## Supplementary information for the manuscript 'Design principles for helices with tunable pitch and Bernal spirals'

Szilard N. Fejer $^{a,b},^*$ Dwaipayan Chakrabarti $^c,^\dagger$ 

Halim Kusumaatmaja<sup>d</sup>,<sup>‡</sup> and David J. Wales<sup>e</sup>§

<sup>a</sup> Department of Chemical Informatics,
University of Szeged, Faculty of Education,
Boldogasszony sgt. 6, H-6725 Szeged, Hungary

<sup>b</sup> Pro-Vitam Ltd., str. Muncitorilor nr. 16, 520032 Sfantu Gheorghe, Romania

<sup>c</sup> School of Chemistry, University of Birmingham,

 $Edg baston, \ Birmingham \ B15 \ 2TT, \ United \ Kingdom$ 

<sup>d</sup> Department of Physics, Durham University,

South Road, Durham DH1 3LE, United Kingdom

<sup>e</sup> University Chemical Laboratories, Lensfield Road, Cambridge CB2 1EW, United Kingdom

<sup>\*</sup>Electronic address: szilard.fejer@cantab.net

<sup>&</sup>lt;sup>†</sup>Electronic address: d.chakrabarti@bham.ac.uk

<sup>&</sup>lt;sup>‡</sup>Electronic address: halim.kusumaatmaja@durham.ac.uk

<sup>&</sup>lt;sup>§</sup>Electronic address: dw34@cam.ac.uk

## I. SUPPLEMENTARY MOVIE 1 LEGEND

This movie shows the fastest rearrangement mechanism between a 20 particle Bernal spiral and a symmetrical cyclic structure, which is a kinetic trap on the energy landscape for 20 particles. The first four rearrangements along the pathway are low-energy 'hinge' motions.

## II. SUPPLEMENTARY MOVIE 2 LEGEND

This movie shows the fastest pathway for inverting the chirality of a left-handed N = 24 helical structure. The rearrangement proceeds exclusively through low-energy 'hinge' motions.

## III. SUPPLEMENTARY MOVIE 3 LEGEND

This movie shows the transformation of a 24-particle spiral into a highly symmetric 'donut'-structure, which is the global minimum for this number of particles. The second rearrangement along the pathway has a high energy barrier, and corresponds to a change in dimerization pattern between the four particles at the lower end of the helix. All other motions are low-energy 'hinge' rearrangements.