

Complete MCB data set C.J. Muller

In the below indicated link you will find the complete MCB data set gathered over a span of more than four years of experiments, with the intent to replicate the “Atomic Probes” result.

https://zenodo.org/communities/muller_mcb_dataset

The complete set contains 191 separate datasets from 191 Bending Beam Assemblies (BBA) or Samples (S). This data is organized in chronological order of conducting the experiments, in the default “sort by Newest” on Zenodo, the last result shows on top. The stored data spans a range from July 2018 to April 2021. Every sample has a unique number, which in general increases towards more recent dates. However, some initially unused older samples may have been used at a later point in time, thus the sample number sequence over time is not consistently continuously increasing.

Every single sample dataset consists of one docx file at the top of the listing, summarizing the entire dataset. It contains detailed information on the experimental circumstances as well as on the drying phase of the junction. Furthermore, all IV curves of the set are shown in this document. The data of every separate IV curve is also available in xls format. The IV curves are obtained via the HP4155 measurement equipment. In this equipment, data is stored in the specific HP4155 machine language, or a .DAT file, which is not readable. The HP4155 has an option to transfer this data to a readable ASCII file or text file. These text files are transferred to excel on a normal PC. It is important to note that the data in these excel files are still identical to the original captured data within the HP4155. Thus, the xls data shows the raw data of the IV curve; there has been zero data manipulation, only data transfer. All the original .DAT files are still available.

The data sets from samples listed on Zenodo are indicated below in a table. How to go about with a dataset of 191 devices? How do I make sense of this all? It is not as bad as it may look at first instance. A lot of the material presented below reflects my own required learning curve.

- Towards the end of 2019 I was still using the pivoting setup with 4.5 mm inner diameter cells. A good understanding of the self-assembly of a single molecule only developed during that time. A remark from my notes December 2019: “As well soft temper as hard temper Au junctions when stopped immediately (motor action) after breaking will “get back” in the drying process (with captured molecule(s)). Be it broken in air or in fluid, nature takes care of it all!”
- In July 2020 (sample 198) a complete understanding of the drying behavior of the 2 mm diameter cell led to the default use of the 2 mm inner diameter cell with paper tip draining.
- During all 2019 and 2020 until November the focus was on the entire -10V to 10V range as to replicate the “Atomic Probes” result. Lots of devices show interesting features at high voltages U , with $|U| > 5$ V. However, due to the large 20 V range and relative fast scan-speed the exact detail and nature of the structure could not be consistently captured.
- Only from November 2020 onwards (device S94) the focus went solely to the high voltage range, either from 7.5 to 10 V or from 9-10 V. This changed the dynamics, most of the relevant data stems from this period. The level of detail in the measurements does require a 1 mV or 2 mV measurement resolution at these high voltages.
- Due to the established standard way of work founded in 2020, the drying procedure of the cell and the starting point of the measurement, the focus on the high voltage range immediately paid off. Not only in terms of the relevance of the data but also in success ratio. Almost every device from November 2020 onwards shows interesting physics.

Date	Device #																				
2018 07	S1																				
2018 11	S13																				
2018 12	S11	S24																			
2019 01	S29	S30																			
2019 04	S31																				
2019 05	S39	S40																			
2019 06	S41	S43	S46																		
2019 07	S49	S50	S51																		
2019 08	S34	S35																			
2019 09	S60	S61	S62	S64	S65	S66															
2019 11	S67	S68	S69	S71	S72	S73	S74	S79													
2019 12	S75	S76	S77	S80	S81	S82	S83	S84	S85	S86	S87										
2020 01	S88	S89	S90	S91	S92	S93	S103	S104	S105	S106	S107	S108									
2020 03	S95	S96	S97	S98	S99+S114	S101	S102	S109	S110	S111	S112	S115	S117	S128	S129	S130	S131	S133	S134	S135	
2020 04	S127	S136	S137	S138	S139	S140	S141	S142	S145	S148	S149	S150	S152	S153	S154						
2020 05	S155	S156	S157	S168	S170	S174	S175														
2020 06	S178	S179	S180	S182	S183	S184															
2020 07	S185	S186	S187	S189	S190	S191	S193	S194	S195	S197	S198	S199	S201	S202	S203	S205	S206	S207			
2020 08	S208	S209	S210	S211	S212	S214	S215	S217	S218	S220	S221	S222	S223	S224	S225	S228					
2020 09	S219	S229	S231	S232	S233	S234	S235	S236	S238	S239	S240	S241	S242	S243	S244	S245					
2020 10	S246	S247	S248	S250	S251	S252															
2020 11	S94	S118	S119	S120	S121	S253	S254	S255	S257	S259	S260	S261	S262	S263	S264						
2020 12	S123	S124	S125	S265	S266	S267	S268	S270	S271	S272	S273	S274	S276								
2021 02	S126	S277	S278																		
2021 03	S143	S279	S280	S281	S282	S283	S284														
2021 04	S287	S288																			

Most of the data relates to BDT (Benzene di-thiol) molecules dissolved in a THF (tetrahydrofuran) solvent. There are, however, several THF only devices: S65, S263, S264, S270, S273, S274, S143, S279, S280. In addition, a few BDTH₂O devices have been created by increasing the humidity to 90% during the self-assembly process: S229, S232, S287, S288.

Coming to an end *the* question to ask is: did I replicate the “Atomic Probes” results? Only those who review the full 191 data sets will know the answer....

Chris Muller