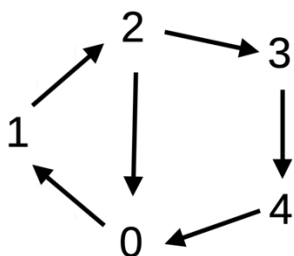SUPPLEMENT TO:

The potential energy minima of nH_2O (n=4,8...,24) in relation to their hydrogen bond cycles

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

Consider the relationships illustrated below.

Here, 0→1→2→3→4 would be one *cycle* (and is equivalent to 4→0→1→2→3, etc.) A second cycle 0→1→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→1→2→3→4 and 0→1→2, is one PCM. It has the *signature* (0,1,2,0,1,2,3,4). The *signature length* is 8, the *cycle sizes* are 5 and 3, and the *cycle count* is 2.

The reversal of the first cycle generates a proto-PCM with one cycle, 4→3→2→1→0, or equivalently 0→4→3→2→1 and has signature (0,4,3,2,1). The signature length is 5, the cycle size is 5, and the cycle count is 1.

The reversal of the second cycle generates a proto-PCM with one cycle, 2→1→0, or 0→2→1 and has signature (0,2,1). The signature length is 3, the cycle size is 3, and the cycle count is 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. For this family, the maximum signature length is 8, the maximum cycle size is 5, and the maximum cycle count is 2.

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 have not been optimized.