SHAPE

Program for the Stereochemical Analysis
of Molecular Fragments by Means of
Continuous Shape Measures and Associated Tools

User's Manual

Version 2.1, March 2013

Miquel Llunell,[†] David Casanova, Jordi Cirera,
Pere Alemany and Santiago Alvarez
Departament de Química Física, Departament de Química Inorgànica, and Institut de Química Teòrica i Computacional - Universitat de Barcelona

[†] *e-mail: llunell@ub.edu*

TABLE OF CONTENTS

About SHAPE

SHAPE calculates continuous shape measures (CShM's) of a set of points (e.g. atomic positions) relative to the vertices of ideal reference polygons or polyhedra (referred in general as "polyhedra" from here on for simplicity), either centered or non centered. The non centered polyhedra are intended to represent structures of clusters without a central atom, whereas centered polyhedra typically represent the coordination sphere (vertices) of a central atom. Throughout this manual we will indistinctly refer to vertices and atoms as synonims. **SHAPE** also calculates deviations from minimal distortion paths and polyhedral interconversion generalized coordinates. This program is based on the algorithm described by Pinsky and Avnir for the calculation of continuous shape measures, and on the definitions of minimal distortion paths and generalized interconversion coordinates. For more information see the following references:

- *Continuous shape measures algorithm:* M. Pinsky, D. Avnir. *Inorg. Chem.*, **37**, 5575 (1998).
- *Minimal distortion paths*: D. Casanova, J. Cirera, M. Llunell, P. Alemany, D. Avnir, S. Alvarez. *J. Am. Chem. Soc.*, **126**, 1755-1763 (2004).
- *Generalized interconversion coordinates*: J. Cirera, E. Ruiz, S. Alvarez. *Chem. Eur. J.*, **12**, 3162 (2006).

It must be noticed that the algorithm used by **SHAPE** does not distinguish the two enantiomers of a chiral shape. Therefore, whenever a chiral reference polyhedron is used, the resulting shape measures may not refer to that specific polyhedron but to its enantiomer.

Using SHAPE

To run the program for calculating shape measures you must simply type

shape *name*[.dat]

assuming the executable has the name "shape" and the input data is in a file *name*.dat (the file name can be given with or without extension). The program will write the results in the *name*.tab file and additional output files as required by optional keywords.

Alternatively, you may inquire the codes that identify the n-vertex reference polyhedra by typing

shape +[*n*]

If the number of vertices is not given, **SHAPE** gives a list of all available reference polyhedra.

To obtain a list of optional keywords type

shape -h

Standard Input File (See Example 1 for a sample input file)

The input file must have the extension .dat (e.g.: *name*.dat), and a name not exceeding 40 characters. It may contain at any position blank lines or comment lines starting by "!". The

program reads all other lines in free format, allowing for any number of blank spaces between the data, and any number of digits for numerical data.

The input file may contain the following data (fields 1-3 are optional, while field 6 can be omitted if a keyword for reading an external coordinates file is used).

1• Title line (up to 80 characters) indicated by the '$' symbol in the first column.

2• Optional comment lines, recognized by the "!" symbol in the first column, allowed at any position of the input file.

3• Keywords (one line for each keyword)

4• Size of the polyhedron (two integer parameters):
- Number of vertices
- Position of the central atom in the coordinates list (0 if there is no central atom); it must be the same for all the structures.

5• Codes of the reference polyhedra chosen (up to 12). These codes can be found in a table below, or can be obtained on screen by typing the symbol "+" when prompted for the input file name (all polyhedra), or "+*n*" (only polyhedra with *n* vertices).

6• One data set for each structure to be analyzed that comprises:
- A label for the structure with up to 15 characters (e.g., the refcode of a CSD structure).
- One line per atom containing a label with up to 4 characters (e.g., an atomic symbol) and cartesian coordinates.

Reference Polyhedra

The ideal geometries of some 90 reference polyhedra are internally defined in **SHAPE**, and identified by acronyms analogous to those defined by IUPAC for some of them. Those geometries meet the following criteria: (i) Regular and semiregular reference polyhedra have all edges of the same length and are spherical (i.e., their vertices are equidistant to the geometric center); this includes the Platonic solids, the prisms and the antiprisms, but not the bipyramids. (ii) For some polyhedra two or more alternative reference shapes are provided, e.g., a *spherical* version with all center-to-vertex distances identical (best suited for coordination polyhedra), a Johnson version with all edges identical (best suited for clusters or boranes), whose acronym starts with a capital J, and a polyhedron with vacant positions (whose acronyms start with a lower case v). More information about reference shapes other than regular polyhedra can be found in our publications:

- *Four vertex polyhedra*: J. Cirera, P. Alemany, S. Alvarez. *Chem. Eur. J.* **10**, 190 (2004).
- *Five vertex polyhedra*: S. Alvarez, M. Llunell. *J. Chem. Soc., Dalton Trans.* 3288 (2000).
- *Six vertex polyhedra*: S. Alvarez, D. Avnir, M. Llunell, M. Pinsky. *New J. Chem.* **26**, 996 (2002).
- *Seven vertex polyhedra*: D. Casanova, P. Alemany, J. M. Bofill, S. Alvarez. *Chem. Eur. J.* **9**, 1281 (2003).
- *Eight vertex polyhedra*: D. Casanova, M. Llunell, P. Alemany, S. Alvarez. *Chem. Eur. J.* **11**, 1479 (2005).

- *Nine vertex polyhedra*: A. Ruiz-Martínez, D. Casanova, S. Alvarez. *Chem. Eur. J.* **14**, 1291 (2008); *Dalton Trans.*, 2583 (2008)

- *Ten vertex polyhedra*: A. Ruiz-Martínez, D. Casanova, S. Alvarez. *Chem. Eur. J.* **15**, 7470 (2009).

- *Twelve, Twenty and Sixty vertex polyhedra:* J. Echeverría, D. Casanova, M. Llunell, P. Alemany, S. Alvarez, *Chem. Commun.* 2717 (2008); S. Alvarez, *Inorg. Chim. Acta* **363**, 4392 (2010).

- *Cubic Lattices*: J. Echeverría, D. Casanova, M. Llunell, P. Alemany, S. Alvarez, *Chem. Commun.* 2717 (2008).

- *Ill-defined coordination numbers and association-dissociation paths*: A. Ruiz-Martínez, D. Casanova, S. Alvarez. *Chem. Eur. J.* **16**, 6567 (2010).

- *Reviews*: S. Alvarez, P. Alemany, D. Casanova, J. Cirera, M. Llunell, D. Avnir. *Coord. Chem. Rev.* **249**, 1693 (2005); S. Alvarez, E. Ruiz, in *Supramolecular Chemistry, From Molecules to Nanomaterials*, J. W. Steed, P. A. Gale, eds., John Wiley & Sons, Chichester, UK, Vol. 5, 1993-2044 (2012).

Input Using an External Atomic Coordinates File

SHAPE is able to handle a large number of structures using atomic coordinate files generated by other programs or downloaded from the Cambridge Structural Database. To use such coordinate files you only need to include before the first numerical data line a keyword that indicates the file type (%conquest or %external) and the name of the coordinates file to be used (optional). In such cases, no coordinates are required in the input file. The user must make sure that all the required data files are in the same directory from which the program is called.

%conquest

With this keyword, **SHAPE** fetches the coordinates from a file with the extension .cor, generated by the CSD ConQuest program. Be sure to check the "orthogonal coordinates" and "hit fragment only" options when exporting the coordinates from within ConQuest; the search fragment must have only the atoms corresponding to the vertices and center of the polyhedron. See Example 2.

– NEW – With this option, the output .tab file includes the refcode and the label of the central atom for each structure, allowing to distinguish crystallographicaly non equivalent fragments within the same crystal structure.

%external

With this keyword, **SHAPE** fetches the coordinates from a file with the extension .shp, with the same format as the item 6 in the .dat file, in which blank and comment lines are also allowed (see Example 3 for a sample file).

If the name of the .cor or .shp file is not specified, **SHAPE** searches a file with the same name as the data file. If the name of the coordinates file is specified, it can go with or without extension (i.e., both %conquest *name* and %conquest *name.cor* are valid).

Output Files

SHAPE writes in a file with the .tab extension and the same root as the input (.dat) file. Other output files are generated when special options are activated (see the "Optional Keywords" and "File Extensions" sections below).

Minimal Distortion Paths

The stereochemistry of structures intermediate between two reference shapes can be characterized by comparison to the minimal distortion path between those two shapes. **SHAPE** calculates the deviation from the minimal distortion path and the generalized coordinate along that path when the %path keyword is included. In that case only two reference shapes can be selected (see Example 5). Since generalized coordinates are meaningful only for those structures that fall along the minimal distortion path, the values given should be taken only as approximate for structures that significantly deviate from that path. For that reason, only generalized coordinates for structures that deviate less than a threshold value from the minimal distortion path are given in the output (.tab) file. The default threshold is set internally at 10%, but can be modified by the user with the help of the %maxdev keyword.

– NEW – With the %path option, version 2.1 generates a set of shape measures relative to the two ideal polyhedra chosen (.pth file), that can be used to represent the minimal distortion pathway in a shape map.

– NEW – The combined use of the %path and %test keywords generates an .xyz file with the coordinates of 21 ideal structures along the minimal distortion pathway, that can be used to make a movie of the interconversion of the two ideal polyhedra (see example 14). In that case, the .tab file is not generated.

