SUPPORTING INFORMATION

The code and data resulting from this study can be found here https://github.com/jensengroup/RMSD_PP_TS and https://sid.erda.dk/sharelink/EPvv68fOTp, respectively. The data files contain the following information:

- run*i*_ts_guess_structures.tar.gz contains TS guess structures obtained by the RMSD-PP and GFN2xTB method in this study during the *i*th run.
- reactions_am.txt contains atom mapped reaction SMILES
- dft_ts_structures.tar.gz contains DFT TS structures for the 89 TSs found in this study as well as the two TSs found by Zimmerman which were not found by the presented procedure
- reactant_product_structures.tar.gz contains the reactant and product structures used as input structures (all 105 obtained from the work of Zimmerman^[11])

Timings

Table S1. examples of wall-times for the RMSD-PP part of the procedure. The examples are for the first parameter set (Table S2), run1, running on a single 2.67 GHz CPU. N_{trials} is the number of trials needed before the reaction completed

Reaction	N _{trials}	wall-time	
75	1	54 s	
55	4	3 min 17 s	

Parameter sets

Table S2. The two parameter sets tested. For each trial three runs are done with the k_{push} and k_{pull} , $1.5*k_{push}$ and $1.5*k_{push}$, and $2.25*k_{push}$ and $2.25*k_{pull}$. The direction is indicated as reactant (R) to product (P) or the other way around. The values were chosen empirically.

Parameter set 1					
Trial	$k_{pull}\left(E_{h} ight)$	$k_{push}\left(E_{h} ight)$	α (1/ a_0)	direction	l
1	-0.02	0.01	0.6	$R \longrightarrow P$	
2	-0.02	0.01	0.3	$P \longrightarrow R$	
3	-0.02	0.01	0.3	$R \longrightarrow P$	
4	-0.03	0.01	0.6	$P \longrightarrow R$	
5	-0.03	0.01	0.6	$R {\longrightarrow} P$	
Parameter set 2					
Trial	$k_{pull}\left(E_{h} ight)$	$k_{push}\left(E_{h} ight)$	α (1/ a_0)	direction	l
1	-0.02	0.008	0.6	$R \longrightarrow P$	
2	-0.02	0.01	0.3	$P \longrightarrow R$	
3	-0.02	0.01	0.3	$R \longrightarrow P$	
4	-0.03	0.01	0.6	$P \longrightarrow R$	
5	-0.03	0.01	0.6	$R {\longrightarrow} P$	

Reactions

	Reaction	Comments
1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
2	$\begin{array}{c} H:B & H:7 & H:5 & H:12 \\ N:1^{\oplus -}B:2^{\oplus} & + & N:3^{\oplus -}B:2^{\oplus} \\ H:9 & H:6 & H:10 & H:11 \end{array} \longrightarrow \begin{array}{c} H:1^{\oplus} H:9 \\ H:5 & N:3^{\oplus} - H:2^{\oplus} H:2^{\oplus} H:6 \\ H:10 & H:12 \\ H:10 & H:12 \\ H:7 \end{array}$	
3	$ \begin{array}{c} H:8 & H:7 \\ H:9 & H:6 \\ H:9 & H:6 \end{array} + \begin{array}{c} H:5 \\ H:10 \\ H:11 \end{array} \xrightarrow{H:10} H:12 \\ H:10 \\ H:11 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:5 \\ H:9 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:5 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:9 \\ H:6 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:9 \\ H:9 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:9 \\ H:9 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:9 \\ H:9 \\ H:9 \\ H:10 \end{array} \xrightarrow{H:10} \begin{array}{c} H:12 \\ H:9 \\ H:10 \\ H:$	
4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
6	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	TS could not be con- firmed to exist by IRC
7	$\begin{array}{c} H:8 & H:7 \\ H:9 & H:6 \\ H:9 & H:6 \end{array} + \begin{array}{c} H:5 \\ H:10 \\ H:11 \end{array} \xrightarrow{H:10} H:7 \\ H:11 \end{array} \xrightarrow{H:9} H:6 \\ H:11 \\ H:11 \end{array} \xrightarrow{H:10} H:7 \\ H:5 \\ H:12 \\ H:11 \\ H:11 \\ H:11 \end{array}$	
8	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
9	$ \begin{array}{c} \overset{H:11}{\underset{B:3}{\leftarrow},H,0} \\ \overset{H:12}{\underset{H:12}{\times},H,13} \end{array} + \begin{array}{c} \overset{H:9}{\underset{H:10}{\times},H,0} \\ \overset{H:9}{\underset{H:10}{\times},H,0} \\ \overset{H:10}{\underset{H:10}{\times},H,0} \\ \overset{H:12}{\underset{H:10}{\times},H,0} \\ \overset{H:12}{\underset{H:10}{\underset{H:10}{\times},H,0} \\ \overset{H:12}{\underset{H:10}{H$	
10	$\begin{array}{c} H:11 & H:14 & H:9 & H.7 \\ B:S^{2} N:0^{6} & + H:8 - B:2^{6} N:0^{6} - H:5 & & H:10 - B:3^{6} N:0^{6} - H:5 & + H:10^{1} B:3^{6} \\ H:12 & H:13 & H:10 & H:6 & & H:12 & H:3 \end{array}$	TS could not be con- firmed to exist by IRC
11	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	TS could not be con- firmed to exist by IRC
12	$ \begin{array}{c} \overset{H_{11}}{\underset{\substack{0 \leq r_{H_{12}}\\H_{12}\\H_{12}\\H_{13}\\$	

Table S3. Table of the 100 studied reactions. Note that Zimmerman's numbering is retained, so some numbers are non-consecutive.

