Supporting Information

Pathfinder – Navigating and Analyzing Chemical Reaction Networks with an Efficient Graph-based Approach

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1 Detailed Chemoton Exploration Settings

1.1 Elementary-step Trial and NT1 Job Settings

NT1 options employed for generating the associative elementary-step trials are summarized in Table 1.

Table 1: Options for the generation of associative elementary-step trials employing the NT1 algorithm. For further explanations consider Ref. 1 and the documentation of the Chemoton code.\(^2\) (\(^*\): for trials involving HIO\(_3\) and H\(_2\)O)

| Setting                      | Value       |
|------------------------------|-------------|
| Molecularity                 |             |
| Bimolecular                  |             |
| # rotamers                   | 3           |
| Max. bond distance per fragment | 1          |
| Unimolecular                 |             |
| Max. bond distance per fragment | 4 (5\(^*\)) |

Additional settings used for elementary-step trials are given in Table 2.

Table 2: Settings employed during structure optimizations and elementary-step trial calculations. For further explanations consider the manuals and source codes of Scine ReaDuct\(^3,4\) and Puffin.\(^5\)

| Calculation Type              | Setting                                      | Value       |
|-------------------------------|----------------------------------------------|-------------|
| Initial Structure Optimization| max_scf_iterations                           | 500         |
|                               | convergence_max_iterations                   | 200         |
|                               | convergence_step_max_coefficient             | 2.0e-3      |
|                               | convergence_step_rms                         | 1.0e-3      |
|                               | convergence_gradient_max_coefficient         | 2.0e-4      |
|                               | convergence_gradient_rms                     | 1.0e-4      |
|                               | convergence_delta_value                      | 1.0e-6      |
|                               | convergence_requirement                      | 3           |
|                               | bfgs_use_trust_radius                        | True        |
|                               | bfgs_trust_radius                            | 0.2         |
|                               | geoopt_coordinate_system                      | internal    |
| Elementary Step Trial Calculation | max_scf_iterations                           | 2000        |
|                               | convergence_max_iterations                   | 600         |
|                               | sd_factor                                     | 1.0         |
|                               | nt_use_micro_cycles                          | True        |
|                               | nt_fixed_number_of_micro_cycles              | True        |
|                               | nt_filter_passes                             | 10          |
| NT1 Scan - General            | nt_total_force_norm                          | 0.1         |
| NT1 Scan - Bimolecular        | nt_number_of_micro_cycles                    | 10          |
| Association                  |                                             |             |
| Model                        | Parameter                                           | Value   |
|------------------------------|-----------------------------------------------------|---------|
| NT1 Scan - Unimolecular      | nt_convergence_repulsive_stop                       | 1.5     |
| Dissociation                 | nt_total_force_norm                                 | 0.1     |
|                              | nt_number_of_micro_cycles                           | 10      |
| NT1 Scan - Unimolecular      | nt_convergence_attractive_stop                      | 0.8     |
| Association                  | nt_total_force_norm                                 | 0.05    |
|                              | nt_number_of_micro_cycles                           | 10      |
| Transition State             | convergence_max_iterations                          | 300     |
| Optimization                 | convergence_step_max_coefficient                    | 2.0e-3  |
|                              | convergence_step_rms                                | 1.0e-3  |
|                              | convergence_gradient_max_coefficient                | 2.0e-4  |
|                              | convergence_gradient_rms                            | 1.0e-4  |
|                              | convergence_requirement                             | 3       |
|                              | convergence_delta_value                             | 1e-6    |
|                              | optimizer                                           | Bofill  |
|                              | bofill_trust_radius                                 | 0.2     |
|                              | geoopt_coordinate_system                             | cartesianWithoutRotTrans |
| IRC                          | convergence_max_iterations                          | 40      |
|                              | sd_factor                                           | 0.6     |
|                              | sd_use_trust_radius                                 | True    |
|                              | sd_trust_radius                                     | 0.1     |
|                              | sd_dynamic_multiplier                               | 1.4     |
|                              | irc_initial_step_size                               | 0.3     |
|                              | stop_on_error                                       | False   |
|                              | convergence_step_max_coefficient                    | 2.0e-3  |
|                              | convergence_step_rms                                | 1.0e-3  |
|                              | convergence_gradient_max_coefficient                | 2.0e-4  |
|                              | convergence_gradient_rms                            | 1.0e-4  |
|                              | convergence_delta_value                             | 1.0e-6  |
|                              | irc_coordinate_system                               | internal |
| IRC Endpoint                 | convergence_max_iterations                          | 500     |
| Optimization                 | convergence_step_max_coefficient                    | 2.0e-3  |
|                              | convergence_step_rms                                | 1.0e-3  |
|                              | convergence_gradient_max_coefficient                | 2.0e-4  |
|                              | convergence_gradient_rms                            | 1.0e-4  |
|                              | convergence_requirement                             | 3       |
|                              | convergence_delta_value                             | 5e-6    |
|                              | bfgs_use_trust_radius                               | True    |
|                              | bfgs_trust_radius                                   | 0.2     |
|                              | geoopt_coordinate_system                             | internal |
| Product Optimization         | convergence_max_iterations                          | 500     |
|                              | convergence_step_max_coefficient                    | 2.0e-3  |
|                              | convergence_step_rms                                | 1.0e-3  |
|                              | convergence_gradient_max_coefficient                | 2.0e-4  |
|                              | convergence_gradient_rms                            | 1.0e-4  |
|                              | convergence_requirement                             | 3       |
|                              | convergence_delta_value                             | 1e-6    |
|                              | bfgs_use_trust_radius                               | True    |
|                              | bfgs_trust_radius                                   | 0.4     |
|                              | geoopt_coordinate_system                             | internal |
1.2 Chemoton: Compound Filters and Exploration Protocol

