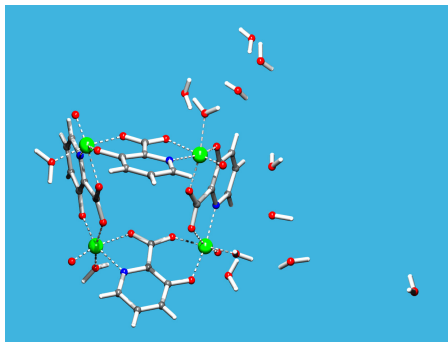


- Structure of  
VO(IV)–3-hydroxypicolinic  
acid complex



### Selected papers

**Resolution and configurational assignment of 3,4,5,6-tetrahydro-2-methyl-2,6-methano-2H-1-benzoxocine derivatives.**

Kurtan, Tibor; Baitz-Gacs, Eszter; Majer, Zsuzsa; Benyei, Attila; Antus, Sandor.  
*Journal of the Chemical Society, Perkin Transactions 1* (2002), (7), 888-894.

**X-ray structures of the tris(2,4-xylyl)phosphane and its trisulfonated derivative: Molecular architecture of a water-soluble sulfonated phosphane with propeller chirality.**

Benyei, Attila C.; Gulyas, Henrik; Ozawa, Yoshiki; Kimura, Kimihiro; Toriumi, Koshiro; Kegl, Tamas; Bakos, Jozsef.  
*Journal of Organometallic Chemistry* (2007), 692(9), 1845-1851.

**Quinoidal Tetrazines: Formation of a Fascinating Compound Class.**

Bostai, Beatrix; Novak, Zoltan; Benyei, Attila C.; Kotschy, Andras.  
*Organic Letters* (2007), 9(17), 3437-3439.

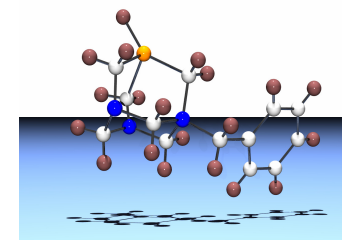
**Complexation properties of the di-, tri-, and tetraacetate derivatives of bis(aminomethyl)phosphinic acid.**

Tircso, Gyula; Benyei, Attila; Kiraly, Robert; Lazar, Istvan; Pal, Robert; Brucher, Erno.  
*European Journal of Inorganic Chemistry* (2007), (5), 701-713.

**Contact:**  
**Dr. Attila Bényei**

✉: 1 Egyetem tér, Debrecen, Hungary H-4032  
☎: (36) 52-512900 Ext. 22486 FAX: (36) 52-512915  
✉: abenyei@delfin.unideb.hu

# Laboratory for X-ray Diffraction



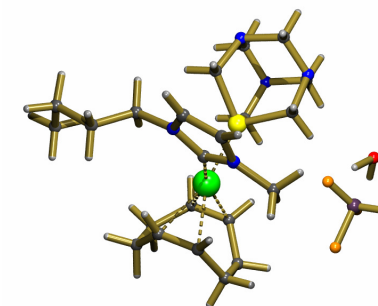
## University of Debrecen, Department of Chemistry

### Specializing in single crystal X-ray diffraction since 1996

**Information:**

**Dr. Attila Bényei**  
crystallographer  
Senior Research Associate

[abenyei@delfin.unideb.hu](mailto:abenyei@delfin.unideb.hu)



## Our Mission

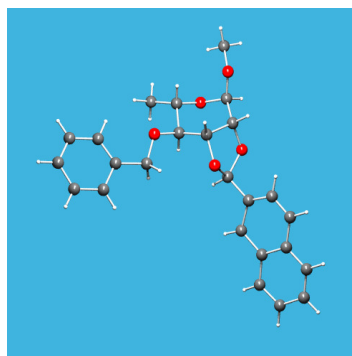
Single crystal X-ray diffraction analysis for academic and industrial research

## Our services

- Single crystal growing
- Solid state structure by single crystal X-ray diffraction
- Determination of absolute configuration
- Structure determination of contaminants
- *ab initio* structure determination from powder diffraction data
- Polymorph screening
- ATR-IR/XRPD study of polymorphs
- Comparison of polymorph structures
- Analysis of hydrogen bond patterns

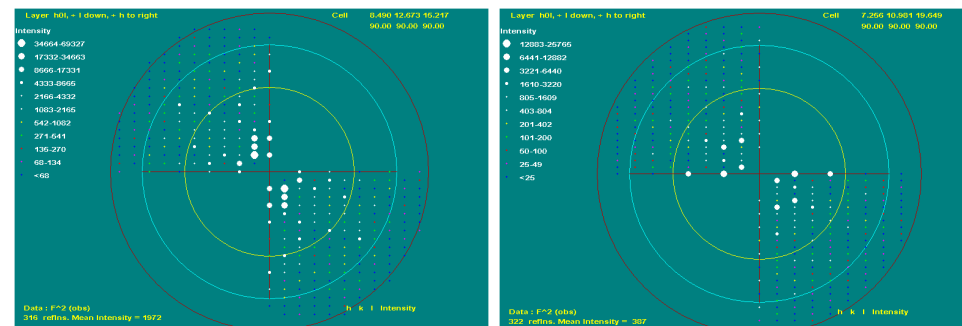
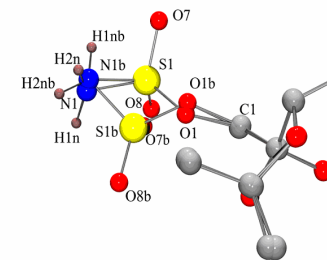
## Instrumentation

- Bruker-Nonius MACH3 Diffractometer
- Oxford Cryosystem Cryostream Cooler (90-370K)
- Thermo Haake computer programmable thermostat for single crystal growing (200-400K)
- CETI optical microscope
- PerkinElmer FT-IR spectrophotometers and FT-IR microscope
- State-of-the-art software and hardware resources
- Fully equipped chemistry laboratory
- Access to GC/HPLC/MS/NMR facilities

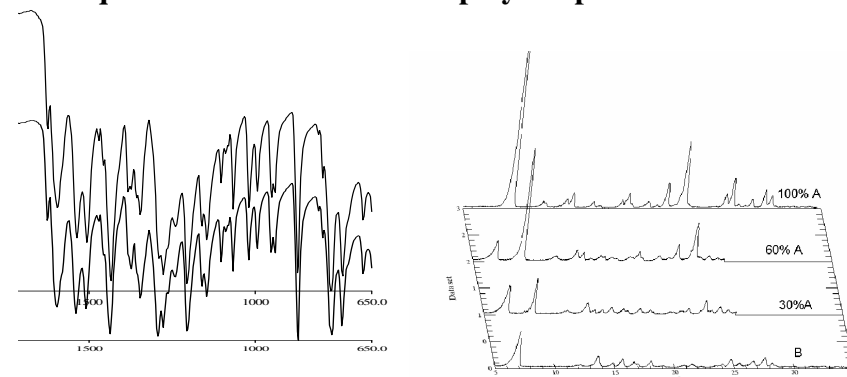


## Example R+D projects

- Single crystal study of sulfonamide polymorphs, diffraction data, structure and hydrogen bond network



- ATR-FTIR – quantitative XRPD of API polymorphs :



## References

200+ solved structures:

- Organic molecules
- Organometallics

20+ pharmaceutical R+D projects

40+ scientific papers

600+ independent citations