13	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} H_{21} \\ g = g = g \\ H_{12} \\ H_{13} \end{array} \end{array} \begin{array}{c} H_{10} \\ H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \end{array} \begin{array}{c} H_{10} \\ H_{10} \\ H_{10} \end{array} \end{array}$	
14	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
15	$\begin{array}{c} \begin{array}{c} & & & & \\ H_{:11} & H_{:14} & & H_{:9} & H_{:7} \\ & & & \\ H_{:12} & H_{:13} & & \\ H_{:10} & H_{:6} & & \\ H_{:10} & H_{:6} & & \\ H_{:10} & H_{:6} & & \\ H_{:10} & H_{:11} & \\ H_{:11} & H_{:11} & \\ \end{array}$	
16	$\substack{H:12 \\ H:12 \\ H:13 \\ H:14 \\ H:10 \\ H:16 \\ H:10 \\ H:16 \\ H:10 \\ H:16 \\ H:10 \\ H:1$	TS confirmed to exist but was not found by the pro- cedure
17	$\begin{array}{c} \begin{array}{c} H_{11}^{(1)} \\ & & \\ H_{14}^{(2)} \\ & & \\ H_{15}^{(2)} \\ & & \\ H_{15}^{(2)} \end{array} \xrightarrow{0.6} \\ & & \\ H_{11}^{(2)} \\ & & \\ H_{11}^{(2)} \end{array} \xrightarrow{0.6} \\ & & \\ H_{11}^{(2)} \\ & & \\ $	
18	$\begin{array}{c} \begin{array}{c} \begin{array}{c} & H:1 \\ & & \\ & \\ H:4 \end{array} \end{array} \xrightarrow{0.6} H:7 \\ H:5 \end{array} + \begin{array}{c} H:10 \\ & \\ & \\ H:11 \end{array} \xrightarrow{0.8} \\ & \\ H:11 \end{array} \xrightarrow{0.8} \begin{array}{c} H:10 \\ & \\ & \\ & \\ & \\ H:11 \end{array} \xrightarrow{0.6} H:7 \\ & \\ & \\ & \\ H:11 \end{array}$	
19	$\begin{array}{c} H_{11}^{+1} & H_{11}^{-1} \\ H_{12}^{-1} - C_{13}^{-1} - C_{13}^{-$	Same bonds broken/- formed as 22 but to different conformations
20	$\begin{array}{c} \begin{array}{c} H:1\\ H:4\\ H:5\\ H:5\end{array} + H:10\\ H:11\end{array} \xrightarrow{H:10} \begin{array}{c} H:1\\ H:10\\ H:11\\ H:11\end{array} \xrightarrow{H:10} \begin{array}{c} H:1\\ H:1\\ H:11\\ H:11\\ H:5\end{array} \xrightarrow{H:10} \begin{array}{c} H:1\\ H:1\\ H:11\\ H:7\end{array}$	TS could not be con- firmed to exist by IRC
21	$ \begin{array}{c} \overset{H_{1}}{\underset{H_{2}}{\overset{0.6}{\underset{H_{5}}{}}}} \\ \overset{H_{1}}{\underset{H_{5}}{}} \end{array} + \overset{H_{10}}{\underset{H_{11}}{\overset{0.6}{\underset{H_{11}}{}}}} \\ \overset{H_{10}}{\underset{H_{11}}{}} \end{array} \longrightarrow \begin{array}{c} \overset{H_{11}}{\underset{H_{14}}{\overset{0.6}{\underset{H_{5}}{}}}} \\ \overset{H_{11}}{\underset{H_{15}}{}} \\ \overset{H_{10}}{\underset{H_{10}}{}} \end{array} $	
22	$\begin{array}{c} H_{11}^{+1} \\ H_{14}^{-C^{2}} \gtrsim c_{13}^{-C^{2}} - C_{13}^{-C^{2}} + H_{11}^{-C^{2}} \\ H_{15}^{-C^{2}} + H_{11}^{-C^{2}} + H_{11}^{-C^{2}} \\ H_{11}^{-C^{2}} + H_{11}^{-$	Same bonds broken/- formed as 19 but to different conformations
23	$ \begin{array}{c} H_{11} \\ H_{22} \\ H_{23} \\ H_{2$	
24	$\begin{array}{c} H_{11}^{+1} & H_{11}^{+1} & H_{11}^{+1} \\ H_{14}^{-2} \geq c_{13}^{-2} = c_{13}^{-2} + H_{11}^{-2} + H_{111}^{-2} & H_{11}^{-2} = c_{13}^{-2} + H_{111}^{-2} + H_{111}^$	
25	$\begin{array}{c} \begin{array}{c} H_{11} \\ \\ H_{14} \\ \\ H_{15} \\ \end{array} \begin{array}{c} 0.6 \\ \\ H_{15} \\ \end{array} \begin{array}{c} H_{11} \\ \\ H_{12} \\ \end{array} \begin{array}{c} 0.6 \\ \\ H_{11} \\ \\ H_{11} \\ \end{array} \begin{array}{c} H_{11} \\ \\ H_{12} \\ \\ H_{12} \\ \end{array} \begin{array}{c} 0.6 \\ \\ H_{12} \\ \\ H_{12} \\ \end{array} \end{array}$	