Selecting Structures with Stereochemical Criteria

A set of structures can be filtered, discarding those that do not meet one of three stereochemical criteria, and the filtered results are written in the *name*.flt (text) and *name*.flt.csv (table) files. The applicable stereochemical criteria are: (i) CShM relative to a reference polyhedron below (or above) a chosen threshold (activated with the %maxcsm and %mincsm keywords, respectively), (ii) deviation from a minimal distortion pathway smaller or larger than a chosen value (%maxdev and %mindev keywords, respectively), and (iii) generalized coordinate along a minimal distortion pathway within a certain range (%mingco and %maxgco keywords). **SHAPE** generates the usual output file for all structures (.tab file), together with a file that contains only the filtered structures (.flt file). See Examples 6 and 7.

User-Defined Reference Shapes

SHAPE can also calculate measures relative to a user-defined reference shape. You only need to prepare a *name*.ref file with the coordinates of your reference shapes (as many as you wish) and use 0 in the input file as the code for each user-defined reference polyhedron (see Example 8). The contents of a .ref file are as follows:

- Abbreviation for the name of the ideal shape (up to 12 characters).
- A line with a more detailed description of the reference shape (up to 50 characters).
- Symmetry label (up to 5 characters)
- Coordinates of the atoms occupying the vertices, followed by those of the central atom if present. Note that in the *name*.ref files the central atom (if present) **must always be at the end of the list of coordinates**, regardless of how are the coordinates of the problem structures arranged in the *name*.dat, *name*.cor or *name*.shp files.

Acknowledgments

The present expanded version of **SHAPE** would have not been possible without the collaboration of David Avnir, Mark Pinsky and Josep M. Bofill in the development of the previous versions. The authors and users of **SHAPE** are in debt with them.

LIST OF REFERENCE SHAPES

Vertices	Code	Label	Shape	Symmetry
2	1	L-2	Linear	$D_{\infty h}$
	2	vT-2	Divacant tetrahedron (V-shape, 109.47º)	C_{2v}
	3	vOC-2	Tetravacant octahedron (L-shape, 90º)	C_{2v}
3	1	TP-3	Trigonal planar	D_{3h}
	2	vT-3	Pyramid‡ (vacant tetrahedron)	C_{3v}
	3	fac-vOC-3	fac-Trivacant octahedron	C_{3v}
	4	mer-vOC-3	mer-Trivacant octahedron (T-shape)	C_{2v}
4	1	SP-4	Square	D_{4h}
	2	T-4	Tetrahedron	T_{d}
	3	SS-4	Seesaw or sawhorse‡ (*cis*-divacant octahedron)	C_{2v}
	4	vTBPY-4	Axially vacant trigonal bipyramid	C_{3v}
5	1	PP-5	Pentagon	D_{5h}
	2	vOC-5	Vacant octahedron‡ (Johnson square pyramid, J1)	C_{4v}
	3	TBPY-5	Trigonal bipyramid	D_{3h}
	4	SPY-5	Square pyramid §	C_{4v}
	5	JTBPY-5	Johnson trigonal bipyramid (J12)	D_{3h}
6	1	HP-6	Hexagon	D_{6h}
	2	PPY-6	Pentagonal pyramid	C_{5v}
	3	OC-6	Octahedron	O_{h}
	4	TPR-6	Trigonal prism	D_{3h}
	5	JPPY-5	Johnson pentagonal pyramid (J2)	C_{5v}
7	1	HP-7	Heptagon	D_{7h}
	2	HPY-7	Hexagonal pyramid	C_{6v}
	3	PBPY-7	Pentagonal bipyramid	D_{5h}
	4	COC-7	Capped octahedron *	C_{3v}
	5	CTPR-7	Capped trigonal prism *	C_{2v}
	6	JPBPY-7	Johnson pentagonal bipyramid (J13)	D_{5h}
	7	JETPY-7	Elongated triangular pyramid (J7)	C_{3v}
8	1	OP-8	Octagon	D_{8h}
	2	HPY-8	Heptagonal pyramid	C_{7v}
	3	HBPY-8	Hexagonal bipyramid	D_{6h}
	4	CU-8	Cube	O_{h}
	5	SAPR-8	Square antiprism	D_{4d}
	6	TDD-8	Triangular dodecahedron	D_{2d}
	7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}
	8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}
	9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}
	10	BTPR-8	Biaugmented trigonal prism	C_{2v}
	11	JSD-8	Snub disphenoid (J84)	D_{2d}
	12	TT-8	Triakis tetrahedron	T_{d}
	13	ETBPY-8	Elongated trigonal bipyramid (see 8)	D_{3h}

Vertices	Code	Label	Shape	Symmetry
9	1	EP-9	Enneagon	D_{9h}
	2	OPY-9	Octagonal pyramid	C_{8v}
	3	HBPY-9	Heptagonal bipyramid	D_{7h}
	4	JTC-9	Triangular cupola (J3) = trivacant cuboctahedron	C_{3v}
	5	JCCU-9	Capped cube (Elongated square pyramid, J8)	C_{4v}
	6	CCU-9	Capped cube	C_{4v}
	7	JCSAPR-9	Capped sq. antiprism (Gyroelongated square pyramid J10)	C_{4v}
	8	CSAPR-9	Capped square antiprism	C_{4v}
	9	JTCTPR-9	Tricapped trigonal prism (J51)	D_{3h}
	10	TCTPR-9	Tricapped trigonal prism	D_{3h}
	11	JTDIC-9	Tridiminished icosahedron (J63)	C_{3v}
	12	HH-9	Hula-hoop	C_{2v}
	13	MFF-9	Muffin	C_s
10	1	DP-10	Decagon	D_{10h}
	2	EPY-10	Enneagonal pyramid	C_{9v}
	3	OBPY-10	Octagonal bipyramid	D_{8h}
	4	PPR-10	Pentagonal prism	D_{5h}
	5	PAPR-10	Pentagonal antiprism	D_{5d}
	6	JBCCU-10	Bicapped cube (Elongated square bipyramid J15)	D_{4h}
	7	JBCSAPR-10	Bicapped square antiprism (Gyroelongated square bipyramid J17)	D_{4d}
	8	JMBIC-10	Metabidiminished icosahedron (J62)	C_{2v}
	9	JATDI-10	Augmented tridiminished icosahedron (J64)	C_{3v}
	10	JSPC-10	Sphenocorona (J87)	C_{2v}
	11	SDD-10	Staggered dodecahedron (2:6:2) #	D_2
	12	TD-10	Tetradecahedron (2:6:2)	C_{2v}
	13	HD-10	Hexadecahedron (2:6:2, or 1:4:4:1)	D_{4h}
11	1	HP-11	Hendecagon	D_{11h}
	2	DPY-11	Decagonal pyramid	C_{10v}
	3	EBPY-11	Enneagonal bipyramid	D_{9h}
	4	JCPPR-11	Capped pent. Prism (Elongated pentagonal pyramid J9)	C_{5v}
	5	JCPAPR-11	Capped pent. antiprism (Gyroelongated pentagonal pyramid J11)	C_{5v}
	6	JAPPR-11	Augmented pentagonal prism (J52)	C_{2v}
	7	JASPC-11	Augmented sphenocorona (J87)	C_s

Vertices	Code	Label	Shape	Symmetry
12	1	DP-12	Dodecagon	D_{12h}
	2	HPY-12	Hendecagonal pyramid	C_{11v}
	3	DBPY-12	Decagonal bipyramid	D_{10h}
	4	HPR-12	Hexagonal prism	D_{6h}
	5	HAPR-12	Hexagonal antiprism	D_{6d}
	6	TT-12	Truncated tetrahedron	T_d
	7	COC-12	Cuboctahedron	O_h
	8	ACOC-12	Anticuboctahedron (Triangular orthobicupola J27)	D_{3h}
	9	IC-12	Icosahedron	I_h
	10	JSC-12	Square cupola (J4)	C_{4v}
	11	JEPBPY-12	Elongated pentagonal bipyramid (J16)	D_{6h}
	12	JBAPPR-12	Biaugmented pentagonal prism (J53)	C_{2v}
	13	JSPMC-12	Sphenomegacorona (J88)	C_s
20	1	DD-20	Dodecahedron †	I_h
24	1	TCU-24	Truncated cube	O_h
	2	TOC-24	Truncated octahedron	O_h
48	1	TCOC-48	Truncated cuboctahedron	O_h
60	1	TRIC-60	Truncated icosahedron (fullerene)	I_h

* Non regular polyhedron, for definition of reference shape see references above.

‡ A regular polyhedron with one or two vertices removed.

§ Spherical distribution of vertices with mass center at the origin (apical-basal bond angles of 104.45°).

† For polyhedra with more than 12 vertices the calculation times may be unpractical, and the user is only allowed to set manually the equivalence between vertices of the problem and reference shapes by means of the %fixperm keyword.

This is a chiral polyhedron; see cautionary note in the "About SHAPE" section.

