

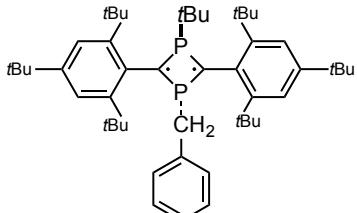
実験報告書様式(一般利用課題・成果公開利用)

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

|  |    |                                  |
|--|----|----------------------------------|
|  <b>MLF Experimental Report</b> |    | 提出日 Date of Report               |
| 課題番号 Project No.   |    | 装置責任者 Name of responsible person |
| 2014A0163  |    | Prof. Yasuhiro Miyake            |
| 実験課題名 Title of experiment  |    | 装置名 Name of Instrument/(BL No.)  |
| Precise analysis of electronic structure of the localized P-heterocyclic singlet biradical                       | D1 |                                  |
| 実験責任者名 Name of principal investigator  |    | 実施日 Date of Experiment           |
| Shigekazu Ito  |    | 2014.11.18-19                    |
| 所属 Affiliation   |    |                                  |
| Department of Applied Chemistry, Tokyo Institute of Technology   |    |                                  |

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)

Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

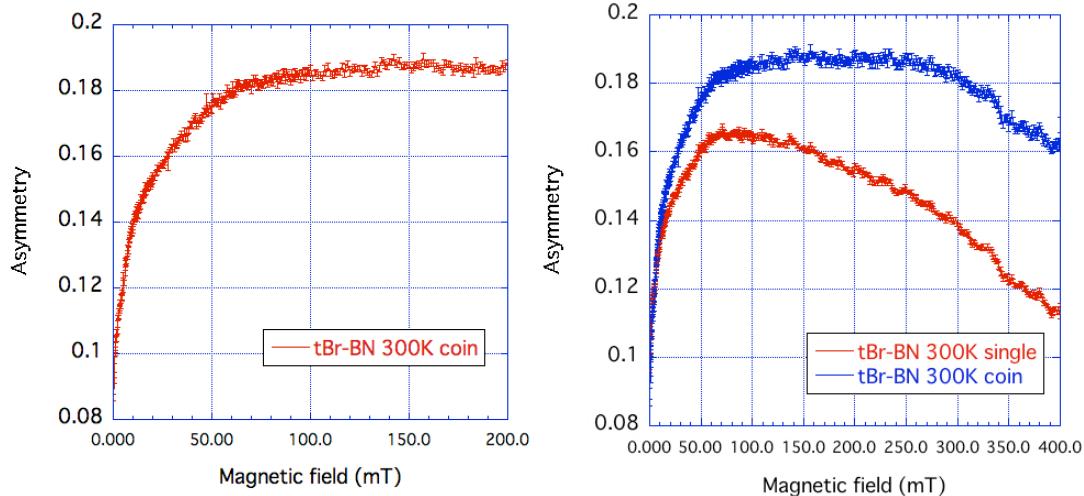
|  |
|--|
| 1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.   |
| 1-Benzyl-3- <i>t</i> -butyl-2,4-Bis(2,4,6-tri- <i>t</i> -butylphenyl)-1,3-diphosphacyclobutane-2,4-diyl (abbreviated as <b>BR</b> )<br>$C_{49}H_{74}P_2$ , pellet of powdered sample |
| Molecular formula:   |
| <br>$tBu = C(CH_3)_3$   |

|  |
|--|
| 2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。)  |
| Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.  |
| <p>The <b>BR</b> sample was compressed as a pellet (20 mmø, 2 mm width) and attached to the center of the detector of MLF D1 muon beam-line. The position of sample was checked by the preparative irradiation of muon beam. Next the level crossing resonance (LCR) experiments were carried out in order to determine the presence of muonium species preliminary. The experimental conditions were as follows:</p> <p>1) Temperature = 300 K, <math>B_{\text{longitudinal}}</math> = 0 to 400 mT<br/>     2) Temperature = 200 K, <math>B_{\text{longitudinal}}</math> = 0 to 200 mT</p> <p>In the experiment under the conditions 2), temporary stops of the beam accumulated, and scans from 200 mT to 400 mT were not carried out.</p> |

## 2. 実験方法及び結果(つづき) Experimental method and results (continued)

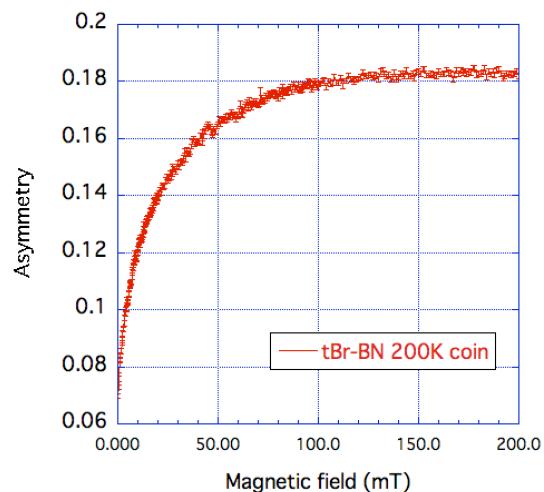
### Results

#### Condition 1)



The lost asymmetry in TF measurement recovers full at relatively low magnetic field of 100 mT, suggesting that the Mu radicals may see relatively small effective magnetic field. DFT calculations (UB3LYP/6-31G\*) for the simplified model molecules suggested that the putatively predominant C-muoniated species would show the hfc parameters of 17 MHz. Indeed the observed data might be consistent to the theoretically predicted results, but characteristic resonance could not be observed in this experiment. The muonium species would be observed under the magnetic field of 50–100 mT. On the other hand, the alternatively possible P-muoniated species would show hfc of 100 MHz, but the characteristic resonance was not determined.

#### Condition 2)



The measurements at 200 K gave almost the same spectrum as the case of 300 K, and no obvious resonance signal was characterized. Because of limit of experiment period, the attempted measurement with the magnetic field of 200–400 mT was not carried out.

Both of the measurements at 300 K and 200 K might not be suitable for characterization. Motion of the molecules was minimized at these temperatures, and width of the resonance peaks might be considerably large. Therefore, the measurements at the higher temperatures would be suitable to observe the characteristic resonances of the muonium species.