26	$ \begin{array}{c} \begin{array}{c} H_{1}^{-1} \\ H_{2}^{-1} \\ H_{2}^{-1} \\ H_{2}^{-1} \\ H_{2}^{-1} \end{array} + \begin{array}{c} H_{1}^{-1} \\ H_{2}^{-1} \\ H_{2}^{-1} \\ H_{2}^{-1} \end{array} \end{array} \xrightarrow{H_{2}^{-1} \\ H_{2}^{-1} \\ H_{2}^{-1} \\ H$	
27	$ \begin{array}{c} \begin{array}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & & \\ & & & \\ \end{array} \xrightarrow{\begin{subarray}{c} & \\$	
28	$\begin{array}{c} H_{11}^{+1} & & H_{11}^{-1} \\ H_{12}^{-1} & & H_{12}^{-1} \\ H_{13}^{-1} & & H_{13}^{-1} \\$	
29	$\begin{array}{c} H:1 \\ H:1 \\ H:4 \\ H:5 \\ H:5 \\ H:1 \\ H:1 \\ H:7 \\ H:5 \\ H:1 \\ H:1 \\ H:7 \\ H:5 \\ H:1 \\ H:7 \\ H:5 \\ H:4 \\ H:7 \\ H:5 \\ H:4 \\ H:7 \\ H:5 \\ H:4 \\ H:7 \\ H:7 \\ H:5 \\ H:4 \\ H:7 \\$	
30	$ \begin{array}{c} \overset{H_{13}}{\underset{H_{14}}{\underset{H_{11}}{\underset{H_{14}}}{H_{14$	
31	$\underset{\substack{H:15}{H_{13}}}{\overset{H_{13}}{\underset{H:14}{H_{11}}}} \underset{\substack{H:15}{f_{13}}}{\overset{H_{12}}{\underset{H:15}{f_{13}}}} \underset{\substack{H:15}{f_{13}}}{\overset{H_{13}}{\underset{H:15}{f_{13}}}} \underset{\substack{H:15}{f_{13}}}{\overset{H_{13}}{\underset{H:15}{f_{13}}}}} \underset{\substack{H:15}{f_{13}}}{\overset{H_{13}}{\underset{H:15}{f_{13}}}} \underset{\substack{H:15}{f_{13}}}{\underset{H:15}{f_{13}}}} \underset{\substack{H:15}{f_{13}}}{\underset{H:15}{f_{13}}} \underset{\substack{H:15}{f_{13}}}}{\underset{H:15}{f_{13}}}} \underset{\substack{H:15}{f_{13}}}}{\underset{H:15}{f_{13}}} \underset{\substack{H:15}{f_{13$	
32	$ \begin{array}{c} \begin{array}{c} H_{113} \\ H_{115} \\ H_{29} \\ H_{21} \\ H_{111} \\ H_{111} \end{array} \begin{array}{c} 0.3 \\ P_{2} \\ P_{2$	
33	$\begin{array}{c} 0:3 \\ C:2 - C:1 - H:4 \\ H:6 \\ H:5 \end{array}$ $\begin{array}{c} H:4 \\ H:5 \\ H:5 \end{array}$ $\begin{array}{c} 0:3 \\ H:5 \\ H:5 \end{array}$ $\begin{array}{c} H:4 \\ C:1 - C:2 \\ H:5 \\ H:6 \end{array}$	
34	$\begin{array}{c} H:3 & H:8 \\ H:1 - C:2 - C:4 - H:6 \\ H:5 & H:7 \end{array} H:1 + H:8 + H:6 - H:5 + H:7 + H:7 + H:6 - H:5 + H:7 + H:6 - H:7 + H:6 - H:5 + H:7 + H:6 - H:7 + H:6 - H:7 + H:7$	
35	$F:10 \qquad \qquad$	TS could not be con- firmed to exist by IRC
36	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
37	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
38	$\overset{H:5}{\underset{H:6}{\leftarrow}} + \overset{H:7}{\underset{H:8}{\overset{H:4}{\longrightarrow}}} \overset{H:4}{\underset{H:8}{\longrightarrow}} \xrightarrow{H:6} \overset{H:6}{\underset{H:8}{\leftarrow}} + \overset{H:5}{\underset{H:8}{\overset{N_3}{\longrightarrow}}} \overset{H:4}{\underset{H:7}{\overset{N_3}{\longrightarrow}}} + \overset{H:5}{\underset{H:7}{\overset{N_3}{\longrightarrow}}} \overset{H:4}{\underset{H:7}{\overset{N_3}{\longrightarrow}}}$	