File Extensions

name.dat	Input file.
name.cor	Name of the coordinates file generated by CSD's ConQuest, specified with the %conquest keyword. Each structure is identified in the output by the refcode and the label of the central atom if present.
name.shp	User-generated coordinates file, optional name specified with the %external keyword.
name.ide	User-defined coordinates for a non-standard reference shape, replaced in **SHAPE 2.1** by *name*.ref. Old files with the .ide extension used with version 2.0 and are still recognized when the %reference (earlier %ideal) keyword is used.
name.tab	Output file with shape measures, path deviations and generalized coordinates.
name.tab.csv	Table of shape measures, path deviations and generalized coordinates in csv (comma separated values) format.
name.flt	Contains the results for only those structures filtered according to shape measure, path deviation function and/or generalized coordinate criteria (see %mincsm, %maxcsm, %mindev, %maxdev, %mingco and %maxgco keywords).
name.flt.csv	Tabular (csv format) version of *name*.flt generated to facilitate data transfer to datasheets or plotting and statistical software.
name.pth	**– NEW –** Gives a set of points for drawing the minimal distortion pathway (in csv format).
name.out	Gives the calculated CShM's and the coordinates of each problem structure and of the closest reference polyhedra, generated when the %fullout keyword is included in the input file before the numerical data (see Example 4). *Note that this option may substantially slow down the calculations*.
name.ref	Contains the coordinates for a user-defined reference shape, required with the %reference keyword.
ID.xyz	Coordinates of the reference polyhedron with acronym ID (see List of Reference Shapes), generated when the %test keyword is used. Readable by programs such as Crystal Maker and Mercury.
name.tst	Geometries of reference shapes (coordinates, distances and angles), generated by the %test keyword.

Optional Keywords §

Keyword	Argument	Description
%conquest [*name*.cor]		Reads the atomic coordinates from a *name*.cor file generated by ConQuest.
%external [*name*.shp]		Reads the atomic coordinates from an external *name*.shp file.
%fixperm	*N*	Calculates the measures for a chosen pairing of vertices of the problem and ideal structures, rather than optimizing the shape measure for all possible pairings (see Examples 9 - 12). To use this option one must first check the ordering of the vertices in the reference shape by looking at the *ID*.xyz file generated with the %test keyword. *N* can adopt one of the following values:
	N = -1	a vertex pairing is given by the user for each set of atomic coordinates. A vertex number for each atom is given right after its coordinates.
	N = 0	the vertices are taken in order of appearance in the list of coordinates, exclusive of the central atom if present.
	N = 1	a vertex pairing is given only once for all the structures present in the input file, in a line appearing before the first set of atomic coordinates.
%fullout		Generates a *name*.out file containing the coordinates of the problem structures and of the closest reference polyhedra, the continuous shape measures and the optimal vertex pairing.
%ideal	*file*	This keyword was used in version 2.0 of **SHAPE** and is replaced in the new version by %reference. However, the program can properly handle input files with the old keyword.
%maxcsm	*y*	Generates output files *name*.flt and *name*.flt.csv with the shape measures for only those structures having at least one shape measure smaller than *y* (*y* is a real number). It is advisable to use this option with only one reference shape.
%maxdev	*y*	Generates *name*.flt and *name*.flt.csv files with the shape measures for only those structures having path deviation functions smaller or equal than *y* (more details as specified for %maxcsm).
%maxgco	*y*	Generates *name*.flt and *name*.flt.csv files with the shape measures for only those structures with generalized coordinates smaller than *y* (more details as specified for %maxcsm).
%mincsm	*x*	Generates *name*.flt and *name*.flt.csv files with the shape measures for only those structures with at least one shape measure larger than *x* (more details as specified for %maxcsm). It is advisable to use this option with only one ideal shape.
%mindev	*x*	Generates *name*.flt and *name*.flt.csv files with the results for only those structures with path deviation functions larger or equal than *x* (more details as specified for %maxcsm).
%mingco	*x*	The program selects structures with shape measures, path deviation functions or generalized coordinates larger than a desired value *x*,

respectively, and writes the filtered results to the *name*.flt and *name*.flt.csv files.

NOTE: The combined use of %max*xxx* and %min*xxx* keywords allows one to select structures within a specific range (between *x* and *y*) of, e.g., generalized coordinates (see Examples 6 and 7). With those options, *name*.flt and *name*.flt.csv files are generated, containing the full output for the filtered structures and a table with only the numerical values in the csv (comma separated values) format, respectively.

%nosymbol — Indicates that no atomic labels are included with the coordinates.

%path — Calculates the *path deviation function* for the minimal distortion interconversion path between two given polyhedra as well as the generalized coordinate. Two and only two reference polyhedra should be coded in the input file with this option. The path is assumed to go from the first (0%) to the second (100%) reference shape specified in the input file.

The generalized coordinate is given only for structures that deviate at most a 10% from the minimal distortion interconversion path. This threshold can be modified with the %maxdev keyword.

%reference *file* — Points to a *file*.ref file containing user-defined reference shapes. The name of the file must be specified only if it is different from that of the data file (see Example 8). This keyword replaces the %ideal keyword of version 2.0 of **SHAPE**, but the program can properly handle input files with the old keyword.

%select *label* — Performs shape measures only for the set of coordinates under the structure label specified and places the results in a file with the name *label*.

%stop *N* — Calculates the shape measures for the first N structures only.

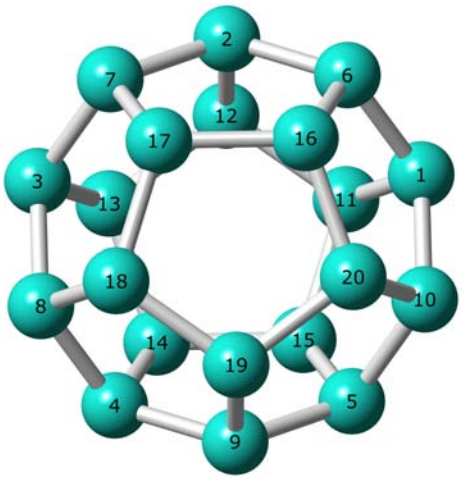
%test — Generates a .tst file with the geometries of the reference shapes (coordinates, distances and angles), and one .xyz file for each ideal shape. The input file must specify the number of vertices and the code of the reference shapes, but no atomic coordinates are required (see Example 13).

%thrdev *x* — This option is replaced in **SHAPE 2.1** by the %mindev and %maxdev keywords.

§ Keywords must appear in the input file before the numerical data.

SHAPE

Examples and Sample Files



Example 1: Standard Input File

Calculate the CShM's of ML_4 fragments relative to two ideal structures: the square (code = 1) and the tetrahedron (code = 2).

Input file example01.dat

```
$ PtL4 structures
! Ligands  Metal
     4       5
! Tetrahedron Square
     2         1
ABOXIY
  N   3.9023   7.5659   14.2563
  C   3.9912   8.8145   16.4883
  S   1.0864   9.0325   13.3242
  Cl  1.4893  10.6356   16.0313
  Pt  2.7159   8.9642   15.0153
!ABZLPT10
!  P   3.9891   1.7349   -5.9463
!  N   2.5932  -0.3213   -2.3836
!  N   3.9661   2.1385   -2.8787
!  Cl  2.6450  -1.1044   -5.4688
!  Pt  3.3098   0.6621   -4.0608
ACACPT
  O   0.6294   1.3760  -1.2703
  O  -0.6294  -1.3760   1.2703
  O  -1.7613   0.9024   0.3486
  O   1.7613  -0.9024  -0.3486
  Pt  0.0000   0.0000   0.0000
```

This input file is equivalent:

```
4 1
2 1
ABOXIY
Pt  2.7159   8.9642   15.0153
N   3.9023   7.5659   14.2563
C   3.9912   8.8145   16.4883
S   1.0864   9.0325   13.3242
Cl  1.4893  10.6356   16.0313
ACACPT
Pt  0.0000   0.0000   0.0000
O   0.6294   1.3760  -1.2703
O  -0.6294  -1.3760   1.2703
O  -1.7613   0.9024   0.3486
O   1.7613  -0.9024  -0.3486
```

Output file example01.tab

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

PtL4 structures

T-4             2 Td    Tetrahedron
SP-4            1 D4h   Square

Structure [ML4 ]          T-4         SP-4
 ABOXIY          ,      31.375,       0.970
 ACACPT          ,      33.440,       0.160
```

Example 2: Atomic coordinates from a .cor file generated by CSD's ConQuest

To generate the .cor file a search must be carried out in ConQuest in which only the atoms in the fragment to be analyzed are defined. A coordinates file is then generated with the results of the search ("Export entries as...") using the "Orthogonal" and "Hit Fragment Only" options.

Input file: example02.dat

```
%conquest coords2
4 1
1 2
```

Coordinates file obtained from ConQuest: coords2.cor

```
DOSDAQ   **FRAG**        1
Pd1          16.04450   0.00000   0.00000     1555011
N1H          17.11627  -1.46619  -0.92483     9655010
N1B          17.11627   1.46619   0.92483     3655010
N1J          14.97273  -1.46619  -0.92483     11555010
N1           14.97273   1.46619   0.92483     1555010
FUBWUU   **FRAG**        1
Pt1           6.35325   1.50775   0.00000     1555001
N1E*          4.67365   2.63675   0.26075     6665002
N2            7.85296   1.80990   1.32660     1555016
N2E*          4.85354   1.20560  -1.32660     6665016
N1            8.03285   0.37875  -0.26075     1555002
LEGFOS   **FRAG**        1
Cr1           5.47182   6.64300   6.21762     1555001
N2            3.90370   5.54292   7.02349     1555003
N1B           7.04319   5.53495   5.40674     3555002
N2B           3.90370   7.74308   7.02349     3555003
N1            7.04319   7.75105   5.40674     1555002
LEGFUY   **FRAG**        1
Cr1           0.00000   0.00000   0.00000     1555001
N2           -1.92134  -0.79300  -0.22619     1555004
N2A           1.92134   0.79300   0.22619     2555004
N1A          -1.33328   1.09218  -1.23891     2555003
N1            1.33328  -1.09218   1.23891     1555003
LEGFUY   **FRAG**        2
Cr2          13.08506   9.95142   5.14071     1555002
N4A*         14.56143   8.60497   5.79769     2766006
N5           13.16165  11.88734   5.96836     1555007
N5A*         13.00848   8.01551   4.31305     2766007
N4           11.60870  11.29788   4.48373     1555006
```

Comment: Notice that the last column in the coordinates file generated by ConQuest is neglected by **SHAPE**. Also the fragment number (e.g., **FRAG** 1) is disregarded.

Output file: example02.tab