The following compound filters with stated settings were always combined and employed:

- TrueMinimumFilter with imaginary_frequency_threshold: -5e-5
- ElementSumCountFilter with atom_type_count: {'H': 7, 'O': 8, 'I': 3}

The SelfReactionFilter, which enables bimolecular associative trials of a compound with itself, was combined as stated in Table 3.

The step-wise generation of elementary-step trials with selected compounds was achieved by altering the settings of the IDFilter. The step-wise generation of elementary-step trials followed the following workflow:

1. Remove and add compound ID’s based on their compound cost to the IDFilter
2. Start the CHEMOTON engine for generating trials
3. Wait until all generated trials and resulting calculations are complete
4. Stop the CHEMOTON engine for generating trials
5. Analyze the resulting CRN with PATHFINDER to determine the compound cost of all compounds
6. Repeat

For the exploration with I₂ and H₂O as starting conditions, a chronological list of the compound IDs with details on which trials were enabled and added to the IDFilter are given in Table 3. The stated IDs were added to the filter in blocks, as can be seen in Table 3. The blocks were formed based on the stated compound cost threshold. If the identical compound cost threshold is stated again in Table 3, the compound cost of the affected IDs dropped below the threshold in the previous exploration step.

Table 3: Protocol for the exploration with I₂ and H₂O as starting conditions. Blocks of compound IDs with compound cost threshold and action to indicate how they were included in the IDFilter.

| Compound Cost [arbitrary unit] | Action | Compound ID |
|-------------------------------|--------|-------------|