39	$ \begin{array}{c} H:3 \\ C:1 \\ H:4 \end{array} \longrightarrow 0:2^{\Theta} = C:1^{\Theta} + H:4 - H:3 $	
40	$\begin{array}{c} H:5 \\ & & \\ H:6 \end{array} \qquad \begin{array}{c} H:7 \\ & & \\ H:8 \end{array} \qquad \begin{array}{c} H:4 \\ & & \\ H:8 \end{array} \qquad \begin{array}{c} H:8 \\ & & \\ H:4 \end{array} \qquad \begin{array}{c} H:8 \\ & & \\ H:4 \end{array} \qquad \begin{array}{c} H:7 \\ & & \\ H:4 \end{array} \qquad \begin{array}{c} H:7 \\ & & \\ H:5 \end{array} \qquad \begin{array}{c} H:7 \\ & & \\ H:6 \end{array} \qquad \begin{array}{c} H:7 \\ & & \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ & \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \\ H:7 \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \\ H:7 \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \\ H:7 \\ H:7 \\ H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7 \end{array} \qquad \begin{array}{c} H:7 \\ H:7$	
41	$\begin{array}{ccccccc} H:5 & & & H:7 & & H:4 \\ & & & & & \\ H:6 & & & H:8 \end{array} \longrightarrow \begin{array}{ccccccccccccccccccccccccccccccccccc$	
42	$\begin{array}{c} H:13 \\ H:4 \\ H:5 \\ H:3 \\ H:10 \\ H:11 \end{array} \xrightarrow{(-1)}{$	
43	$\begin{array}{c} H:13 \\ H:4 \\ H:5 \\ H:5 \\ H:3 \\ H:10 \\ H:11 \end{array} \xrightarrow{(2)^{-2} + 12}_{H:9} \\ H:10 \\ H:$	
44	$\begin{array}{c} \overset{H:13}{\underset{H:5}{\overset{(2)}{\underset{H:10}{\overset{(2)}{\underset{H:10}{\overset{(2)}{\underset{H:11}{\overset{(2)}{\underset{H:12}{\underset{H:12}{\overset{(2)}{\underset{H:12}{\underset{H:12}{\overset{(2)}{\underset{H:12}{\atop{H:12}{\underset{H:12}{\atop_{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\atop_{H:12}{\underset{H:12}{\atop_{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\atop_{H:12}{\underset{H:12}{\atop_{H:12}{\atop_{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\underset{H:12}{\atop_{H:12}{\underset{H:12}{\atop_{H:12}{\atop_{H:12}{\underset{H:12}{\atop_{H:12}{\underset{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{\atop_{H:12}{$	
45	$\begin{array}{c} H:13 \\ H:4 \\ H:5 \\ H:5 \\ H:3 \\ H:11 \end{array} \xrightarrow{(-2)}{(-2)} (-1) (-1) (-1) (-1) (-1) (-1) (-1) (-1)$	
46	$\begin{array}{c} H:13 \\ H:4 \\ F:2 \\ H:5 \\ H:3 \\ H:10 \\ H:11 \end{array} \xrightarrow{(1,2)} F:12 \\ H:10 \\ H:9 \\ H:9$	
47	$\begin{array}{c} \begin{array}{c} \begin{array}{c} +1.3 \\ +.10 \\15 \\ +.10 \\ +.10 \\15 \end{array} \begin{array}{c} +1.4 \\ +.10 \\15 \end{array} \begin{array}{c} +.14 \\ +.12 \\15 \end{array} \begin{array}{c} +.14 \\ +.12 \end{array} \begin{array}{c} +.14 \\ +.12 \\12 \end{array} \end{array}$	
48	$\underset{\substack{H_{2} \\ H_{3} \\ H_{6} \\ H_{10} \\ H_{11} \\ H_{12} \\ $	
49	$ \begin{array}{c} \overset{H:13}{\underset{H:6}{\overset{H:13}{\underset{H:6}{\underset{H:6}{\underset{H:11}{\underset{H:11}{\underset{H:11}{\underset{H:12}{\underset{H:6}{\underset{H:6}{\underset{H:12}{H$	
50	$\overset{\text{H}_{13}}{\underset{\text{H}_{6}}{\overset{\text{H}_{13}}{\underset{\text{H}_{11}}{\overset{\text{H}_{13}}{\underset{\text{H}_{11}}{\overset{\text{H}_{12}}{\underset{\text{H}_{12}}{\overset{\text{H}_{12}}{\underset{\text{H}_{11}}{\overset{\text{H}_{12}}{\underset{\text{H}_{11}}{\overset{\text{H}_{12}}{\underset{\text{H}_{12}}{\overset{\text{H}_{12}}{\underset{\text{H}_{11}}{\overset{\text{H}_{12}}{\underset{H}_{11}}{\overset{H}_{12}}{\overset{H}_{12}}{\overset{H}_{12}}{\overset{H}_{12}}{\overset{H}_{12}}{\underset{H}_{11}}{\overset{H}_{12}}{H$	
51	$ \begin{array}{c} \overset{H_{13}}{\underset{H_{4}}{\overset{H_{13}}{\underset{H_{6}_{H_{10}} \overset{H_{13}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\underset{H_{11}}{\underset{H_{11}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{11}}{\underset{H_{11}}{\underset{H_{12}}{\underset{H_{11}}{\underset{H_{11}}{\overset{H_{12}}{\underset{H_{12}}{\underset{H_{11}}{\underset{H_{11}}{\underset{H_{12}}{\underset{H_{12}}{\underset{H_{12}}{\underset{H_{11}}{\underset{H_{11}}{\underset{H_{12}}{$	