```
--------------------------------------------------------------------------------

SP-4            1 D4h   Square
T-4             2 Td    Tetrahedron

Structure [ML4 ]         SP-4          T-4
 DOSDAQ   1 Pd1 ,       5.271,       36.847
 FUBWUU   1 Pt1 ,       5.184,       36.789
 LEGFOS   1 Cr1 ,       5.047,       36.698
 LEGFUY   1 Cr1 ,       5.234,       36.822
 LEGFUY   2 Cr2 ,       5.100,       36.733
```

Example 3: Input with external coordinates

Input file: example03.dat

```
! keyword, name of coords. file
%external      geometries
4 1
2 1
```

External file: geometries.shp

```
ABOXIY
  Pt  2.7159   8.9642   15.0153
  N   3.9023   7.5659   14.2563
  C   3.9912   8.8145   16.4883
  S   1.0864   9.0325   13.3242
  Cl  1.4893  10.6356   16.0313
ACACPT
  Pt  0.0000   0.0000   0.0000
  O   0.6294   1.3760  -1.2703
  O  -0.6294  -1.3760   1.2703
  O  -1.7613   0.9024   0.3486
  O   1.7613  -0.9024  -0.3486
```

Output file as in example01.tab

Example 4: Use of the %fullout Option

Input file: example04.dat, as in Example 1 with the %fullout keyword added:

```
$ Example 4 – Four-coordinate complexes, %fullout option
%fullout
4 1
2 1
ABOXIY
 Pt  2.7159   8.9642   15.0153
 N   3.9023   7.5659   14.2563
 C   3.9912   8.8145   16.4883
 S   1.0864   9.0325   13.3242
 Cl  1.4893  10.6356   16.0313
ACACPT
 Pt  0.0000   0.0000   0.0000
 O   0.6294   1.3760  -1.2703
 O  -0.6294  -1.3760   1.2703
 O  -1.7613   0.9024   0.3486
 O   1.7613  -0.9024  -0.3486
```

Output files: example04.tab (see example01.tab) and example04.out:

```
--------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
--------------------------------------------------------------------------------

Example 4: Four-coordinate complexes, %fullout option
--------------------------------------------------------------------------------

Ideal structures   ML4
T-4              2 Td    Tetrahedron
SP-4             1 D4h   Square

--------------------------------------------------------------------------------

Structure     1    [ABOXIY]
    Pt          2.7159   8.9642  15.0153
    N           3.9023   7.5659  14.2563
```

```
    C          3.9912   8.8145  16.4883
    S          1.0864   9.0325  13.3242
    Cl         1.4893  10.6356  16.0313


 T-4          Ideal structure    CShM =   31.37468
    Pt      M          2.6370   9.0025  15.0231
    N       L1         4.0461   8.7682  13.9529
    C       L2         2.9073   8.1375  16.5607
    S       L3         1.1733   8.3606  14.2286
    Cl      L4         2.4214  10.7439  15.3500


 SP-4         Ideal structure    CShM =    0.96957
    Pt      M          2.6370   9.0025  15.0231
    N       L1         3.7673   7.4669  14.0426
    C       L2         4.0241   8.9797  16.6579
    S       L4         1.2499   9.0254  13.3883
    Cl      L3         1.5068  10.5382  16.0036

--------------------------------------------------------------------------------

Structure     2    [ACACPT]
    Pt         0.0000   0.0000   0.0000
    O          0.6294   1.3760  -1.2703
    O         -0.6294  -1.3760   1.2703
    O         -1.7613   0.9024   0.3486
    O          1.7613  -0.9024  -0.3486


 T-4          Ideal structure    CShM =   33.43969
    Pt      M          0.0000   0.0000   0.0000
    O       L1         0.3779   0.9502  -0.8463
    O       L2        -0.3779  -0.9502   0.8463
    O       L3        -1.1497   0.6333   0.1977
    O       L4         1.1497  -0.6333  -0.1977


 SP-4         Ideal structure    CShM =    0.15954
    Pt      M          0.0000   0.0000   0.0000
    O       L1         0.5669   1.4252  -1.2695
    O       L3        -0.5669  -1.4252   1.2695
    O       L2        -1.7245   0.9500   0.2965
    O       L4         1.7245  -0.9500  -0.2965

--------------------------------------------------------------------------------
```

Example 5: Deviation from a Minimal Distortion Pathway

Input file: example05.dat:

```
$ Example 5 – Six-coordinate complexes, %path option
%path
   6  2
   3  4
BOYGOL
S2          -3.02522  14.98464   5.51132
Re1         -2.01859  15.17612   3.40291
S3          -2.17289  12.84935   3.26636
S6          -3.39746  17.02591   3.63698
S1           0.03863  14.89916   4.42076
S5          -0.52591  16.54038   2.22545
S4          -3.10277  14.76411   1.37960
BOYGOL10
S4          -3.10243  14.76411   1.37689
Re1         -2.01775  15.17612   3.39621
S2          -3.02386  14.98464   5.50049
S3          -2.17209  12.84935   3.25994
S1           0.03972  14.89916   4.41207
S6          -3.39657  17.02591   3.62983
S5          -0.52536  16.54038   2.22108
BOZCAU
S2           0.69939   1.53300   5.44636
Mo1         -0.40113   1.75609   3.21129
S3          -1.78709   3.67403   4.01926
S2B         -1.50164   1.53300   0.97623
S1           1.40580   0.08654   2.66152
S1B         -2.20805   0.08654   3.76107
S3B          0.98484   3.67403   2.40333
LIDKEO
S6           0.32602  15.18437  14.42702
Zr1          2.69911  16.39788  15.02023
S5           1.53570  16.00081  17.37198
S3           5.20997  16.42018  14.60756
S4           2.88922  13.81919  15.56890
S2           2.48141  17.42623  12.74821
S1           3.04257  18.76688  15.79633
MARSIH
S2           5.04452   0.58097  10.04321
Ti1          4.61060   0.61541   7.54130
S3           5.75074  -1.61199   7.95608
S6           4.33426  -0.20342   5.34729
S1           2.59925  -0.65331   8.49150
S5           6.54438   1.75909   6.96978
S4           3.11547   2.40223   7.47819
MARSIH
S2           5.04452   0.58097  10.04321
Ti2          4.25297  -1.81575   9.98445
S3           5.75074  -1.61199   7.95608
S9           5.87017  -2.47681  11.55377
S1           2.59925  -0.65331   8.49150
S8           3.91311  -4.13376   9.42357
S7           2.77452  -1.68916  11.78932
POJFOJ
S2           0.81532   2.72459   4.24025
Ti1         -0.20836   4.25976   5.95223
S3           2.08147   5.28307   5.54063
S9          -1.92082   2.72459   6.34306
S1          -0.31827   5.54322   3.74035
S8          -1.78359   5.95191   6.45995
S7           0.78176   3.84167   7.97794
```

Output file: example05.tab:

```
--------------------------------------------------------------------------------

Example 5 – Six-coordinate complexes, %path option

OC-6            3 Oh    Octahedron
TPR-6           4 D3h   Trigonal prism

Minimal distorsion path analysis:
   from OC-6 (0%) to TPR-6 (100%)
   Deviation threshold to calculate Generalized Coordinate: 10.0000

Structure [ML6 ]         OC-6        TPR-6     DevPath    GenCoord
 BOYGOL          ,      12.011,       0.954,        7.2,        84.0
 BOYGOL10        ,      12.012,       0.957,        7.2,        84.0
 BOZCAU          ,       1.142,      11.245,        6.5,        25.4
 LIDKEO          ,      10.707,       1.236,        5.5,        79.1
 MARSIH          ,       0.993,      12.826,       10.6,           -
 MARSIH          ,       1.105,      11.783,        8.1,        25.0
 POJFOJ          ,       5.203,       5.085,        8.6,        54.6
```

Comment: For the first fragment of structure MARSIH the generalized coordinate is omitted because it is calculated only for structures with a DevPath value smaller than a threshold of 10% set by default. That threshold can be modified by the user (see Example 6).

Results for plotting a shape map, file example05.csv:

```
Structure      ,        OC-6,       TPR-6
 BOYGOL          ,      12.011,       0.954
 BOYGOL10        ,      12.012,       0.957
 BOZCAU          ,       1.142,      11.245
 LIDKEO          ,      10.707,       1.236
 MARSIH          ,       0.993,      12.826
 MARSIH          ,       1.105,      11.783
 POJFOJ          ,       5.203,       5.085
```

Minimal distortion pathway file: example05.pth :

