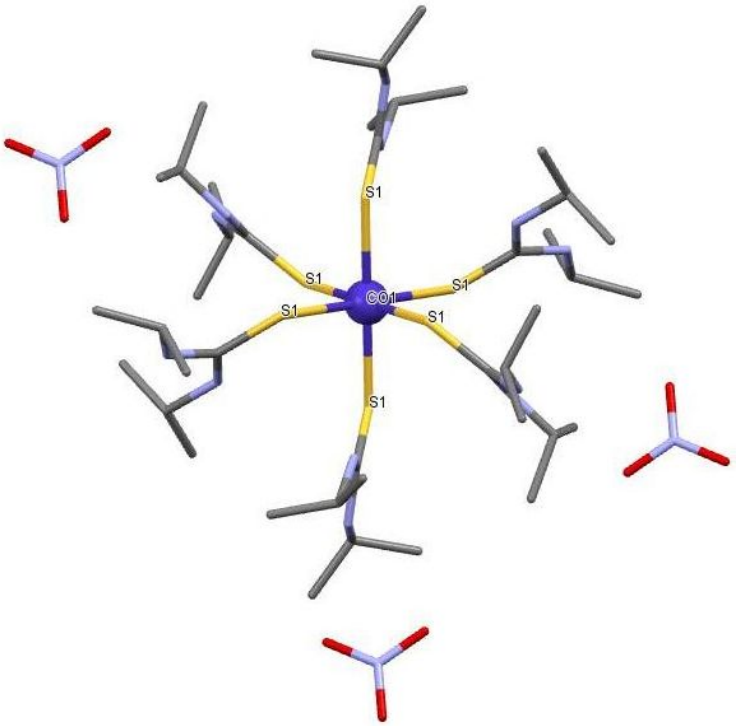
Low-temperature EPR spectroscopy of high-spin cobalt complexes with unusual valence Co(III).

student of the 2nd course 201 group
Makarenko Anatoly Konstantinovich

Experimental methods and samples for research



Structural view of the synthesized complex

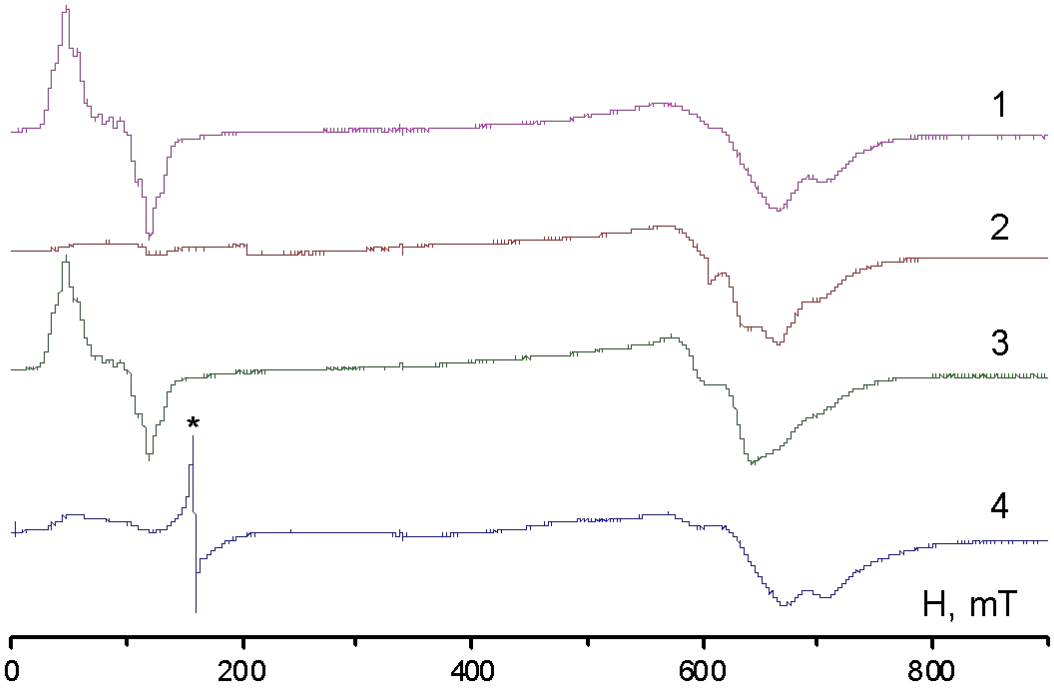
Used samples:

