Supporting Information: Context-Driven Exploration of Chemical Reaction Networks

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1 Exploration Data

The processed exploration data are given in the files `structures.json` and `paths.json`.

The file `structures.json` contains information on the explored molecular structures. It is structured as a map, where the key is a unique ID for the structure and the value is in turn a map which contains the following keys: `type`, `coordinates`, and `energy`. The key `type` has the value `unique` if the node is a molecular configuration, `ts` if it is a transition state, and `minimum` if it is an endpoint of a minimum energy path. The value of the key `coordinates` is the structure's atomic coordinates. The charge and spin multiplicity of all structures is zero and one, respectively. If the structure has the type `minimum` or `ts` the key `energy` has as a value the PBE/DZ[1,2] single-point energy, otherwise `null`. Energies and Cartesian coordinates are in atomic units.

The file `paths.json` contains the processed reaction paths. If there was more than one reaction path present for a reaction, the one with the lowest reaction barrier was taken (one for the forward and one for the backward reaction). It is structured as a list of maps, where each map contains the keys `reactants`, `reactant_minimum`, `ts`,

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`product_minimum`, and `products`. The values of the keys `reactant_minimum`, `ts`, and `product_minimum` reference the reactant, transition state, and product structures of a reaction path, respectively. The values of the keys `reactants` and `products` reference the molecular configurations in `reactant_minimum` and `product_minimum`, respectively.

2 Reaction Network

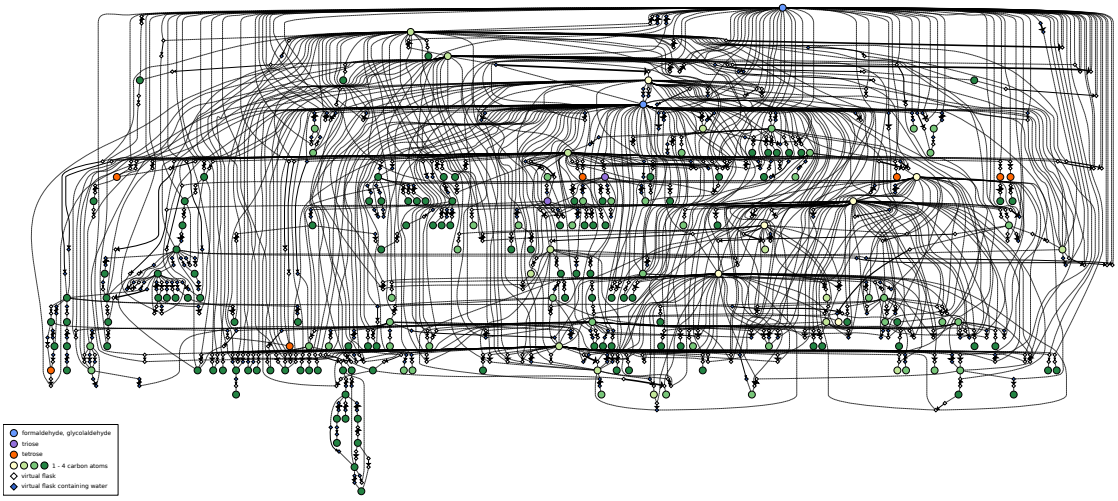

Figure 1: Reaction network generated from formaldehyde, glycolaldehyde, and water (the last not shown explicitly) consisting of reactions with activation barriers below 100 kJ/mol.

References

(1) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.

(2) Dunning, T. H. Gaussian Basis Functions for Use in Molecular Calculations. I. Contraction of (9s5p) Atomic Basis Sets for the First-Row Atoms. *J. Chem. Phys.* **1970**, *53*, 2823–2833.