```
        OC-6_pth,       TPR-6_pth
          16.737,           0.000
          15.355,           0.035
          14.002,           0.144
          12.681,           0.329
          11.398,           0.593
          10.158,           0.940
           8.966,           1.371
           7.828,           1.890
           6.748,           2.497
           5.732,           3.195
           4.785,           3.984
           3.911,           4.865
           3.116,           5.837
           2.403,           6.901
           1.777,           8.055
           1.241,           9.298
           0.798,          10.626
           0.450,          12.038
           0.201,          13.530
           0.050,          15.097
           0.000,          16.737
```

Example 6: Use of the %maxdev Keyword

In this example we select from the coordinates file nickel.cor those structures that deviate at most a 5% from the square-tetrahedron pathway.

Input file: example06.dat:

```
$ Example 6- Four coordinate Ni complexes, %maxdev option
!             Atomic coordinates in file nickel.cor
!             Writes results for structures that deviate at most
!                   a 5% from the tetrahedron-square pathway.
%conquest nickel
%path
%maxdev 5.0
   4  1
   1  2
```

ConQuest generated coordinates file: nickel.cor (only first lines shown):

```
ACTPNI  **FRAG**        1
Ni1          2.71219   2.81088   1.41507     1555010
P1           4.69038   2.60714   2.35529     1555012
Cl1          2.08358   0.76327   2.15287     1555001
P2           0.82300   2.98937   0.30206     1555013
C1           3.11326   4.57241   0.99635     1555002
ADUVOL  **FRAG**        1
Ni1          6.37726   3.85616  10.65061     1555001
C1           8.04704   3.64539   9.74674     1555008
Cl2          6.42565   6.01430  10.27734     1555003
C22          4.70946   4.05219  11.58132     1555055
Cl1          6.31751   1.69381  10.91760     1555002
ASBRNI  **FRAG**        1
Ni1          3.19481   1.63191   9.58172     1555001
P1           1.95029  -0.32618   9.47129     1555005
Br3          5.26621   0.96957  10.51781     1555004
Br1          1.88263   3.13514  10.85158     1555002
Br2          3.47447   2.28428   7.30800     1555003
```

Output file: example06.tab (only first lines shown):

```
------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
------------------------------------------------------------------------------

Example 6- Four coordinate Ni complexes, %maxdev option

SP-4            1 D4h   Square
T-4             2 Td    Tetrahedron

Minimal distorsion path analysis:
   from SP-4 (0%) to T-4 (100%)

Deviation threshold to calculate Generalized Coordinate:  5.000%

Structure [ML4 ]         SP-4          T-4     DevPath    GenCoord
 ACTPNI   1 Ni1 ,       0.712,      28.619,        5.4,           -
 ADUVOL   1 Ni1 ,       0.463,      32.253,        9.2,           -
 ASBRNI   1 Ni1 ,      32.428,       0.314,        7.5,           -
 AWELET   1 Ni3 ,       0.109,      30.780,        0.9,         5.4
 AWELUJ   1 Ni1 ,       0.056,      33.227,        3.7,         3.8
 AZERAY   1 Ni1 ,      30.356,       2.583,       21.0,           -
```

```
 BAJWOZ   1 Ni1 ,      28.722,       2.264,       16.4,          -
 BAQZEY   1 Ni1 ,       0.062,      33.375,        4.1,        4.0
 BAVCEH   1 Ni1 ,       0.050,      33.367,        3.7,        3.6
 BAZRID   1 Ni1 ,       0.035,      33.357,        3.1,        3.0
 BAZRID   2 Ni2 ,       0.243,      28.800,        0.1,        8.0
 BAZSUR   1 Ni1 ,       0.944,      33.963,       16.9,          -
 BEFDIZ02 1 Ni1 ,       1.025,      34.017,       17.7,          -
 BEGDAT   1 Ni1 ,       0.002,      33.335,        0.7,        0.7
 BIPKER   1 Ni1 ,      30.909,       1.126,       13.1,          -
 BIVFOB   1 Ni1 ,       0.464,      33.467,       11.3,          -
 BONHIV   1 Ni1 ,       0.995,      33.997,       17.4,          -
 CABQUS   1 Ni1 ,       0.093,      33.395,        5.1,          -
 CADJEW   1 Ni1 ,      33.353,       0.056,        3.9,      100.0
 CADJEW   2 Ni2 ,      33.343,       0.059,        4.0,      100.0
```

Filtered output file: example06.flt (only first lines shown):

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

Example 6- Four coordinate Ni complexes, %maxdev option

SP-4            1 D4h   Square
T-4             2 Td    Tetrahedron

Minimal distorsion path analysis:
   from SP-4 (0%) to T-4 (100%)


Filtered results
  Only structures within the following boundaries are given in this file:
  Path deviation function (%):   0.000 -   5.000
  Generalized coordinate (%):    0.000 - 100.000

Structure [ML4 ]         SP-4          T-4     DevPath    GenCoord
 AWELET   1 Ni3 ,       0.109,      30.780,        0.9,        5.4
 AWELUJ   1 Ni1 ,       0.056,      33.227,        3.7,        3.8
 BAQZEY   1 Ni1 ,       0.062,      33.375,        4.1,        4.0
 BAVCEH   1 Ni1 ,       0.050,      33.367,        3.7,        3.6
 BAZRID   1 Ni1 ,       0.035,      33.357,        3.1,        3.0
 BAZRID   2 Ni2 ,       0.243,      28.800,        0.1,        8.0
 BEGDAT   1 Ni1 ,       0.002,      33.335,        0.7,        0.7
 CADJEW   1 Ni1 ,      33.353,       0.056,        3.9,      100.0
 CADJEW   2 Ni2 ,      33.343,       0.059,        4.0,      100.0
 CAVLIV   1 Ni2 ,       0.014,      33.227,        1.7,        1.9
 CEPXIF   1 Ni1 ,      28.550,       0.405,        1.9,       91.6
 CIKTIZ   1 Ni1 ,       0.101,      31.838,        2.6,        5.2
 CLTPNI03 1 Ni1 ,      25.471,       0.898,        1.4,       86.0
 COPYEM   1 Ni5 ,      32.736,       0.038,        2.1,       99.0
 CSINIA   1 Ni1 ,       0.883,      25.608,        1.5,       15.3
 CSINIA   2 Ni2 ,       1.332,      23.721,        1.4,       18.8
 CSINIB   1 Ni1 ,       2.102,      22.707,        4.3,       23.6
 CSINIB   2 Ni2 ,       1.346,      24.716,        3.4,       18.9
 DARBII   1 Ni2 ,       0.004,      33.336,        1.1,        1.1
```

Other files generated: example06.pth *and* example06.csv (see Example 5).

Example 7: Use of the %maxgco and %mingco Keywords

Select from the coordinates file nickel.cor those structures that are in the middle of the interconversion pathway between the square and the tetrahedron.

Input file: example07.dat (only first lines shown):

```
$ Example 7- Four coordinate Ni complexes, %maxgco option
!             Reads atomic coordinates from file nickel.cor
!             Selects structures that are in the middle of
!             the planarization pathway (40 < GenCoord < 60%).
%conquest nickel
%path
%mingco 40.
%maxgco 60.
%maxdev  10.
   4  1
   1  2
```

Output file: example07.tab:

```
------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
------------------------------------------------------------------------------

Example 7- Four coordinate Ni complexes, %maxgco option

SP-4            1 D4h   Square
T-4             2 Td    Tetrahedron

Minimal distorsion path analysis:
   from SP-4 (0%) to T-4 (100%)

Deviation threshold to calculate Generalized Coordinate: 10.000%

Structure [ML4 ]         SP-4          T-4     DevPath    GenCoord
 ACTPNI   1 Ni1 ,       0.712,      28.619,        5.4,        13.7
 ADUVOL   1 Ni1 ,       0.463,      32.253,        9.2,        11.1
 ASBRNI   1 Ni1 ,      32.428,       0.314,        7.5,        98.4
 AWELET   1 Ni3 ,       0.109,      30.780,        0.9,         5.4
 AWELUJ   1 Ni1 ,       0.056,      33.227,        3.7,         3.8
 AZERAY   1 Ni1 ,      30.356,       2.583,       21.0,           -
 BAJWOZ   1 Ni1 ,      28.722,       2.264,       16.4,           -
 BAQZEY   1 Ni1 ,       0.062,      33.375,        4.1,         4.0
 BAVCEH   1 Ni1 ,       0.050,      33.367,        3.7,         3.6
 BAZRID   1 Ni1 ,       0.035,      33.357,        3.1,         3.0
 BAZRID   2 Ni2 ,       0.243,      28.800,        0.1,         8.0
 BAZSUR   1 Ni1 ,       0.944,      33.963,       16.9,           -
 BEFDIZ02 1 Ni1 ,       1.025,      34.017,       17.7,           -
 BEGDAT   1 Ni1 ,       0.002,      33.335,        0.7,         0.7
 BIPKER   1 Ni1 ,      30.909,       1.126,       13.1,           -
 BIVFOB   1 Ni1 ,       0.464,      33.467,       11.3,           -
 BONHIV   1 Ni1 ,       0.995,      33.997,       17.4,           -
 CABQUS   1 Ni1 ,       0.093,      33.395,        5.1,         5.0
 CADJEW   1 Ni1 ,      33.353,       0.056,        3.9,       100.0
 CADJEW   2 Ni2 ,      33.343,       0.059,        4.0,       100.0
 CADJEW   3 Ni3 ,      33.363,       0.109,        5.4,       100.1
```

Filtered output file: example07.flt:

```
------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
------------------------------------------------------------------------------

Example 7- Four coordinate Ni complexes, %maxgco option

SP-4            1 D4h   Square
T-4             2 Td    Tetrahedron

Minimal distorsion path analysis:
   from SP-4 (0%) to T-4 (100%)


Filtered results
  Only structures within the following boundaries are given in this file:
  Path deviation function (%):   0.000 -  10.000
  Generalized coordinate (%):   40.000 -  60.000

Structure [ML4 ]         SP-4          T-4     DevPath    GenCoord
 DUKNED   1 Ni1 ,      12.738,       6.199,        0.2,       59.3
```

Other files generated: example07.pth *and* example07.csv (see Example 5).