-powder in a vial filled with helium

-powder in the vacuum oil

-monocrystalline sample

Results and discussion

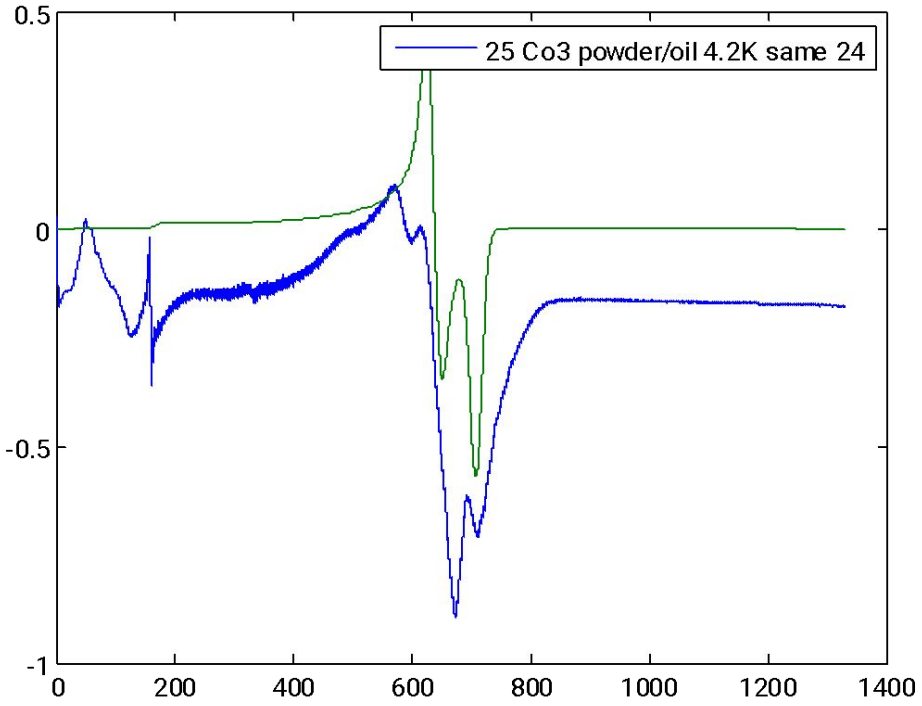


The EPR spectra of powder sample of Co(III) (T=15K) .

1. Spectra without turning
2. Spectra rotate 90 degrees.
3. Spectra rotate 90 degrees.(repeat)
4. Spectra with the use of vacuum oil without turning.

(*- impurities from the glass).