4
| Condition | Description | Initial State | Final State |
|-----------|-------------|---------------|-------------|
| 0.45      | Starting conditions - Always in IDFilter | 614b303c2a814a60bb4e696a | 614b30322a814a60bb4e6968 |
| < 100     | Always in IDFilter | 614b3d952a814a60bb4e6968 | 614fda422a814a1c224a4efb |
|           | SelfReactionFilter inactive | 614fda422a814a1c224a4efb | 614fda422a814a1c224a4efb |
| < 200     | In IDFilter until all trials of this block are complete | 614b671d2a814a3532259307 | 614b671d2a814a353225930f |
|           | SelfReactionFilter active | 614b671d2a814a353225930f | 614b671d2a814a353225930f |
|           | Only trials with starting compounds and compound with a cost < 100 | 614b671d2a814a353225930f | 614b671d2a814a353225930f |
| < 225     | In IDFilter until all trials of this block are complete | 6155e1cc2a814a4a57c0b8e | 614e2232a814a1c224a4ee7 |
|           | SelfReactionFilter active | 614e2232a814a1c224a4ee7 | 614e2232a814a1c224a4ee7 |
|           | Only trials with starting compounds and compound with a cost < 100 | 614e2232a814a1c224a4ee7 | 614e2232a814a1c224a4ee7 |
| < 232     | In IDFilter until all trials of this block are complete | 615509712a814a0cd81e42e0 | 6177c87e2a814a399675f5b14 |
|           | Actions identical to compounds with a cost < 225 | 6177c87e2a814a399675f5b14 | 6177c87e2a814a399675f5b14 |
| < 242     | In IDFilter until all trials of this block are complete | 617c76f42a814a225b1a7ea5 | 617c76f42a814a225b1a7ea5 |
|           | Actions identical to compounds with a cost < 225 | 617c76f42a814a225b1a7ea5 | 617c76f42a814a225b1a7ea5 |
| < 246     | In IDFilter until all trials of this block are complete | 616f6902a814a1c224a4f00 | 617a9052a814a702b39352a |
|           | Actions identical to compounds with a cost < 225 | 617a9052a814a702b39352a | 617a9052a814a702b39352a |
< 250 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 6179b1742a814a702b393232 |
| 6168ff2a814a55aa49b5f7 |
| 61519b62a814a1c224a4ff1 |
| 6144fb52a814a1c224a4eeb |
| 615c9e72a814a4b6d933 |
| 6154a0482a814a0ed81e42cb |

< 253 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 6178e2862a814a399675b24 |
| 6178d5592a814a399675b22 |
| 614bf20d2a814a3532259319 |
| 617cc5a2a814a225b1a7eb |
| 616599682a814a55aa49b5cc |

< 255 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 61503242a814a44a57c0b3 |
| 615508092a814a0ed81e42df |
| 6157ecc2d814a55aa49b5d4 |
| 6177c928a814a399675b0c |
| 618101122a814a72610d3c19 |

< 255 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 61813b342a814a72610d3c1b |
| 61548dd42a814a0ed81e42c8 |
| 6181df62a814a72610d3c24 |
| 6158c7772a814a44a57c0bbf |
| 617c5fde2a814a225b1a7eb1 |
| 6154a2ba2a814a0ed81e42cc |
| 614482572a814a1ec224a4ec9 |

< 260 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 61535a9d2a814a1ba66a2003 |
| 6151dc502a814a44bde5d935 |
| 617b76702a814a702b393535 |
| 6155b59f2a814a44a57c0b89 |
| 618475d2a814a2fbfffe4 |
| 617f8b0a2a814a7cc75a86eb |
| 615db1a2a814a1e224a4f12 |

< 260 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 6159f79d2a814a44a57c0b7c |
| 618aca9d2a814a7e8e392691 |
| 6189b1d2a814a7e8e392683 |

< 268 \text{ In IDFilter until all trials of this block are complete}

| Actions identical to compounds with a cost $< 225 |
|--------------------------------------------------|
| 615494662a814a0cd81e42ca |
| 614be8ab2a814a3532259317 |
| 615018ba2a814a1ec224a4f01 |
| 61501c532a814a1c224a4f02 |
| 614af5992a814a2fbfffe4 |
| 615195492a814a47a7671a05 |
| 61785df2a814a399675b18 |
| 6155555a2a814a0ed81e42f3 |
| 6150c52a2a814a1c224a4f0d |
| Cost | Actions | Cost | Actions |
|------|---------|------|---------|
| < 268 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | < 268 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| 268  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | 268  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| < 280 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | < 280 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| 280  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | 280  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| < 295 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | < 295 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| 295  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | 295  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| < 299 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | < 299 | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
| 299  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. | 299  | In **IDFilter** until all trials of this block are complete. Actions identical to compounds with a cost < 225. |
< 308 In IDFilter until all trials of this block are complete
Actions identical to compounds with a cost < 225

< 308 In IDFilter until all trials of this block are complete
Actions identical to compounds with a cost < 225

< 310 In IDFilter until all trials of this block are complete
Actions identical to compounds with a cost < 225

< 314 In IDFilter until all trials of this block are complete
Actions identical to compounds with a cost < 225