52	$ \begin{array}{c} \begin{array}{c} & & & & & \\ & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ &$	
53	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} & H_{13} \\ H_{7} \\ H_{8} \\ H_{8} \\ H_{11} \end{array} \end{array} \begin{array}{c} H_{12} \\ H_{11} \end{array} \end{array} \begin{array}{c} \begin{array}{c} H_{13} \\ H_{12} \\ H_{11} \end{array} \end{array} \begin{array}{c} \begin{array}{c} H_{13} \\ H_{13} \\ H_{11} \end{array} \end{array} \begin{array}{c} \begin{array}{c} H_{13} \\ H_{13} \\ H_{11} \end{array} \end{array} \begin{array}{c} \begin{array}{c} H_{13} \\ H_{13} \\ H_{12} \end{array} \begin{array}{c} H_{13} \\ H_{12} \end{array} \begin{array}{c} H_{13} \\ H_{13} \\ H_{12} \end{array} \begin{array}{c} H_{13} \\ H_{13} \end{array} \begin{array}{c} H_{13} \\ H_{13} \end{array} \begin{array}{c} H_{13} \\ H_{13} \\ H_{12} \end{array} \end{array} \begin{array}{c} H_{13} \\ H_{13} \\ H_{12} \end{array} \end{array} \begin{array}{c} H_{13} \\ H_{13} \\ H_{13} \end{array} \end{array} $	
54	$\overset{H:13}{\underset{H:8}{\overset{H:13}{\underset{H:0}{\overset{G_{1}}{\underset{H:11}{\overset{H:12}{\underset{H:11}{\overset{H:14}{\underset{H:11}{\overset{H:14}{\underset{H:11}{\overset{H:14}{\underset{H:12}{\overset{H:14}{\underset{H:12}{\overset{H:14}{\underset{H:12}{\overset{H:14}{\underset{H:12}{\overset{H:14}{\underset{H:12}{\overset{H:14}{\underset{H:11}{\overset{H:14}{\underset{H:12}{\overset{H:14}{\underset{H:11}{\underset{H:11}{\overset{H:14}{\underset{H:11}{\underset{H:11}{\overset{H:14}{\underset{H:11}{\underset{H:11}{\overset{H:14}{\underset{H:11}{\underset{H:11}{\overset{H:14}{\underset{H:11}{\underset{H:11}{\underset{H:11}{\overset{H:14}{\underset{H:111}{\underset{H:111}{\underset{H:11}{\underset{H:111}{\underset{H:11}{\underset{H:111}{\underset{H:11}{\underset{H:11}{\underset{H:11}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:11}{\underset{H:111}{\underset{H:11}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:111}{\underset{H:11}{\underset{H:11}{\underset{H:11}{\underset{H:11}{H:1$	TS could not be con- firmed to exist by IRC
55	$ \begin{array}{c} \begin{array}{c} & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$	
56	$\begin{array}{c} H:5 \\ C_{1} \\ H:6 \\ H:6 \end{array} + \begin{array}{c} H:10 \\ H:9 \\ O:4 \\ H:8 \end{array} \xrightarrow{H:7} H:7 \\ H:8 \\ H:8 \\ O:2 \\ H:8 \\ O:2 \\ H:5 \end{array}$	
57	$\begin{array}{c} H:5 \\ C:1 \\ H:6 \\ H:6 \\ H:7 \\ H:8 \\ H:7 \\ H:8 \\ H:7 \\$	
58	$\overset{H:5}{\underset{H:6}{\overset{C1}{\longrightarrow}}} + \overset{H:10}{\underset{H:8}{\overset{H:7}{\longrightarrow}}} + \overset{H:7}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{H:7}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{H:7}{\underset{H:6}{\overset{C1}{\longrightarrow}}} + \overset{H:8}{\underset{H:10}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:10}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{C1}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{O.4}{\longrightarrow}}} + \overset{O.4}{\underset{H:8}{\overset{O.4}{$	
59	$\overset{\text{H:5}}{\underset{\text{H:6}}{\overset{\text{C}2}{\overset{\text{C}2}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:7}}{\overset{\text{H:8}}{\overset{H:8}}{\overset{H:8}}\overset{\overset{H:8}}{\overset{H:8}}{\overset{H:8}}{\overset{H:8}}{\overset{H:8}}$	
60	$ \underset{H,6}{\overset{H,2}{\underset{H,6}{\overset{O,2}{\overset{H}}}}} + \underset{H,6}{\overset{H,20}{\underset{H,8}{\overset{H,7}{\overset{H}}}}} + \underset{H,6}{\overset{H,20}{\underset{H,8}{\overset{H,7}{\overset{H}}}} + \underset{H,7}{\overset{H,7}{\underset{H,8}{\overset{H,7}{\overset{H}}}} + \underset{H,7}{\overset{H,7}{\underset{H,8}{\overset{H,7}{\overset{H,7}{\overset{H}}}}} + \underset{H,7}{\overset{H,7}{\underset{H,8}{\overset{H,7}{\overset{H}}{\overset{H,7}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}{\overset{H}}}{\overset{H}}}}}}}}$	
61	$\begin{array}{ccccccc} H:5 & & & & H:10 \\ H:5 & & & & H:9 \\ H:6 & & & & H:9 \\ H:6 & & & & H:8 \end{array} \xrightarrow{H:7} & & & H:7 \\ H:7 & & & & H:7 \\ H:7 & & & & H:7 \\ H:8 & & & & H:7 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9 \\ H:8 & & & & H:9 \\ H:7 & & & & H:9 \\ H:8 & & & & H:9$	
62	$\begin{array}{c} \begin{array}{c} H:6 \\ H:8 \\ H:7 \\ H:7 \\ H:9 \end{array} \xrightarrow{H:10} H:10 \\ H:9 \\ H:9 \\ H:7 \\ H:9 \\ H:7 \\ H:5 \end{array}$	
63	$\begin{array}{c} H:6 \\ H:8 \\ H:7 \\ H:7 \\ H:7 \\ H:9 \end{array} \xrightarrow{H:10} H:10 \\ $	
64	$\begin{array}{c} \begin{array}{c} H:6 \\ H:6 \\ H:8 \\ H:7 \\ H:7 \\ H:9 \end{array} \xrightarrow{H:10} H:10 \\ H:8 \\ H:7 \\ H:9 \\ H:7 \\ H:9 \end{array} H:6 \\ H:6 \\ H:10 \\ H:8 \\ H:7 \\ H:9 \\ $	

