



Automation: the new frontier for Allotrope?

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Allotrope for automation?

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AFO

Allotrope Foundation Ontologies

Defines terms & their relationships consistently across laboratory domains

- Standardized vocabulary out of the box

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{a:1}
{b:2}

ASM

Allotrope Simple Models

Provides standardized text-based representation (JSON) of laboratory data

- Easy to use
- Standard tooling
- Validation
- Extensible

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ADM

Allotrope Data Models

Establishes schema for consistent use of ontologies to describe laboratory items

- Existing models could cover up to 80% of our needs
- New models for simple instruments can be created quickly

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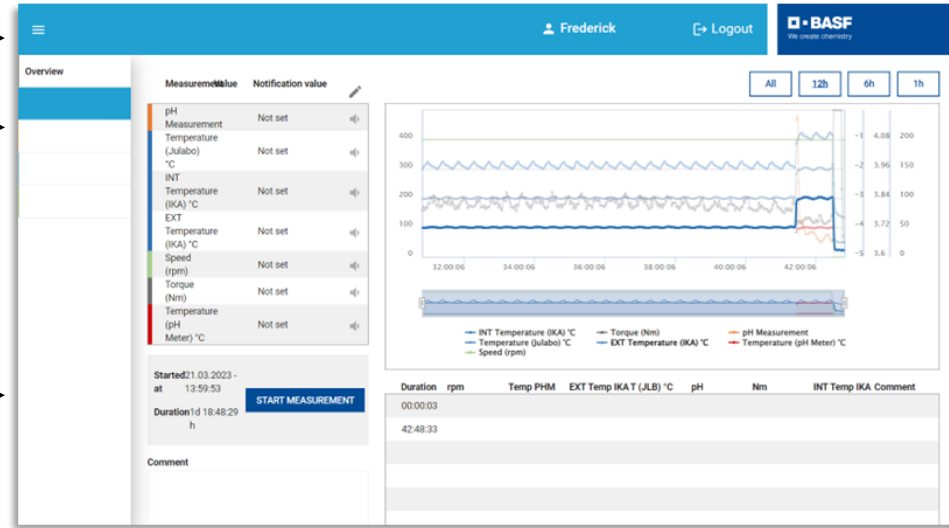


- Benefit from the community's experience
- Data modelling group

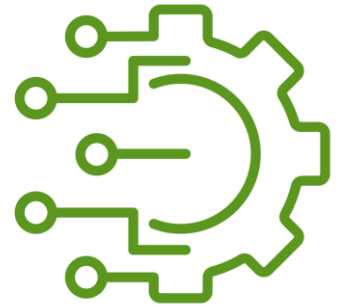
Our use case synthesis monitoring



Sensors producing data over hours, days, weeks



All data are linked logically together by the experimental setup



Visualization
Integration
Analytics

Key enabler: Standardized data format – ASM



Proof of Concept

Allotrope Simple Models

contributed by BASF

39	pH Sensor	Measuring the acidity or alkalinity of a solution over time (Time series data)
40	Pressure Monitoring	Measuring the amount of force or stress being applied to a material over time (Time series data)
48	Stirring	Modeling the operation of a stirrer, a device used to stir a substance or solution.
52	Temperature Monitoring	Measuring the temperature of an object, substance or environment using a sensor or a device over time (Time series data)

PoC implementation time

About 2 weeks for a single developer

Technical implementation

Python package

- collection of basic fields (e.g. sample identifier)
- implementation of various models
- based on pydantic

API

- standardized data endpoint
- model instance validation endpoint

A close-up photograph of a hand holding a light-colored wooden block. The block has the word "LIVE" printed on it in a bold, black, sans-serif font. The background is a solid, light green color.

LIVE

A close-up photograph of a hand holding a light-colored wooden block. The block has the word "DEMO" printed on it in a bold, black, sans-serif font. The background is a solid, light green color.

DEMO

Is Allotrope ready for automation?

ASMs do these things well

- simple to implement
- data models development can be very quick for simple instruments
- very well suited to not just represent data, but facilitate its use in downstream workloads

...yet there are some gaps...

- no concept of experiment – each sensor / instrument is independent – some metadata redundancy
- missing concept of workflow
- the structure of older and newer models differs

...and some questions

- Are newer versions of models backward compatible?
- How to handle different precision levels in different parts of a measurement?
- How to handle measurements done in a unit different to that of the model?

ASM is a promising data standard for use in automation workloads



We create chemistry