< 316 In IDFilter until all trials of this block are complete
Actions identical to compounds with a cost < 225
For the exploration with HIO$_3$ and H$_2$O as starting conditions, the list of when and how the compound IDs were added to the **IDFilter** are given in Table 4. The stated IDs were added to the filter as block defined by the given compound cost threshold. If the identical compound cost threshold is stated again in Table 3, the compound cost of the affected IDs dropped below the threshold in the previous exploration step.
Table 4: Protocol for the exploration with HIO₃ and H₂O as starting conditions. Blocks of compound IDs with compound cost threshold and action to indicate how they were included in the IDFilter.

| Compound Cost [arbitrary unit] | Action | Compound ID |
|-------------------------------|--------|-------------|
| 0.45                          | Starting compound - Always in IDFilter | 614b303c2a814a600bb4e696a |
| 1.0                           | In IDFilter until all trials of this block are complete | 616722872a814a55aa49b5e6 |
| < 28                          | In IDFilter until all trials of this block are complete | 61deb5052a814a044c297012 |
|                               | SelfReactionFilter inactive | 61dc88c32a814a044c29701b |
|                               | Only trials with starting compound (H₂O) | 61de012a814a044c297006 |
|                               |                             | 61dcba8d02a814a044c297013 |
|                               |                             | 61dca078a814a044c297010 |
|                               |                             | 61dcb7172a814a044c297016 |
|                               |                             | 61dce51a32a814a044c29701a |
|                               |                             | 61dcc22b2a814a044c297018 |
| < 28                          | In IDFilter until all trials of this block are complete | 61dcd2a2a814a044c297021 |
|                               | SelfReactionFilter active | 61de96d32a814a1b90216277 |
|                               | Only trials with starting compound (H₂O) | 61ebac612a814a28c66cbe67 |
|                               |                             | 61ef50f2a814a28c66cbe25 |
|                               |                             | 61eaf972a814a044c297019 |
|                               |                             | 61e0e7742a814a28c66cbe0c |
|                               |                             | 61e102832a814a28c66cbe0e |
| < 34                          | In IDFilter until all trials of this block are complete | 61e10982a814a28c66cbe0f |
|                               | SelfReactionFilter active | 61dcb8ad2a814a044c297020 |
|                               | Only trials with starting compound (H₂O) | 61ecb5c0a2a814a28c66cbe06 |
|                               |                             | 61e09b062a814a28c66cbe04 |
|                               |                             | 61ecc99a32a814a28c66cbe34 |
|                               |                             | 61e0e7742a814a28c66cbe0c |
| < 34                          | In IDFilter until all trials of this block are complete | 61e222382a814a28c66cbe1d |
|                               | SelfReactionFilter active | 620b28f62a814a0c263b4f38 |
|                               | Only trials with starting compound (H₂O) | 620060c8f2a814a0c263b4f27 |
|                               |                             | 620ba9952a814a0c263b4f2d |
|                               |                             | 620a9892a814a0c263b4f34 |
|                               |                             | 62005ead2a814a0d205ef67 |
2 Details on Paths for the Disproportionation and Comproportionation

In the following sections, the output given by PathFinder of the discussed paths is stated. This includes each reaction equation of the path, where the first molecular formula given is the one of the visited compound node. The total length of the path is given as Cost. The overall reaction equation and the corresponding overall reaction energy is stated as well. The reaction barriers represented in the reaction profiles as well as the maximum barrier of the path are listed.

2.1 Disproportionation of I$_2$

2.1.1 Literature$^6,7$ Path

\[
\begin{align*}
I_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow HI_0(c:0, m:1) + HI(c:0, m:1) \\
HI_0(c:0, m:1) + HI(c:0, m:1) & \rightarrow I_2O(c:0, m:1) + H_2O(c:0, m:1) \\
I_2O(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow H_2I_2O_2(c:0, m:1) \\
H_2I_2O_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow H_3I_2O_3(c:0, m:1) + HI(c:0, m:1) \\
H_3I_2O_3(c:0, m:1) & \rightarrow HIO_2(c:0, m:1) + H_2O(c:0, m:1) \\
HI_0(c:0, m:1) + I_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow H_2I_2O_3(c:0, m:1) + HI(c:0, m:1) \\
H_2I_2O_3(c:0, m:1) & \rightarrow HI_3(c:0, m:1) + HI(c:0, m:1)
\end{align*}
\]