65	$\begin{array}{c} \begin{array}{c} H:6 \\ H:8 \\ H:7 \\ H:7 \\ H:7 \\ H:9 \end{array} \xrightarrow{H:10} H:10 \\ H:8 \\ H:7 \\ H:9 \\ H:7 \\ H:11 \end{array} \xrightarrow{H:10} H:10 \\ H:8 \\ H:7 \\ H:11 \\ H:8 \\ H:7 \\ H:11 \\ H:9 \\ H:7 \\ H:11 \\ H:11 \\ H:9 \\ H:7 \\ H:11 \\ H:7 \\ H:11 \\ H:9 \\ H:7 \\ H:11 \\ H:7 \\ H:7 \\ H:7 \\ H:7 \\ H:7 \\ H:11 \\ H:7 \\ H:$	
66	$\begin{array}{c} \begin{array}{c} \begin{array}{c} H:11 \\ C:12^{-}C:13 \\ H:14 \\ H:15 \end{array} \\ \begin{array}{c} H:16 \\ H:19 \\ H:2 \end{array} \\ \begin{array}{c} H:10 \\ H:7 \\ H:16 \\ $	
67	$\begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} H:2\\ H:3\\ H:3\\ \end{array} \end{array} \xrightarrow{H:2} \begin{array}{c} H:8\\ H:7\\ H:6 \end{array} \xrightarrow{H:7} \begin{array}{c} H:6\\ H:7\\ H:8\\ H:3\\ \end{array} \xrightarrow{H:7} \begin{array}{c} H:2\\ H:3\\ H:9 \end{array} \xrightarrow{H:7} \begin{array}{c} H:7\\ H:8\\ H:3\\ H:9 \end{array}$	
68	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	TS could not be con- firmed to exist by IRC
69	$\begin{array}{cccc} H:3 & & H:4 \\ H:3 & & H:2 \\ Si:1 & & H:5 \\ H:5 & & H:4 \end{array} \longrightarrow \begin{array}{c} H:4 \\ H:3 - Si:1 - H:2 \\ H:5 \end{array}$	
70	$H_{0,2}H_{1} + O_{3,2}H_{1} + O_{3$	
71	$\begin{array}{c} H_{11}^{H_{11}} & 0.6 \\ C_{12} \gtrsim C_{13} \\ H_{15} \\ H_{15} \end{array} \xrightarrow{\begin{array}{c} 0.6 \\ H_{17} \\ H_{15} \\ H_{15} \\ H_{15} \end{array}} \xrightarrow{\begin{array}{c} 0.6 \\ H_{17} \\ C_{13} \\ H_{15} \\ H_{14} \end{array}} \xrightarrow{\begin{array}{c} 0.6 \\ H_{17} \\ C_{13} \\ H_{15} \\ H_{14} \end{array}}$	
72	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
73	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
74	$\begin{array}{c} H_{13} \\ H_{11} \\ H_{13} \\ H_{13} \\ H_{12} \\ H_{13} \\ H_{12} \\ H_{13} \\ H_{13$	
75	$\begin{array}{c} \begin{array}{c} \begin{array}{c} H:16\\ H:2\\ H:9\\ H:9\\ H:7\\ H:15\end{array} \end{array} \xrightarrow{H:16} H:10\\ H:12\\ H:16\\ H:16\\ H:17\end{array} \xrightarrow{H:10} H:12\\ H:12\\ H:12\\ H:12\\ H:14\\ H:12\\ H:14\\ H:16\\ H:7\end{array}$	
76	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
77	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	

