",
    tag: "color",
    attrs: (r: "0", g: "0", b: "1"),
    children: (),
   ),
   "\n ",
    tag: "color",
    attrs: (r: "1", g: "0", b: "1"),
    children: (),
   ),
   "\n ",
 ),
),
"\n ",
 tag: "fonttable",
 attrs: (:),
 children: (
   "\n
   (
     tag: "font",
     attrs: (id: "3", charset: "iso-8859-1", name: "Arial"),
     children: (),
```

```
),
    "\n
 ),
),
"\n
 tag: "page",
  attrs: (
    id: "34",
    BoundingBox: "0 0 538.51 785.11",
    HeaderPosition: "36",
    FooterPosition: "36",
    PrintTrimMarks: "yes",
    HeightPages: "1",
   WidthPages: "1",
  children: (
    "\n
    (
      tag: "group",
      attrs: (
        id: "32",
        BoundingBox: "94.39 138.98 186.30 160.69",
        Z: "18",
      ),
      children: (
        "\n
        (
          tag: "fragment",
          attrs: (
            id: "16",
            BoundingBox: "94.39 138.98 115.75 160.69",
            Z: "2",
          ),
          children: (
                               ш,
            "\n
            (
              tag: "n",
              attrs: (id: "15", p: "94.50 160.50", Z: "1", AS: "N"),
             children: (),
            ),
            "\n
             tag: "n",
             attrs: (id: "17", p: "105.07 154.40", Z: "3", AS: "N"),
             children: (),
            ),
            "\n
             tag: "n",
             attrs: (id: "19", p: "115.63 160.50", Z: "5", AS: "N"),
              children: (),
            ),
            "\n
             tag: "n",
```

```
attrs: (
        id: "21",
        p: "105.07 142.20",
        Z: "7",
        Element: "8",
        NumHydrogens: "1",
        NeedsClean: "yes",
        AS: "N",
      ),
      children: (
        "\n
        (
          tag: "t",
          attrs: (
            p: "102.34 144.93",
            BoundingBox: "102.34 138.98 112.85 145.03",
            LabelJustification: "Left",
            LabelAlignment: "Left",
          ),
          children: (
                                        ۳,
            "\n
            (
              tag: "s",
              attrs: (font: "3", size: "7", color: "0", face: "96"),
              children: ("OH",),
            ),
            "\n
          ),
        ),
        "\n
      ),
    ),
    "\n
     tag: "b",
     attrs: (id: "18", Z: "4", B: "15", E: "17", BS: "N"),
     children: (),
    ),
    "\n
     tag: "b",
     attrs: (id: "20", Z: "6", B: "17", E: "19", BS: "N"),
     children: (),
    ),
                       Ϊ,
    "\n
      tag: "b",
      attrs: (id: "22", Z: "8", B: "17", E: "21", BS: "N"),
     children: (),
    ),
   "\n
 ),
),
"\n
  tag: "fragment",
```

```
attrs: (
  id: "24",
  BoundingBox: "164.94 138.98 186.30 160.69",
  Z: "10",
),
children: (
                     п,
  "\n
  (
    tag: "n",
    attrs: (id: "23", p: "165.05 160.50", Z: "9", AS: "N"),
   children: (),
  ),
 "\n
   tag: "n",
   attrs: (id: "25", p: "175.62 154.40", Z: "11", AS: "N"),
   children: (),
  ),
  "\n
   tag: "n",
   attrs: (id: "27", p: "186.18 160.50", Z: "13", AS: "N"),
   children: (),
  ),
  "\n
   tag: "n",
    attrs: (
     id: "29",
      p: "175.62 142.20",
     Z: "15",
      Element: "8",
      NumHydrogens: "0",
      NeedsClean: "yes",
     AS: "N",
    ),
    children: (
      "\n
      (
        tag: "t",
        attrs: (
          p: "172.89 144.93",
          BoundingBox: "172.89 138.98 178.34 145.03",
         LabelJustification: "Left",
        ),
        children: (
          "\n
          (
            tag: "s",
            attrs: (font: "3", size: "7", color: "0", face: "96"),
           children: ("0",),
         ),
          "\n
       ),
      ),
      "\n
```

```
),
    ),
   "\n
    (
     tag: "b",
      attrs: (id: "26", Z: "12", B: "23", E: "25", BS: "N"),
      children: (),
    ),
    "\n
    (
      tag: "b",
      attrs: (id: "28", Z: "14", B: "25", E: "27", BS: "N"),
      children: (),
    ),
    "\n
      tag: "b",
      attrs: (
        id: "30",
        Z: "16",
        B: "25",
        E: "29",
        Order: "2",
        BS: "N",
      ),
      children: (),
   ),
   "\n
  ),
),
"\n
(
  tag: "graphic",
  attrs: (
   id: "31",
    SupersededBy: "35",
    BoundingBox: "152.64 149.84 128.04 149.84",
    Z: "17",
    GraphicType: "Line",
    ArrowType: "FullHead",
    HeadSize: "2250",
  ),
  children: (),
),
"\n
  tag: "arrow",
  attrs: (
    id: "35",
    BoundingBox: "128.04 147.16 152.64 152.38",
    Z: "17",
    FillType: "None",
    ArrowheadHead: "Full",
    ArrowheadType: "Solid",
    HeadSize: "2250",
    ArrowheadCenterSize: "1969",
```

```
ArrowheadWidth: "563",
                Head3D: "152.64 149.84 0",
                Tail3D: "128.04 149.84 0",
                Center3D: "212.99 225.59 0",
                MajorAxisEnd3D: "237.59 225.59 0",
                MinorAxisEnd3D: "212.99 250.18 0",
              ),
              children: (),
            ),
            "\n
          ),
        ),
        "\n
      ),
    ),
    "\n",
  ),
)
  "": "CDXML",
  alpha: none,
  AminoAcidTermini: "HOH",
  bgalpha: none,
  bgcolor: "1",
  BoldWidth: "1.60",
  BondLength: "12.20",
  BondSpacing: "20",
  BondSpacingAbs: none,
  BoundingBox: "94.39 138.98 186.30 160.69",
  CaptionColor: none,
  CaptionFace: none,
  CaptionFont: "3",
  CaptionJustification: "Left",
  CaptionLineHeight: none,
  CaptionSize: "7",
  CartridgeData: none,
  ChainAngle: "120",
  ChemPropAnalysis: "Elemental Analysis: ",
  ChemPropBoilingPt: "Boiling Point: ",
  ChemPropCLogP: none,
  ChemPropCMR: none,
  ChemPropCritPres: "Critical Pres: ",
  ChemPropCritTemp: "Critical Temp: ",
  ChemPropCritVol: "Critical Vol: ",
  ChemPropEForm: "Heat of Form: ",
  ChemPropExactMass: "Exact Mass: ",
  ChemPropFormula: "Chemical Formula: ",
  ChemPropGibbs: "Gibbs Energy: ",
  ChemPropHenry: "Henry's Law: ",
  ChemPropLogP: "Log P: ",
  ChemPropMeltingPt: "Melting Point: ",
  ChemPropMolWt: "Molecular Weight: ",
  ChemPropMOverZ: "m/z: ",
  ChemPropMR: "MR: ",
  ChemPropName: "",
  ChemProptPSA: "tPSA: ",
```

```
color: "0",
Comment: none,
CreationDate: none,
.. (51 pairs omitted),
```