Cost [a.u.]: 420.3517271348526
1 $I_2(c:0, m:1) + 1 H_2O(c:0, m:1) + 2 HI_0(c:0, m:1) = 3 HI(c:0, m:1) + 1 HI_0(c:0, m:1)$

Overall Rxn Energy [kJ / mol]: 316.72
Barriers [kJ / mol]: [174.43, 108.3, 204.66, 58.82, 83.22]
Max. Barrier [kJ / mol]: 204.66

2.1.2 PathFinder Path

\[
\begin{align*}
I_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow HI_0(c:0, m:1) + HI(c:0, m:1) \\
HI_0(c:0, m:1) + I_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow H_2I_2O_2(c:0, m:1) + HI(c:0, m:1) \\
H_2I_2O_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow H_3I_2O_3(c:0, m:1) + HI(c:0, m:1) \\
H_3I_2O_3(c:0, m:1) & \rightarrow HI_2(c:0, m:1) + H_2O(c:0, m:1) \\
HI_2(c:0, m:1) + I_2(c:0, m:1) + H_2O(c:0, m:1) & \rightarrow H_2I_2O_3(c:0, m:1) + HI(c:0, m:1) \\
H_2I_2O_3(c:0, m:1) & \rightarrow HI_3(c:0, m:1) + HI(c:0, m:1)
\end{align*}
\]

Cost [a.u.]: 320.80480369274903
3 $I_2(c:0, m:1) + 3 H_2O(c:0, m:1) = 5 HI(c:0, m:1) + 1 HI_3(c:0, m:1)$

Overall Rxn Energy [kJ / mol]: 585.75
2.2 Comproportionation of HIO$_3$ and HI

2.2.1 Literature$^6,7$ Path

\begin{align*}
\text{HIO}_3(c:0, m:1) + \text{HI}(c:0, m:1) & \rightarrow \text{HIO}_2(c:0, m:1) + \text{HIO}(c:0, m:1) \\
\text{HIO}_2(c:0, m:1) + \text{HIO}(c:0, m:1) + \text{HIO}(c:0, m:1) & \rightarrow \text{I}_2\text{O}(c:0, m:1) + \text{H}_3\text{IO}_3(c:0, m:1) \\
\text{I}_2\text{O}(c:0, m:1) + \text{H}_2\text{O}(c:0, m:1) & \rightarrow \text{HIO}(c:0, m:1) + \text{HIO}(c:0, m:1) \\
\text{HIO}(c:0, m:1) + \text{HI}(c:0, m:1) & \rightarrow \text{I}_2(c:0, m:1) + \text{H}_2\text{O}(c:0, m:1)
\end{align*}

Cost [a.u.]: 159.00697318658905

1 $\text{HIO}_3(c:0, m:1) + 2 \text{HI}(c:0, m:1) = 1 \text{H}_3\text{IO}_3(c:0, m:1) + 1 \text{I}_2(c:0, m:1)$

Overall Rxn Energy [kJ / mol]: -209.99

Barriers [kJ / mol]: [30.93, 46.13, 119.79, 39.91]

Max. Barrier [kJ / mol]: 119.79

2.2.2 Pathfinder Path

\begin{align*}
\text{HIO}_3(c:0, m:1) + \text{HI}(c:0, m:1) & \rightarrow \text{H}_2\text{IO}_3(c:0, m:1) \\
\text{H}_2\text{IO}_3(c:0, m:1) + \text{HI}(c:0, m:1) & \rightarrow \text{I}_2(c:0, m:1) + \text{H}_2\text{O}(c:0, m:1) + \text{HIO}_2(c:0, m:1)
\end{align*}

Cost [a.u.]: 24.695543461067764

1 $\text{HIO}_3(c:0, m:1) + 2 \text{HI}(c:0, m:1) = 1 \text{I}_2(c:0, m:1) + 1 \text{H}_2\text{O}(c:0, m:1) + 1 \text{HIO}_2(c:0, m:1)$

Overall Rxn Energy [kJ / mol]: -186.81

Barriers [kJ / mol]: [19.23, 24.23]

Max. Barrier [kJ / mol]: 24.23

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