

## P23 – Analysis of Pyridine Coordination Compounds using Single Molecule Force Spectroscopy

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Multivalency is a fundamental effect in supramolecular Chemistry (e.g. recognition in devices), Nanotechnology (e.g. self organization) or Biochemistry (e.g. transduction of signals) [1]. It can increase binding constants disproportionately high and thereby shift balances strongly to complex side. Thus it is important to gain a deeper knowledge on multivalent interactions. Single Molecule Force Spectroscopy (SMFS) is a direct measurement of forces [2] and an therefore an ideal tool to study multivalency on the molecular level.

Here we present first results of SMFS on a monovalent pyridine coordination compound in an aqueous solution of Fe(II). The pyridine was coupled to Au covered tips and Au surfaces, using thiol chemistry and Polyethylene-glycol (PEG) as spacer with well known stretching properties [3]. Force-distance measurements were performed at different pulling velocities to calculate molecular properties as bond lifetime, bond width and thermal force [4]. Our results are the basement for further analysis on multivalent pyridines. Furthermore, an astonishing repeatability of rupture events along few sawtooth pathways in force-distance space allowed us to analyze rupture events of successive bonds in series separately [5].

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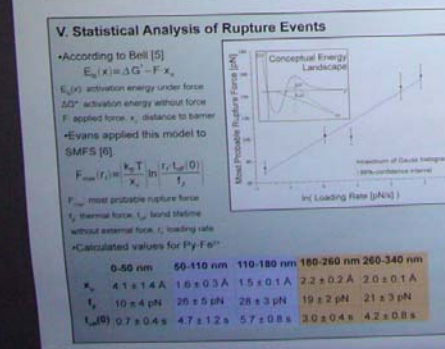
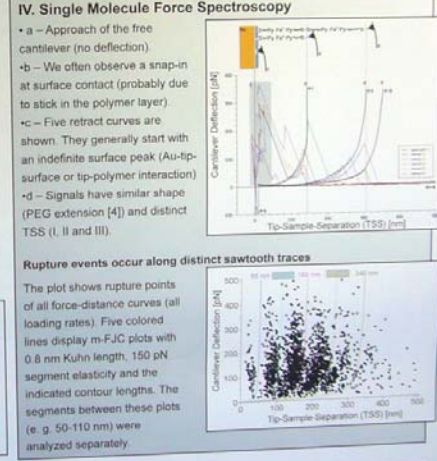
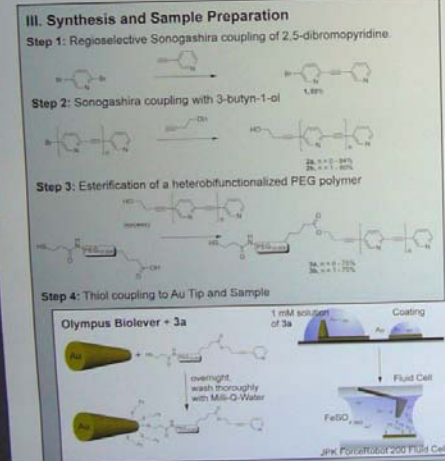
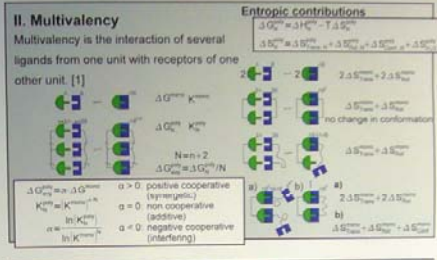
# Analysis of Pyridine Coordination Compounds using Single Molecule Force Spectroscopy

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### I. Abstract

Multivalency is a fundamental effect in supramolecular Chemistry, Nanotechnology and Biochemistry [1]. It can increase binding constants disproportionately high and thereby shift balances strongly to complex side. Thus it is important to gain a deeper knowledge on multivalent interactions. Single Molecule Force Spectroscopy (SMFS) is a direct measurement of forces [2] and therefore an ideal tool to study multivalency on the molecular level. Here we present first results of SMFS on a monovalent pyridine coordination compound in an aqueous solution of Fe<sup>3+</sup>. Force-distance measurements were performed at different pulling velocities to calculate molecular properties as bond lifetime, bond width and thermal force [3].



### VI. Summary and Outlook

The monovalent pyridine coordination compound 3a with Fe<sup>3+</sup> was analyzed by SMFS. We used PEG as separator to exclude tip-surface interactions and its well known extension behavior as model for curve analysis. Forces of single molecular rupture events were measured at different pulling velocities. Surprisingly, most rupture events occurred along distinct sawtooth paths in force-distance space. This was utilized to perform statistical analysis according to models by Bell and Evans separately for each peak.

Next step will be the analysis of di- and trivalent pyridine coordination compounds such as 3b. SMFS measurements under the same conditions might show multivalent effects. MD simulations will be used to gain a deeper understanding of the concerning energy landscapes. Moreover, our experiments can be extended to other metal ions and ligands.

**References**

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This work was funded by SFB 765