

# SHAPE

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

## User's Manual

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## TABLE OF CONTENTS

About <b>SHAPE</b>	3
Using <b>SHAPE</b>	3
Standard input file	3
Reference polyhedra	4
Input using an external atomic coordinates file	5
Output files	6
Minimal distortion paths	6
Selecting structures with stereochemical criteria	6
User-defined reference shapes	7
Acknowledgments	7
List of reference shapes	8
File extensions	11
Optional keywords	12
Examples and sample files	14

## 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 synonyms. **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 crystallographically 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
<b>2</b>	1	L-2	Linear	$D_{\infty h}$
	2	vT-2	Divacant tetrahedron (V-shape, 109.47°)	$C_{2v}$
	3	vOC-2	Tetravacant octahedron (L-shape, 90°)	$C_{2v}$
<b>3</b>	1	TP-3	Trigonal planar	$D_{3h}$
	2	vT-3	Pyramid <sup>‡</sup> (vacant tetrahedron)	$C_{3v}$
	3	fac-vOC-3	fac-Trivacant octahedron	$C_{3v}$
	4	mer-vOC-3	mer-Trivacant octahedron (T-shape)	$C_{2v}$
<b>4</b>	1	SP-4	Square	$D_{4h}$
	2	T-4	Tetrahedron	$T_d$
	3	SS-4	Seesaw or sawhorse <sup>‡</sup> ( <i>cis</i> -divacant octahedron)	$C_{2v}$
	4	vTBPY-4	Axially vacant trigonal bipyramid	$C_{3v}$
<b>5</b>	1	PP-5	Pentagon	$D_{5h}$
	2	vOC-5	Vacant octahedron <sup>‡</sup> (Johnson square pyramid, J1)	$C_{4v}$
	3	TBPY-5	Trigonal bipyramid	$D_{3h}$
	4	SPY-5	Square pyramid <sup>§</sup>	$C_{4v}$
	5	JTBPY-5	Johnson trigonal bipyramid (J12)	$D_{3h}$
<b>6</b>	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)	$C_{5v}$
<b>7</b>	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)	$C_{3v}$
<b>8</b>	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
<b>9</b>	1	EP-9	Enneagon	D <sub>9h</sub>
	2	OPY-9	Octagonal pyramid	C <sub>8v</sub>
	3	HBPY-9	Heptagonal bipyramid	D <sub>7h</sub>
	4	JTC-9	Triangular cupola (J3) = trivacant cuboctahedron	C <sub>3v</sub>
	5	JCCU-9	Capped cube (Elongated square pyramid, J8)	C <sub>4v</sub>
	6	CCU-9	Capped cube	C <sub>4v</sub>
	7	JCSAPR-9	Capped sq. antiprism (Gyroelongated square pyramid J10)	C <sub>4v</sub>
	8	CSAPR-9	Capped square antiprism	C <sub>4v</sub>
	9	JTCTPR-9	Tricapped trigonal prism (J51)	D <sub>3h</sub>
	10	TCTPR-9	Tricapped trigonal prism	D <sub>3h</sub>
	11	JTDIC-9	Tridiminished icosahedron (J63)	C <sub>3v</sub>
	12	HH-9	Hula-hoop	C <sub>2v</sub>
	13	MFF-9	Muffin	C <sub>s</sub>
<b>10</b>	1	DP-10	Decagon	D <sub>10h</sub>
	2	EPY-10	Enneagonal pyramid	C <sub>9v</sub>
	3	OBPY-10	Octagonal bipyramid	D <sub>8h</sub>
	4	PPR-10	Pentagonal prism	D <sub>5h</sub>
	5	PAPR-10	Pentagonal antiprism	D <sub>5d</sub>
	6	JBCCU-10	Bicapped cube (Elongated square bipyramid J15)	D <sub>4h</sub>
	7	JBCSAPR-10	Bicapped square antiprism (Gyroelongated square bipyramid J17)	D <sub>4d</sub>
	8	JMBIC-10	Metabidiminished icosahedron (J62)	C <sub>2v</sub>
	9	JATDI-10	Augmented tridiminished icosahedron (J64)	C <sub>3v</sub>
	10	JSPC-10	Sphenocorona (J87)	C <sub>2v</sub>
	11	SDD-10	Staggered dodecahedron (2:6:2) <sup>#</sup>	D <sub>2</sub>
	12	TD-10	Tetradecahedron (2:6:2)	C <sub>2v</sub>
	13	HD-10	Hexadecahedron (2:6:2, or 1:4:4:1)	D <sub>4h</sub>
<b>11</b>	1	HP-11	Hendecagon	D <sub>11h</sub>
	2	DPY-11	Decagonal pyramid	C <sub>10v</sub>
	3	EBPY-11	Enneagonal bipyramid	D <sub>9h</sub>
	4	JCPPR-11	Capped pent. Prism (Elongated pentagonal pyramid J9)	C <sub>5v</sub>
	5	JCPAPR-11	Capped pent. antiprism (Gyroelongated pentagonal pyramid J11)	C <sub>5v</sub>
	6	JAPPR-11	Augmented pentagonal prism (J52)	C <sub>2v</sub>
	7	JASPC-11	Augmented sphenocorona (J87)	C <sub>s</sub>