Example 8: Use of a user-defined reference polyhedron

Input file: example08.dat

```
$ Cyclen complexes in cis conformation
%path
   6   5
   4   0
TUKWEB
N4           2.04091   3.92389  10.64074
N3          -0.83988   4.13831  10.95260
N1           2.23124   4.94238  13.37296
N6           2.07351   2.22997  13.43397
Zn1          0.62860   3.58403  12.61024
N5          -0.85563   1.90834  12.62380
N2          -0.64030   5.09248  13.74584
NAXJIF
N2           1.57673   0.92781   9.50033
N3           2.08309   1.65282   6.59555
N1           1.20034   3.81264  10.25045
N4           1.64134   4.56300   7.29441
Ag1          0.31080   2.65820   8.13611
S1          -1.91668   3.16393   9.58508
S3          -1.13006   1.56080   6.07099
```

Ideal polyhedron file: example08.ref

```
dvCU
Divacant cube
C2v
   0.000  0.000   0.000
   0.000  0.000   1.000
   0.000  1.000   0.000
   1.000  0.000   0.000
```

```
   1.000  1.000   0.000
   1.000  1.000   1.000
   0.500  0.500   0.500
```

Note *that in the* .ref *file the coordinates of the central atom must be in the last line*.

Alternatively one could use an ideal polyhedron file dvcube.ide *introducing the* `%ideal dvcube` *instruction in the input file*.

Output file: example08.tab

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

Cyclen complexes in cis conformation

TPR-6           4 D3h   Trigonal prism
dvCU            0 C2v   Divacant cube

Minimal distorsion path analysis:
   from TPR-6 (0%) to dvCU (100%)

Deviation threshold to calculate Generalized Coordinate: 10.000%

Structure [ML6 ]        TPR-6         dvCU     DevPath    GenCoord
 TUKWEB         ,       1.967,       3.699,        3.8,       43.7
 NAXJIF         ,       6.955,       0.602,        7.0,       82.8
```

Other files generated: *example08.pth*, *example08.csv* (see Example 5).

Example 9. Large Polyhedra: Specifying a Vertex Pairing with the %fixperm Option

Dodecahedron

It is first necessary to run **SHAPE** with the %test keyword, to obtain the coordinates of the reference dodecahedron, whereupon the files dodec.tst and DD-20.xyz are generated.

Test file: dodec.dat

```
%test
   20  0
    1
```

Output file: dodec.tst

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

Ideal structures   L20

-------------------------------------------------------------------------
DD-20           1 Ih    Dodecahedron
-------------------------------------------------------------------------

   M     0.0000   0.0000   0.0000
   L     1.1135   0.8090  -0.2629
```

L	-0.4253	1.3090	-0.2629
L	-1.3764	0.0000	-0.2629
L	-0.4253	-1.3090	-0.2629
L	1.1135	-0.8090	-0.2629
L	0.4253	1.3090	0.2629
L	-1.1135	0.8090	0.2629
L	-1.1135	-0.8090	0.2629
L	0.4253	-1.3090	0.2629
L	1.3764	0.0000	0.2629
L	0.6882	0.5000	-1.1135
L	-0.2629	0.8090	-1.1135
L	-0.8507	0.0000	-1.1135
L	-0.2629	-0.8090	-1.1135
L	0.6882	-0.5000	-1.1135
L	0.2629	0.8090	1.1135
L	-0.6882	0.5000	1.1135
L	-0.6882	-0.5000	1.1135
L	0.2629	-0.8090	1.1135
L	0.8507	0.0000	1.1135

Distances

	L1	L2	L3	L4	L5	L6	L7	L8
X	1.4013	1.4013	1.4013	1.4013	1.4013	1.4013	1.4013	1.4013
L1		1.6180	2.6180	2.6180	1.6180	1.0000	2.2882	2.8025
L2			1.6180	2.6180	2.6180	1.0000	1.0000	2.2882
L3				1.6180	2.6180	2.2882	1.0000	1.0000
L4					1.6180	2.8025	2.2882	1.0000
L5						2.2882	2.8025	2.2882
L6							1.6180	2.6180
L7								1.6180

	L9	L10	L11	L12	L13	L14	L15	L16
X	1.4013	1.4013	1.4013	1.4013	1.4013	1.4013	1.4013	1.4013
L1	2.2882	1.0000	1.0000	1.6180	2.2882	2.2882	1.6180	1.6180
L2	2.8025	2.2882	1.6180	1.0000	1.6180	2.2882	2.2882	1.6180
L3	2.2882	2.8025	2.2882	1.6180	1.0000	1.6180	2.2882	2.2882
L4	1.0000	2.2882	2.2882	2.2882	1.6180	1.0000	1.6180	2.6180
L5	1.0000	1.0000	1.6180	2.2882	2.2882	1.6180	1.0000	2.2882
L6	2.6180	1.6180	1.6180	1.6180	2.2882	2.6180	2.2882	1.0000
L7	2.6180	2.6180	2.2882	1.6180	1.6180	2.2882	2.6180	1.6180
L8	1.6180	2.6180	2.6180	2.2882	1.6180	1.6180	2.2882	2.2882
L9		1.6180	2.2882	2.6180	2.2882	1.6180	1.6180	2.2882
L10			1.6180	2.2882	2.6180	2.2882	1.6180	1.6180
L11				1.0000	1.6180	1.6180	1.0000	2.2882
L12					1.0000	1.6180	1.6180	2.2882
L13						1.0000	1.6180	2.6180
L14							1.0000	2.8025
L15								2.6180

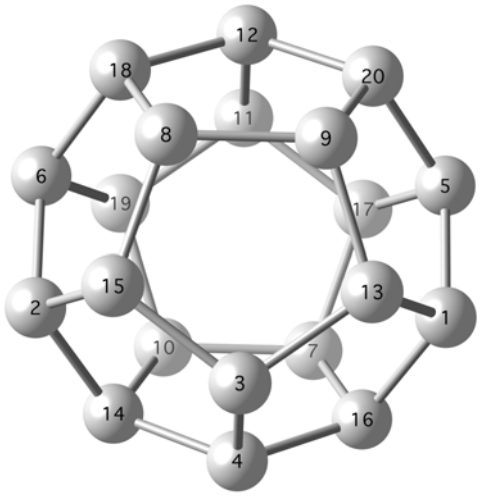
	L17	L18	L19	L20
X	1.4013	1.4013	1.4013	1.4013
L1	2.2882	2.6180	2.2882	1.6180
L2	1.6180	2.2882	2.6180	2.2882
L3	1.6180	1.6180	2.2882	2.6180
L4	2.2882	1.6180	1.6180	2.2882
L5	2.6180	2.2882	1.6180	1.6180
L6	1.6180	2.2882	2.2882	1.6180
L7	1.0000	1.6180	2.2882	2.2882
L8	1.6180	1.0000	1.6180	2.2882
L9	2.2882	1.6180	1.0000	1.6180
L10	2.2882	2.2882	1.6180	1.0000
L11	2.6180	2.8025	2.6180	2.2882
L12	2.2882	2.6180	2.8025	2.6180

```
    L13         2.2882    2.2882    2.6180    2.8025
    L14         2.6180    2.2882    2.2882    2.6180
    L15         2.8025    2.6180    2.2882    2.2882
    L16         1.0000    1.6180    1.6180    1.0000
    L17                   1.0000    1.6180    1.6180
    L18                             1.0000    1.6180
    L19                                       1.0000

  AnglesLXL

            L1        L2        L3        L4        L5        L6        L7        L8
    L1           70.5288 138.1897 138.1897  70.5288  41.8103 109.4712 180.0000
    L2                    70.5288 138.1897 138.1897  41.8103  41.8103 109.4712
    L3                             70.5288 138.1897 109.4712  41.8103  41.8103
    L4                                      70.5288 180.0000 109.4712  41.8103
    L5                                              109.4712 180.0000 109.4712
    L6                                                       70.5288 138.1897
    L7                                                                70.5288

      ...

This reference structure cannot be used without FIXPERM option

-------------------------------------------------------------------------------
```

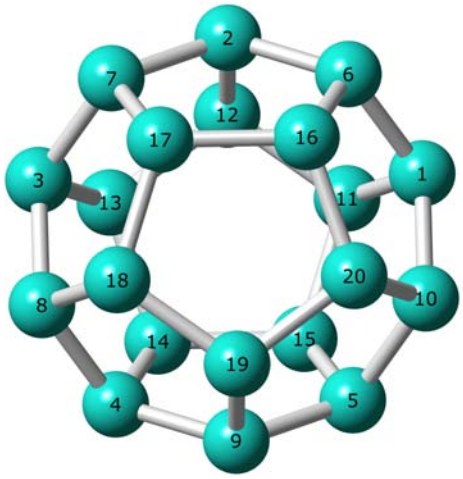
From the DD-20.xyz *we can generate the file containing the coordinates of the reference dodecahedron:* example09.ref

```
DD-20
Dodecahedron
Ih
    1.1135   0.8090  -0.2629
   -0.4253   1.3090  -0.2629
   -1.3764   0.0000  -0.2629
   -0.4253  -1.3090  -0.2629
    1.1135  -0.8090  -0.2629
    0.4253   1.3090   0.2629
   -1.1135   0.8090   0.2629
   -1.1135  -0.8090   0.2629
    0.4253  -1.3090   0.2629
    1.3764   0.0000   0.2629
    0.6882   0.5000  -1.1135
   -0.2629   0.8090  -1.1135
   -0.8507   0.0000  -1.1135
   -0.2629  -0.8090  -1.1135
    0.6882  -0.5000  -1.1135
    0.2629   0.8090   1.1135
   -0.6882   0.5000   1.1135
   -0.6882  -0.5000   1.1135
    0.2629  -0.8090   1.1135
    0.8507   0.0000   1.1135
    0.0000   0.0000   0.0000
```

Then a vertex of the ideal dodecahedron should be assigned to each vertex of the problem structure. As an example, we show here the skeleton of dodecahedrane (left) and the ideal polyhedron (right) with their atom numberings, that have been used to make the vertex assignment at the end of each coordinates line in the input file *example09.dat*.



