

Dataset for publication “Laser Absorption Shock Tube Study of C₁ to C₄ n-Alkyl Formate Pyrolysis”

M. Döntgen, A. Wildenberg, K.A. Heufer

Guide to shock tube data

- <fuel>_overview.json Overview of all included .json files, identified key metadata
- <fuel>_<id>_<p5>_<T5>_<phi>.json
 - DOI journal publication identifier
 - fuel fuel name (fuel abbreviation)
 - Date date of experiment
 - p5 / bar pressure after shock reflection / bar
 - T5 / K temperature after shock reflection / K
 - tign / ms ignition delay time / ms
 - 1st stage / ms first stage timing / ms
 - p1 / bar initial pressure / bar
 - T1 / K initial temperature / K
 - v_isw / m/s incident shock wave velocity / m/s
 - operator,exp arbitrary operator identifier
(consistent throughout all experiments)
 - mix molar fractions of mixture composition
 - formula element count of the fuel
 - phi equivalence ratio of the mix
 - Tmix / K temperature of the mixing vessel / K
 - Date,mix date of mixture preparation
 - pfuel,mix / mbar fuel partial pressure in the mix / mbar
 - operator,mix arbitrary operator identifier
(consistent throughout all experiments)
 - p4,fill / bar driver absolute filling pressure (“air” and “helium”) / bar
 - pControlPiston,He / bar helium holding pressure in control piston / bar
 - pMainPiston,He / bar helium holding pressure in main piston / bar
 - sensors list of all sensors used in the experiment
 - x / mm sensor position relative to endwall / mm
 - type sensor type as defined by manufacturer
 - serial number specific sensor serial number for identification
 - conditioner type signal conditioner type as defined by manufacturer
 - conditioner serial number specific signal conditioner serial number for identification
 - BNC unit type BNC cable connector type as defined by Manufacturer
 - BNC unit serial number specific BNC cable connector serial number for identification

- DAQ unit type data acquisition unit type as defined by manufacturer
- DAQ unit serial number specific data acquisition unit serial number for identification
- unit raw signal unit
- sens / bar/V sensor sensitivity for unit conversion
- loss factor losses due to diaphragm opening and shock attenuation
- NASA string containing all relevant NASA parameters for thermodynamic property prediction in the NASA format
- _comment additional information, e.g. where to find the raw data
- t / ms time data / ms
- p_S<i>(t) / V pressure trace raw data / V

Guide to IR absorption data

- <fuel>_<id>_IR_<p5>_<T5>_<phi>.json
 - DOI journal publication identifier
 - fuel fuel name (fuel abbreviation)
 - Date date of experiment
 - p5 / bar pressure after shock reflection / bar
 - T5 / K temperature after shock reflection / K
 - p1 / bar initial pressure / bar
 - T1 / K initial temperature / K
 - mix molar fractions of mixture composition
 - formula element count of the fuel
 - phi equivalence ratio of the mix
 - xSample / mm position of sample path relative endwall / mm
 - xTrigger / mm position of triggering sensor relative to endwall / mm
 - module information about laser module
 - type designation of laser module
 - serial number serial number of laser module
 - vCentral / cm-1 central wavenumber of laser module
 - software version version of the laser control software
 - nAveraging
 - transfer number of acquisitions for the noise measurement
 - background number of acquisitions for the background measurement
 - sample number of acquisitions for the transient measurement
 - tBackgroundIntegration / ms time for integration of the background
 - tPretrigger / ms time which will be recorded before the trigger signal
 - dfrep / MHz repetition rate for the dual comb setup
 -
 - _comment additional information, e.g. where to find the raw data
 - I0 / - transient reference signal, recorded during pretrigger
 - std / - transient standard deviation of sample to reference signal, recorded during pretrigger
 - T_{static} / - transmission (I/I0) of static measurement (with p1 filled)
 - std_{static} / - as <std / ->, but for static measurement

- t / ms time / ms
- transmission / - transient transmission (I/I₀), one list of length <t / ms> for each wavenumber

Guide to quantum mechanical data

- smi SMILES of compound (only for stable compounds, not for TS)
- xyz / Angstrom geometry of minimum energy conformer / Angstrom
- q / e charge / e
- multiplicity / - spin multiplicity / -
- SPE / h/p single point energy of optimized geometry / h/p
- ZPE / h/p zero point energy of optimized geometry / h/p
- #Elec.Levels / - number of electronic levels / states / configurations
- v / cm-1 harmonic frequencies of internal degrees of freedom / 1/cm
- v_im / cm-1 imaginary frequency / 1/cm (only for TS)
- normal mode / - normal modes of internal degrees of freedom
- method ORCA command line used to obtain results (geometry optimization + frequency calculation)
- scan dictionary of all one-dimensional hindered rotor scan information (keys are tuples of axis-determining atom IDs)
 - axis list of atoms determining the rotational axis
 - <step-nr.> identifier of scan step
 - xyz / Angstrom geometry of scan step / Angstrom
 - SPE / h/p single point energy of scan step / h/p
 - method ORCA command line used to obtain results
- SPE-CC DLPNO-CCSD(T)/cc-pVXZ results
 - <X> basis set size; X = 2, 3, 4 for D, T, Q, respectively
 - SPE / h/p single point energy / h/p
 - T1diag / - T1 diagnostics for multi-reference check
 - method ORCA command line used to obtain results