

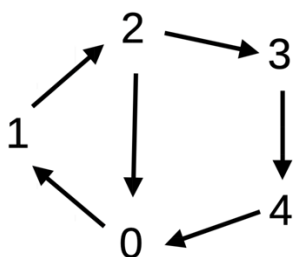
SUPPLEMENT TO:

## The potential energy minima of $n\text{H}_2\text{O}$ ( $n=4,8,\dots,24$ ) in relation to their hydrogen bond cycles

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The following example explains the terms "cycle", "cycle reversal", "signature", "ledger", "family", "parent" and "child proto-PCM".

Consider the relationships illustrated below.



Here,  $0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 4$  would be one **cycle** (and is equivalent to  $4 \rightarrow 0 \rightarrow 1 \rightarrow 2 \rightarrow 3$ , etc.) A second cycle  $0 \rightarrow 1 \rightarrow 2$  is a smaller cycle within. Note that **reversing** the smaller cycle would interrupt the bigger cycle and vice versa.

Thus, the configuration above with two cycles,  $0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 4$  and  $0 \rightarrow 1 \rightarrow 2$ , is one PCM. It has the **signature** (0,1,2,0,1,2,3,4).

The reversal of the first cycle generates a proto-PCM with one cycle,  $4 \rightarrow 3 \rightarrow 2 \rightarrow 1 \rightarrow 0$ , or equivalently  $0 \rightarrow 4 \rightarrow 3 \rightarrow 2 \rightarrow 1$  and has signature (0,4,3,2,1).

The reversal of the second cycle generates a proto-PCM with one cycle,  $2 \rightarrow 1 \rightarrow 0$ , or  $0 \rightarrow 2 \rightarrow 1$  and has signature (0,2,1).

These exhaust all combination of reversals. The **ledger**, is therefore [0,1,2,0,1,2,3,4;0,2,1;0,4,3,2,1] and defines the **family**. The ledger exhaustively lists all possible combinations of reversals.

The **parent** is the input to the Hydrocycler program and is normally an optimized configuration. In the example above, it is the configuration with the signature (0,1,2,0,1,2,3,4). The **child proto-PCMs** are the output configurations: (0,4,3,2,1) and (0,2,1) and are not optimized.