Dodecahedrane ($C_{20}H_{20}$)



Ideal Dodecahedron

Input file: example09.dat

```
$ Example 9 - Dodecahedra with %fixperm option
%fixperm -1
  20  0
   1
dodecahedrane
  C1          28.44679      3.45463    -33.58569  10
  C2          24.39894      3.55118    -33.55192   8
  C3          26.41729      2.81375    -32.26794  19
  C4          26.38756      2.03139    -33.59312   9
  C5          28.47186      4.77961    -34.36851   1
  C6          24.42402      4.87616    -34.33474   3
  C7          27.16565      3.11796    -35.70969  15
  C8          25.70516      5.21282    -32.21073  17
  C9          27.24385      5.17612    -32.22357  16
  C10         25.62696      3.15466    -35.69686  14
  C11         26.45352      5.51703    -35.65248  12
  C12         26.48325      6.29939    -34.32731   2
  C13         27.68524      3.69624    -32.26352  20
  C14         25.14496      2.48854    -34.38902   4
  C15         25.19311      3.75568    -32.24273  18
  C16         27.63709      2.42910    -34.40981   5
  C17         27.67770      4.57510    -35.67770  11
  C18         25.23372      5.90168    -33.51061   7
  C19         25.18557      4.63454    -35.65691  13
  C20         27.72585      5.84224    -33.53140   6
Ar_hydrate_55707
 O1           0.39296     32.61596     -6.56135    2
 O2           0.30563     25.36797     -5.10327    9
 O3          -1.88792     31.99342     -5.04347    7
 O4           2.69910     31.92412     -5.11326    6
 O5           0.36408     26.80783     -2.69137   19
 O6           2.58651     25.99050     -6.62116    5
 O7          -2.00051     26.05980     -6.55136    4
 O8           0.33451     31.17609     -8.97325   12
 O9          -1.90822     28.33327     -2.74310   18
 O10         -0.90229     30.94117     -2.71661   17
 O11          1.75336     30.90105     -2.75702   16
 O12         -1.98021     29.71995     -8.85174   13
 O13         -3.26688     30.19314     -6.57660    3
 O14          2.67880     28.26397     -2.81289   20
 O15          3.96547     27.79078     -5.08803   10
 O16          1.60087     27.04275     -8.94802   15
 O17         -1.05477     27.08287     -8.90761   14
```

```
 O18          3.97579    30.08372    -6.68680    1
 O19          2.60681    29.65064    -8.92153   11
 O20         -3.27720    27.90021    -4.97783    8
```

Output file: example09.tab

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

Example 9 - Dodecahedra with %fixperm option

DD-20           1 Ih    Dodecahedron

Fixed vertices permutation used for CShM
(specific permutation for each fragment)

Structure [L20 ]        DD-20
 dodecahedrane  ,       0.000
 Ar_hydrate_5570,       0.075
```

Example 10: Truncated Icosahedron

Input file: fullerene.dat

```
$ Truncated icosahedra: C60 in C60H60 and In48Na12 in Na172In197Ni2
%fixperm -1
  60  0
   1

C60
   C1          0.005146    0.007254    0.003476  35
   C2          1.458757    0.007257    0.003476  34
   C3          1.907989    1.389770    0.003240  16
   C4          0.731948    2.244255    0.003047  57
   C5         -0.444088    1.389769    0.003238  17
   C6         -1.573237    1.756575    0.737186  18
   C7         -0.692556   -0.953037    0.737745  36
   C8          2.156466   -0.953034    0.737747  33
   C9          3.037135    1.756579    0.737190  15
   C10         0.731946    3.431330    0.737225  58
   C11         3.332048   -0.570871    1.502179  32
   C12         3.763628    0.756279    1.501828  31
   C13         3.037103    2.992887    1.501655  55
   C14         1.907956    3.813075    1.501639  56
   C15        -0.444061    3.813072    1.501634  60
   C16        -1.573211    2.992880    1.501650  59
   C17        -2.299724    0.756269    1.501826  38
   C18        -1.868146   -0.570881    1.502175  37
   C19         0.034164   -1.953560    1.501771   8
   C20         1.429747   -1.953559    1.501772   7
   C21        -0.692575   -2.189974    2.738343  49
   C22        -1.868623   -1.335620    2.738313   9
   C23         2.156486   -2.189970    2.738343  47
   C24         3.332537   -1.335613    2.738314   6
   C25         4.212753    1.374358    2.738298  30
   C26         3.764379    2.757156    2.738009  14
   C27         1.458799    4.431737    2.738000  54
   C28         0.005090    4.431737    2.737998  52
   C29        -2.300475    2.757146    2.738006  19
   C30        -2.748849    1.374346    2.738296  39
```

```
   C31          0.005106   -2.416864    3.925583  50
   C32          1.458809   -2.416861    3.925581  48
   C33          3.764380   -0.742262    3.925571   5
   C34          4.212758    0.640532    3.925282  29
   C35          3.332525    3.350500    3.925266  13
   C36          2.156480    4.204856    3.925236  53
   C37         -1.868632    3.350493    3.925264  20
   C38         -0.692587    4.204851    3.925233  51
   C39         -2.300472   -0.742271    3.925572  10
   C40         -2.748848    0.640522    3.925280  40
   C41          1.907964   -1.798191    5.161946  46
   C42          3.037112   -0.977998    5.161931  45
   C43         -1.573201   -0.978008    5.161927  41
   C44         -0.444052   -1.798196    5.161943  42
   C45         -2.299718    1.258603    5.161750  21
   C46         -1.868150    2.585751    5.161403  22
   C47          0.034157    3.968433    5.161808  11
   C48          1.429737    3.968437    5.161810  12
   C49          3.763626    1.258612    5.161751  28
   C50          3.332044    2.585757    5.161403  27
   C51          0.731958   -1.416450    5.926355  44
   C52         -1.573230    0.258297    5.926392   1
   C53         -0.692561    2.967916    5.925832  23
   C54          2.156460    2.967922    5.925834  26
   C55          3.037140    0.258303    5.926392   4
   C56          0.005146    2.007624    6.660108  24
   C57          1.458754    2.007626    6.660106  25
   C58          1.907991    0.625113    6.660343   3
   C59          0.731957   -0.229374    6.660537  43
   C60         -0.444084    0.625111    6.660340   2
!
In48Na12
    In2     19.548    4.583   50.605  54
    In2     20.537    7.431   50.590  53
    In3     18.517    3.387   53.161  52
    In3     20.476    9.033   53.131  12
    In3     21.079    2.476   49.105  56
    In3     23.039    8.122   49.075  13
    In6     27.501    1.869   62.126  10
    In6     28.500    4.744   62.110  41
    In6     32.632    0.044   54.005   7
    In6     33.630    2.920   53.989  47
    In8     22.947   -0.194   60.595  39
    In8     28.848   -2.293   51.256  34
    In8     26.198    9.170   60.545   2
    In8     32.099    7.072   51.206   5
    In10    28.974   -0.296   60.575   9
    In10    30.992    5.516   60.543  42
    In10    31.518   -1.201   56.548   8
    In10    33.535    4.611   56.517  48
    In18    18.443    4.977   55.792  51
    In18    19.443    7.856   55.777  11
    In18    23.651    3.125   47.550  55
    In18    24.650    6.004   47.535  14
    In21    27.517   -2.391   59.038  37
    In21    29.114   -2.959   56.511  36
    In21    31.141    8.048   58.982  44
    In21    32.738    7.480   56.455  46
    In22    31.462    2.039   49.825  32
    In22    23.723    4.791   62.074  21
    In23    19.374    0.519   53.202  60
    In23    20.939   -0.037   50.726  58
    In23    22.927   10.753   53.148  26
    In23    24.491   10.197   50.671  27
```

```
    In28    24.534   1.899  62.164  40
    In28    26.152   6.559  62.139   1
    In28    31.339  -0.521  51.394  33
    In28    32.957   4.140  51.369   6
    In30    31.414   0.485  59.022  49
    In30    32.418   3.376  59.007  50
    In35    24.440  -2.337  58.971  38
    In35    27.684  -3.491  53.838  35
    In35    28.693   9.912  58.906  43
    In35    31.936   8.758  53.772  45
    In48    20.240  -0.840  55.905  59
    In48    23.417  -1.970  50.876  57
    In48    24.457  11.310  55.840  25
    In48    27.635  10.179  50.811  28
    In51    29.090   2.852  47.971  31
    In51    21.201   5.658  60.458  22
    Na12    24.351  -3.935  53.504  17
    Na12    22.565  -3.300  56.331  18
    Na12    29.594  11.168  53.423   4
    Na12    27.808  11.804  56.250   3
    Na48    28.040   5.954  47.142  30
    Na48    26.342   1.060  47.168  15
    Na48    20.614   8.595  58.896  23
    Na48    18.915   3.701  58.923  20
    Na48    26.276  -1.885  49.115  16
    Na48    20.006   0.345  59.040  19
    Na48    29.821   8.325  49.060  29
    Na48    23.550  10.555  58.985  24
```

Output file: fullerene.tab

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

Truncated icosahedra: C60 in C60H60 and In48Na12 in Na172In197Ni2

TIC-60          1 Ih    Truncated Icosahedron

Fixed vertices permutation used for CShM
(specific permutation for each fragment)

Structure [L60 ]       TIC-60
 C60             ,       0.003
 In48Na12        ,       0.150
```

Example 11: Use of the %fixperm 1 Option

Compare the skeletons of phenylacetylenes and of disilyne with that of acetylene using the same permutation for all structures in a file.

