**1. Gluing algorithm for self-assembly**

In order to construct the configuration space, we begin at a net and proceed with an algorithm called gluing at vertex connections with exterior angle 1200 until a final folded state is reached. An analogy could be made between gluing of edges and the formation of a stable bond during self-assembly of octahedra. Briefly the algorithm is as follows:

1. Begin with a net *S­0*.

2. Choose any vertex connection *v0* of *S0*, and glue the emanating edges. These may only be glued by rotating rigidly the dihedral angle about self-assembly hinges that meet at *v0.* Let *S1* be the new set of faces, edges, and vertices formed by this gluing.

3. Continue recursively by defining *Sk+1* as the gluing of a vertex connection *vk* in *Sk*.

4. Terminate the process when there are no available vertex connections, or gluing is impossible.

For a process terminating after *n* *gluings*, the resulting set of states (*S0*, . . . , *Sn*) produced is called a pathway of *S­0*; e.g. the set {1, 12, 34, 66, 83} shown in Figure 2 is a self-assembling pathway of net 1, where state 1 is the starting net (*S0*), state 83 is the final state (*Sn*) and states 12, 34 and 66 are intermediates. When panels at vertex connection 1200 are glued, they always meet at the dihedral angle corresponding to an octahedron (83). As a consequence, all pathways terminate at a unique state — a perfectly folded convex octahedron (Isomer I). The complete set of states that results from all possible nets of the octahedron by gluing at vertex connections with 1200 angle is the configuration space *C* of the octahedron comprising of 30 states. These 30 states can be divided into five transition states of intermediates where the states {1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11} represent initial states, the sets {12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22}, {34, 35, 36, 37, 38, 39} and {66} represent intermediate transition states and {83} is the final state. When gluing algorithm is followed for both types of vertex connections at 1200 and 1800 angles, the complete set of states we obtain is the configurations space *Є,* comprising of 84 states*.*