78	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
79	$ \begin{array}{c} \overset{H_{3}}{\underset{H_{9}}{\overset{H_{16}}{\overset{G_{12}}{\overset{G_{12}}{\overset{G_{12}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{11}}{\overset{H_{16}}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}}{\overset{H_{16}}}{\overset{H_{16}}{\overset{H_{16}}{\overset{H_{16}}{H_{1$	
80	$ \begin{array}{c} \overset{H:8}{\underset{H:9}{\overset{H:16}{\underset{H:15}{\overset{G_{1}}{\underset{H:15}{\overset{G_{2}}{\underset{H:15}{\overset{H:14}{\underset{H:11}{\overset{H:10}{\underset{H:11}{\overset{H:10}{\underset{H:11}{\overset{H:10}{\underset{H:11}{\underset{H:11}{\overset{H:12}{\underset{H:11}{\overset{H:13}{\underset{H:11}{\overset{H:13}{\underset{H:11}{\overset{H:13}{\underset{H:11}{\underset{H:11}{\overset{H:13}{\underset{H:11}{\overset{H:13}{\underset{H:11}{\underset{H:11}{\overset{H:13}{\underset{H:11}{\underset{H:11}{\overset{H:13}{\underset{H:15}{H:15$	
81	$ \begin{array}{c} \overset{H:8}{\underset{H:9}{\overset{G:1}{\underset{H:7}{\overset{C3}{\underset{H:7}{\overset{C3}{\underset{H:15}{\overset{H:14}{\underset{H:11}{\overset{H:10}{\underset{H:11}{\overset{H:10}{\underset{H:11}{\overset{H:10}{\underset{H:12}{\underset{H:12}{\overset{H:13}{\underset{H:12}{\underset{H:12}{\overset{H:13}{\underset{H:12}{\underset{H:12}{\overset{H:13}{\underset{H:12}{\underset{H:12}{\overset{H:13}{\underset{H:12}{\underset{H:12}{\overset{H:13}{\underset{H:12}{\underset{H:12}{\overset{H:13}{\underset{H:12}$	
82	$\overset{H:8}{\underset{H:9}{\overset{H:16}{\underset{C2}{\overset{C3}{\underset{C2}{\overset{C3}{\underset{H:15}{\overset{H:16}{\underset{H:11}{\overset{H:10}{\underset{H:16}{\underset{H:16}{\underset{H:16}{\overset{H:13}{\underset{H:16}{\underset{H:16}{\overset{H:13}{\underset{H:16}{\underset{H:16}{\overset{H:13}{\underset{H:16}{H:16$	
83	$ \begin{array}{c} \overset{H_{1}8}{\underset{H_{2}7}{\overset{H_{1}16}{\underset{H_{1}7}{\overset{H_{1}16}{\underset{H_{1}5}{\overset{H_{1}16}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{2}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}}{\underset{H_{1}1}{\underset{H_{1}1}{\underset{H_{1}1}{H_$	
84	$ \begin{array}{c} \overset{H_{8}}{\underset{H_{7}}{\overset{H_{16}}{\underset{H_{15}}{\overset{G}{\underset{H_{15}}{\overset{H_{14}}{\underset{H_{15}}{\overset{H_{14}}{\underset{H_{11}}{\overset{H_{10}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{12}}{\overset{H_{13}}{\underset{H_{13}}{\underset{H_{13}}{\underset{H_{13}}{\overset{H_{13}}{\underset{H_{13}}}{\underset{H_{13}}{\underset{H_{13}}}{\underset{H_{13}}{\underset{H_{13}}}{\underset{H_{13}}}{\underset$	TS confirmed to exist but was not found by the pro- cedure
85	$ \begin{array}{c} \overset{\mu_{3}}{\underset{\mu_{3}}{\overset{\mu_{16}}{\underset{\mu_{7}}{\overset{\mu_{16}}{\underset{\mu_{15}}{\overset{\mu_{14}}{\underset{\mu_{11}}{\underset{\mu_{11}}{\underset{\mu_{12}}{\underset$	
85	$ \begin{array}{c} \overset{\mu_{3}}{\underset{n_{3}}{\overset{\mu_{12}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{13}}{\overset{\mu_{14}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}{\underset{n_{12}}{\overset{\mu_{13}}{\underset{n_{12}}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}}{\underset{n_{12}}{\underset{n_{12}}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}}{\underset{n_{12}}}{\underset{n_{12}}{\underset{n_{12}}{\underset{n_{12}}}{n$	
85 86 87	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \\ \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \\ \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \end{array} \\ \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \end{array} \\ \begin{array}{c} \\ \\ \end{array} \end{array} \\ \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \end{array} \\ \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \end{array} \end{array} \\ \begin{array}{c} \\ \end{array} \end{array} \\ \begin{array}{c} \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \end{array} \end{array} \\ \end{array} \end{array} \\ \begin{array}{c} \\ \end{array} \end{array} \end{array} \\ \begin{array}{c} \\ \end{array} \end{array} \end{array} \\ \end{array} \end{array} \\ \begin{array}{c} \\ \end{array} \end{array} \end{array} \\ \end{array} \end{array} \\ \begin{array} \end{array} \end{array} \\ \begin{array} \end{array} \end{array} \\ \begin{array} \end{array} \end{array} \\ \begin{array}{c} \end{array} \end{array} \end{array} \end{array} \\ \end{array} \end{array} \\ \end{array} \end{array} \end{array} \end{array} \end{array} \\ \end{array} \end{array} \\ \end{array} \end{array}$	
85 86 87 88	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c}$	
85 86 87 88 89	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c}$	