Input file: example11.dat

```
%conquest
%fixperm 1
   4  0
   0
 2 1 4 3
```

Ideal shape file: example11.ref

```
ACET
Linear acetylene
Dinfh
           0.558100    0.424900    0.000000
           0.441900    0.575100    0.000000
           0.668900    0.293500    0.000000
           0.331100    0.706500    0.000000
```

ConQuest coordinates file (only first few lines shown): example11.cor

```
XONNOE  **FRAG**        1
Si1         12.73812  12.02248  32.82539     1555001
Si1E        12.02248  12.73812  34.67421     6557001
C1          12.46423  12.56259  31.05319     1555002
C1E         12.56259  12.46423  36.44641     6557002
ASIJER  **FRAG**        1
C7A          4.39115   8.06144   6.76854     2676012
C7           4.01895   7.80998   5.66677     1555012
C4A          4.81373   8.33510   8.11653     2676007
C4           3.59637   7.53633   4.31879     1555007
ASIJER  **FRAG**        2
C14A         3.63340   4.06486   5.66615     2666024
C14          4.00217   4.31791   6.76917     1555024
C11A         3.21994   3.77463   4.32712     2666019
C11          4.41562   4.60814   8.10820     1555019
CIFWUJ  **FRAG**        1
C1D         -1.38304   0.00000   4.17935     5556001
C1          -0.25053   0.00000   3.78587     1555001
C2D         -2.73089   0.00000   4.67877     5556002
C2           1.09731   0.00000   3.28645     1555002
COBSUI  **FRAG**        1
C44A         4.72609  10.27316   6.83506     2676097
C44          3.61994  10.30689   6.38301     1555097
C45A         6.06242  10.24539   7.37753     2676098
C45          2.28361  10.33465   5.84054     1555098
```

Output file: example11.tab

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

ACET            0 Dinfh Linear acetylene

Fixed vertices permutation used for CShM
   2   1   4   3

Structure [L4  ]         ACET
 XONNOE   1     ,       2.915
 ASIJER   1     ,       0.329
 ASIJER   2     ,       0.317
 CIFWUJ   1     ,       0.311
 COBSUI   1     ,       0.328
 DPHACT01 1     ,       0.241
 DPHACT01 2     ,       0.217
 DPHACT02 1     ,       0.305
 DPHACT02 2     ,       0.310
 DPHACT03 1     ,       0.323
```

```
 DPHACT03 2     ,       0.321
 DPHACT05 1     ,       0.270
 DPHACT05 2     ,       0.272
 DPHACT06 1     ,       0.277
 DPHACT06 2     ,       0.294
 DPHACT07 1     ,       0.316
 DPHACT07 2     ,       0.308
 DPHACT08 1     ,       0.300
 DPHACT08 2     ,       0.296
 DPHACT09 1     ,       0.308
 KURCEG   1     ,       0.308
 OCAYIA   1     ,       0.310
 OCAYIA01 1     ,       0.317
 PUZBIV   1     ,       0.330
 UKOLIP   1     ,       0.305
 YALSOT   1     ,       0.310
```

Example 12: Use of the %fixperm 0 **Option**

To be used with the example12.cor and example12.ide files. Compares the skeletons of phenylacetylenes and of disilyne with that of acetylene by comparing the *i*-th atom of each structure with the corresponding atom of the reference structure (%fixperm 0).

Input file: example12.dat

```
%conquest example12
%fixperm 0
   4  0
   0
```

This input file is equivalent to:

```
%conquest example12
%fixperm 1
   4  0
   0
 1 2 3 4
```

Ideal shape file: example12.ref is identical to example11.ref.

Output file: example12.tab

```
-------------------------------------------------------------------------------
S H A P E   v2.1         Continuous Shape Measures calculation
(c) 2013  Electronic Structure Group, Universitat de Barcelona
                  Contact:  llunell@ub.edu
-------------------------------------------------------------------------------

ACET            0 Dinfh Linear acetylene

Fixed vertices permutation used for CShM
   1   2   3   4

Structure [L4  ]         ACET
 XONNOE   1     ,       2.915
 ASIJER   1     ,       0.329
 ASIJER   2     ,       0.317
 CIFWUJ   1     ,       0.311
```

Example 13: Getting coordinates of Internally Defined Reference Shapes

Input file: example13.dat

```
$ Generate 9-vertices reference shapes
%test
  9 1
  1 8
```

Output files: example13.tst, EP-9.xyz and CSAPR-9.xyz.

EP-9.xyz:

```
 10

N          0.00000000    0.00000000    0.00000000
H          1.00000000    0.00000000    0.00000000
H          0.76604444    0.64278761    0.00000000
H          0.17364818    0.98480775    0.00000000
H         -0.50000000    0.86602540    0.00000000
H         -0.93969262    0.34202014    0.00000000
H         -0.93969262   -0.34202014    0.00000000
H         -0.50000000   -0.86602540    0.00000000
H          0.17364818   -0.98480775    0.00000000
H          0.76604444   -0.64278761    0.00000000
```

CSAPR-9.xyz:

```
 10

N          0.00000000    0.00000000    0.00000000
H          0.00000000    0.00000000    1.00000000
H          0.93222657    0.00000000    0.36187516
H          0.00000000    0.93222657    0.36187516
H         -0.93222657    0.00000000    0.36187516
H          0.00000000   -0.93222657    0.36187516
H          0.56059535    0.56059535   -0.60947986
H         -0.56059535    0.56059535   -0.60947986
H         -0.56059535   -0.56059535   -0.60947986
H          0.56059535   -0.56059535   -0.60947986
```

Example 14: Generating Coordinates of Structures Along a Minimal Distortion Path

Input file: movie.dat

```
$ Generation of xyz files for a minimal distortion pathway
%test
%path
   6 1
   3 4
```

Output file: movie.tst (see Example 9)

Coordinates files: TPR-6.xyz and OC-6.xyz (coordinates of the two ideal shapes), and movie.xyz (structures along the path, only the first four structures shown):

```
7

N          0.00000000    0.00000000    0.00000000
H          0.81649658    0.00000000   -0.70710678
H         -0.40824829    0.70710678   -0.70710678
H         -0.40824829   -0.70710678   -0.70710678
```

```
H          0.81649658   0.00000000   0.70710678
H         -0.40824829   0.70710678   0.70710678
H         -0.40824829  -0.70710678   0.70710678
  7

N          0.00000000   0.00000000   0.00000000
H          0.81051792   0.02011845  -0.70020322
H         -0.42268205   0.69186989  -0.70020322
H         -0.38783588  -0.71198833  -0.70020322
H          0.81051792  -0.02011845   0.70020322
H         -0.38783588   0.71198833   0.70020322
H         -0.42268205  -0.69186989   0.70020322
  7

N          0.00000000   0.00000000   0.00000000
H          0.80453927   0.04023689  -0.69329966
H         -0.43711580   0.67663300  -0.69329966
H         -0.36742346  -0.71686989  -0.69329966
H          0.80453927  -0.04023689   0.69329966
H         -0.36742346   0.71686989   0.69329966
H         -0.43711580  -0.67663300   0.69329966
  7

N          0.00000000   0.00000000   0.00000000
H          0.79856061   0.06035534  -0.68639610
H         -0.45154956   0.66139610  -0.68639610
H         -0.34701105  -0.72175144  -0.68639610
H          0.79856061  -0.06035534   0.68639610
H         -0.34701105   0.72175144   0.68639610
H         -0.45154956  -0.66139610   0.68639610
```

Viewing the structures in Crystal Maker:

1. Load the multiple structure file generated by **SHAPE 2.1** (***File*** > ***Import*** > ***XYZ*** > movie.xyz)
2. All the snapshots appear in the ***Views*** panel.
3. In the Window menu, select ***Play Views***. Suggested settings:

   0.1 sec per frame

   Loop – back and forth

   Full screen

Generating a QuickTime movie:

Click on the Overview window's ***Actions*** button  to display a popup menu (lower left corner in the bottom Views palette) and choose ***Save as Movie***.

Movies are saved in QuickTime format (extension .mov). You can customize your movie settings, including the type and quality of compression, frame rate, and so on, using the ***Movie Options*** command.