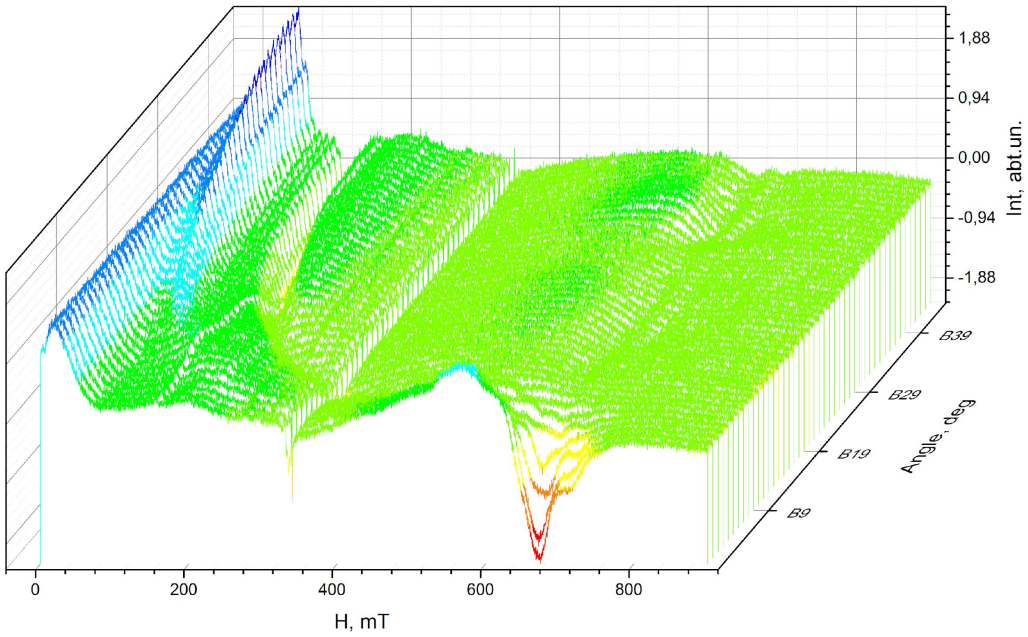
Results and discussion



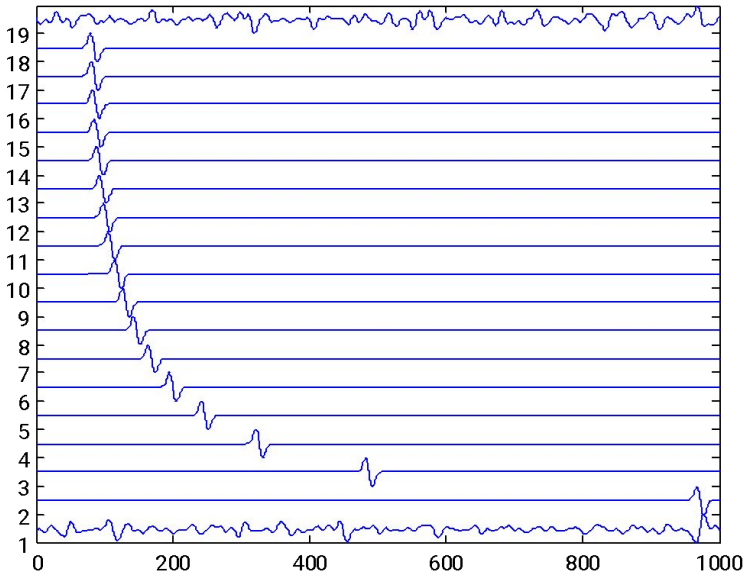
The EPR spectra of powder sample of Co(III) (blue) and simulated spectrum (green)
The simulation parameters S = 2; D = 3.465, E = 0.0055; g=2; the Temperature Of 4.2 K.

Results and discussion

Research of the angular dependence, Temperature 16K.



Experimental spectra



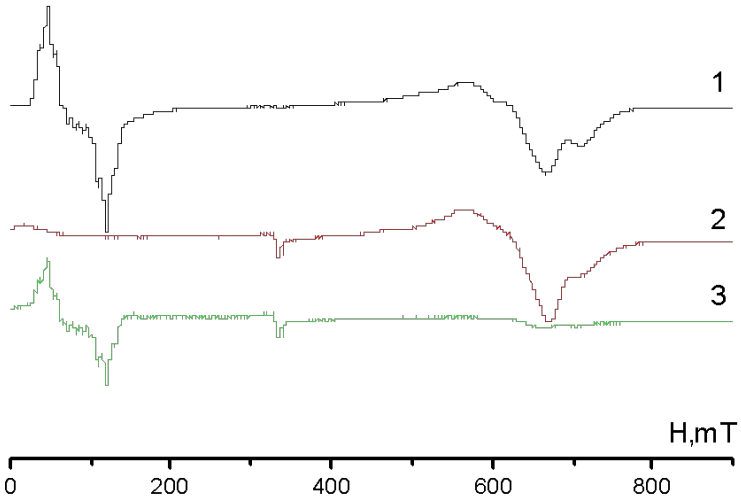
Simulated spectra

The simulation parameters:

S = 2; D = 3.4, E = 0.102 ; g=2;

Results and discussion

Research of spectra of the crystalline sample (temperature 4.2 K)



1. Powder spectra
2. Crystalline spectrum, orientation of 0 degrees.
3. Crystalline spectrum, orientation of 90 degrees.

Conclusion

- For the observed data, it was concluded that the line in the area 100mT on the ESR spectra of the crystalline sample belongs to our complex Co(III). This means that for accurate research of our we need accurate knowledge of its orientation.

- Working with the powder sample, we spotted “torquing effect” , which was eliminated by using vacuum grease

- In the future we will make more accurate simulation of the powder and crystal samples for accurate experimental determination of the magnetic parameters and their comparison with the results of quantum-chemical calculations.

References:

1. **Halogen atom effect on the magnetic anisotropy of pseudotetrahedral Co(II) complexes with a quinoline ligand / Denis V. Korchagin, Gennadii V. Shilov, Sergey M. Aldoshin, Roman B. Morgunov, Artem D. Talantsev, Elena A. Yureva / Polyhedron 102 (2015) 147–151 / DOI: 10.1016/j.poly.2015.09.044**

2. **Deborah Brazzolotto , Marcello Gennari, Shengying Yu, Jacques Pecaut, Mathieu RouziÀres, RodolpheClerac, Maylis Orio, and Carole Duboc. An Experimental and Theoretical Investigation on Pentacoordinated Cobalt(III) Complexes with an Intermediate S=1 Spin State:How Halide Ligands Affect their Magnetic Anisotropy. Chemistry . A European Journal Full Paper/ DOI :10.1002/chem.201502997**

3. **J. Krzystek, Joshua Telser, Luca A. Pardi, David P. Goldberg, Brian M.Hoffman, and Louis-Claude Brunel, High-Frequency and -Field Electron Paramagnetic Resonance of High-Spin Manganese(III) in Porphyrinic Complexes. Inorg.Chem. 1999,38,6121-6129/ DOI: 10.1021/ic9901970.**

4. http://www.EasySpin.org