

Supporting Information to

Systematic Enumeration of Elementary Reaction Steps in Surface Catalysis

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Data Description

The data described is hosted at rnet.theo.ch.tum.de. The $[\text{CHO}]_{1-4}$ molecule datasets are provided as numbered lists of SMILES strings. For technical reasons an “empty” molecule ($[\text{x}]$) is included as the last entry in each list. Reaction datasets are provided as numbered lists of reactions for each $[\text{CHO}]_n$ set. The number after each SMILES string corresponds to the numbering in the corresponding molecule list.

A python function for checking isomorphism of arbitrary SMILES strings is provided as a Jupyter notebook.