91	$\underset{\substack{H_{12} \\ H_{12} \\ H_{11} \\ H_{14} \\ H_{14} \\ H_{16} \\ H_{16}$	
92	$\underset{\substack{H_{12} \\ H_{12} \\ H_{14} \\ H_{14} \\ H_{16} \\ H_{17} \\ H_{16} \\ H_{17} \\ H_{17} \\ H_{17} \\ H_{17} \\ H_{17} \\ H_{18} \\ H_{16} \\ H_{17} \\ H_{17} \\ H_{18} \\ H_{16} \\ H_{17} \\ H_{18} \\ H_{18} \\ H_{17} \\ H_{18} \\ H_{18} \\ H_{17} \\ H_{18} \\ H_{18}$	Same bonds broken/- formed as 93 but to different conformations
93	$\underset{\substack{H_{12} \\ H_{12} \\ H_{14} \\ H_{14} \\ H_{16} \\ H_{16}$	Same bonds broken/- formed as 92 but to different conformations
96	$\begin{array}{c} \begin{array}{c} \begin{array}{c} H_{11}^{+1} & H_{11}^{-1} \\ H_{12}^{-1} & H_{12}^{-1} \\ H_{12}^{-1} \\$	TS could not be con- firmed to exist by IRC
97	$\begin{array}{c} \begin{array}{c} \begin{array}{c} H_{11}^{+1} & H_{11}^{+1} \\ H_{12} & H_{11}^{-1} & H_{12}^{-1} \\ H_{12} & H_{12}^{-1} \\ H_{12} & H_{12}^{-1} \\ H_{12} & H_{12}^{-1} \end{array}$	
98	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
99	$ \begin{array}{c} \overset{H_{18}}{\underset{_{H_{21}}}{\overset{_{H_{13}}}{\underset{_{H_{26}}}{\overset{_{H_{13}}}{\underset{_{H_{26}}}{\overset{_{H_{13}}}{\underset{_{H_{26}}}{\overset{_{H_{26}}}{\underset{_{H_{26}}}{\underset{_{H_{26}}}{\overset{_{H_{26}}}{\underset{_{H_{26}}}{\underset{_{H_{26}}}{\overset{_{H_{26}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}{\underset{_{H_{16}}}}{\underset{_{H_{16}}}$	
100	$\begin{array}{c} \begin{array}{c} H_{12}^{10} & H_{13}^{10} \\ H_{20}^{-10} c_{11}^{-1} & H_{14}^{11} \\ H_{20}^{-10} c_{11}^{-1} & H_{14}^{11} \\ H_{20}^{-10} & H_{14}^{-10} \\ H_{21}^{-10} & H_{14}^{-10} \\ H_{21}^{-10} & H_{14}^{-10} \\ H_{21}^{-10} & H_{21}^{-10} \\ H_{21}^{-10} \\ H_{21}^{-10} \\ H_{2$	
101	$\begin{array}{c} \begin{array}{c} H_{18} & H_{13} & H_{14} \\ H_{20} & C_{10} & C_{11} \\ C_{11} & C_{12} \\ H_{21} & H_{16} \\ H_{21} & H_{16} \\ H_{21} & H_{16} \\ H_{21} \\ $	
102	$\underset{\substack{n=1\\n=1}}{\overset{n+1}{\underset{n=1}{n}}} \underset{\substack{n=1\\n=1}{n}}{\overset{n+1}{\underset{n=1}{n}}} + \underset{\substack{n=1\\n=1}{n}}{\overset{n+1}{\underset{n=1}{n}}} + \underset{\substack{n=1\\n=1\\n=1}{n}}{\overset{n+1}{\underset{n=1}{n}}} + \underset{\substack{n=1\\n=1\\n=1}{n}}{\overset{n+1}{\underset{n=1\\n=1}{n}}} + \underset{\substack{n=1\\n=1\\n=1}{n}}{\overset{n+1}{\underset{n=1\\n=1}{n}}} + \underset{\substack{n=1\\n=1\\n=1}{n}}{\overset{n+1}{\underset{n=1\\n=1}{n}}} + \underset{\substack{n=1\\n=1\\n=1}{n}}{\overset{n+1\\n=1\\n=1\\n=1}{n}} + \underset{\substack{n=1\\n=1\\n=1\\n=1}{n}}{\overset{n+1\\n=1\\n=1\\n=1\\n=1\\n=1}{n}}{n+1\\n=1\\n=1\\n=1\\n=1\\n=1\\n=1\\n=1\\n=1\\n=1\\n=$	

Table S4. Table of the 9 reactions where a TS could not be confirmed

#	Туре	Reaction/Structure	Comments
6	intended	$\begin{array}{c} \bigoplus_{H \\ H_2N \\ H \\ $	A minimum is found at the indicated
6	interme- diate	H ₂ N H H H ₂ N H H	structure. The TS correspond to a conformational change





#	Туре	Reaction/Structure	Comments
30	intended	H H H H H H H H H H	TS correspond to different but similar reaction. The H from ammonia goes
30	Other reaction	$F_{3}C$ H H H $F_{3}C$ H $H_{2}N$ H H $H_{2}N$ H H $H_{2}N$ H H H $H_{2}N$ H	to the carbonyl oxygen atom instead
34	intended		No re-optimization: Both sides of IRC go to product Re-optimization: TS
34	Other reaction		reaction
40	intended	$H \rightarrow H \rightarrow H \rightarrow H \rightarrow H_{2} \rightarrow H_{2$	TS goes to reactant along both directions of the IRC
44	intended		TS corresponds to a different reaction
44	Other reaction		
70	intended	$C_{I} \xrightarrow{C_{I}}_{O} \xrightarrow{H}_{H} \xrightarrow{H}_{H} \xrightarrow{H}_{O} \xrightarrow{H}_{O} \xrightarrow{H}_{O} \xrightarrow{H}_{H} \xrightarrow{H}_{O} \xrightarrow{H}_{O} \xrightarrow{H}_{H} \xrightarrow{H}_{O} \xrightarrow{H}_{O} \xrightarrow{H}_{H} \xrightarrow{H}_{O} $	No Re-optimization: 2 imaginary fre- quencies (below 150 cm^{-1}). IRC can only be followed in reactant direction. Re-optimization: No imaginary frequen- cies left
80	intended		The IRC stops al- most immediately in both directions while still at the proposed TS structure.
81	intended		Reaction equivalent to 80. No re-optimization: 2 imaginary frequencies, IRC stops almost immediately in reactant direction. Re-optimization: Find reaction with different reactan 22 /25

Table S5. 7 Reactions for which TSs were found by the RMSD-PP procedure but where the TSs given in \square went to different reactants/products during the IRC



Barrier estimates



Figure S1. Barrier estimate from GFN2-xTB compared to DFT (UB3LYP/6-31G**) barriers for the 6 runs shown in Figure 2. k_{pull} and k_{push} values are given in Hartree per atom. For each point is indicated the pull strength (color) and the push strength (size). Reactions, where the search was unsuccessful are labelled with red edges.



Figure S2. Barrier estimate from DFT single point energy evaluations compared to DFT (UB3LYP/6-31G**) barriers for the 6 runs shown in Figure 2. k_{pull} and k_{push} values are given in Hartree per atom. For each point is indicated the pull strength (color) and the push strength (size). Reactions, where the search was unsuccessful are labelled with red edges.

REFERENCES

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