Vertices	Code	Label	Shape	Symmetry
<b>12</b>	1	DP-12	Dodecagon	D <sub>12h</sub>
	2	HPY-12	Hendecagonal pyramid	C <sub>11v</sub>
	3	DBPY-12	Decagonal bipyramid	D <sub>10h</sub>
	4	HPR-12	Hexagonal prism	D <sub>6h</sub>
	5	HAPR-12	Hexagonal antiprism	D <sub>6d</sub>
	6	TT-12	Truncated tetrahedron	T <sub>d</sub>
	7	COC-12	Cuboctahedron	O <sub>h</sub>
	8	ACOC-12	Anticuboctahedron (Triangular orthobicupola J27)	D <sub>3h</sub>
	9	IC-12	Icosahedron	I <sub>h</sub>
	10	JSC-12	Square cupola (J4)	C <sub>4v</sub>
	11	JEPBPY-12	Elongated pentagonal bipyramid (J16)	D <sub>6h</sub>
	12	JBAPPR-12	Biaugmented pentagonal prism (J53)	C <sub>2v</sub>
	13	JSPMC-12	Sphenomegacorona (J88)	C <sub>s</sub>
<b>20</b>	1	DD-20	Dodecahedron <sup>†</sup>	I <sub>h</sub>
<b>24</b>	1	TCU-24	Truncated cube	O <sub>h</sub>
	2	TOC-24	Truncated octahedron	O <sub>h</sub>
<b>48</b>	1	TCOC-48	Truncated cuboctahedron	O <sub>h</sub>
<b>60</b>	1	TRIC-60	Truncated icosahedron (fullerene)	I <sub>h</sub>

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

<sup>‡</sup> 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°).

<sup>†</sup> For polyhedra with more than 12 vertices the calculation times may be impractical, 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

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

## Optional Keywords §

Keyword	Argument	Description
%conquest	[ <i>name.cor</i> ]	Reads the atomic coordinates from a <i>name.cor</i> file generated by ConQuest.
%external	[ <i>name.shp</i> ]	Reads the atomic coordinates from an external <i>name.shp</i> file.
%fixperm	<i>N</i>	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 <i>ID.xyz</i> file generated with the %test keyword. <i>N</i> can adopt one of the following values:
	<i>N</i> = -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.
	<i>N</i> = 0	the vertices are taken in order of appearance in the list of coordinates, exclusive of the central atom if present.
	<i>N</i> = 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 <i>name.out</i> file containing the coordinates of the problem structures and of the closest reference polyhedra, the continuous shape measures and the optimal vertex pairing.
%ideal	<i>file</i>	This keyword was used in version 2.0 of <b>SHAPE</b> and is replaced in the new version by %reference. However, the program can properly handle input files with the old keyword.
%maxcsm	<i>y</i>	Generates output files <i>name.flt</i> and <i>name.flt.csv</i> with the shape measures for only those structures having at least one shape measure smaller than <i>y</i> ( <i>y</i> is a real number). It is advisable to use this option with only one reference shape.
%maxdev	<i>y</i>	Generates <i>name.flt</i> and <i>name.flt.csv</i> files with the shape measures for only those structures having path deviation functions smaller or equal than <i>y</i> (more details as specified for %maxcsm).
%maxgco	<i>y</i>	Generates <i>name.flt</i> and <i>name.flt.csv</i> files with the shape measures for only those structures with generalized coordinates smaller than <i>y</i> (more details as specified for %maxcsm).
%mincsm	<i>x</i>	Generates <i>name.flt</i> and <i>name.flt.csv</i> files with the shape measures for only those structures with at least one shape measure larger than <i>x</i> (more details as specified for %maxcsm). It is advisable to use this option with only one ideal shape.
%mindev	<i>x</i>	Generates <i>name.flt</i> and <i>name.flt.csv</i> files with the results for only those structures with path deviation functions larger or equal than <i>x</i> (more details as specified for %maxcsm).
%mingco	<i>x</i>	The program selects structures with shape measures, path deviation functions or generalized coordinates larger than a desired value <i>x</i> ,

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

**NOTE:** The combined use of %maxxxx and %minxxx 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.

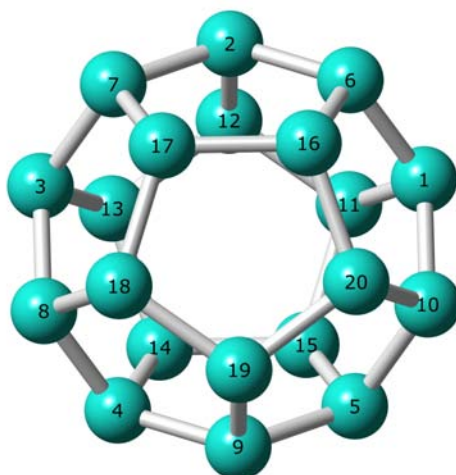
%nosymbol		Indicates that no atomic labels are included with the coordinates.
%path		Calculates the <i>path deviation function</i> for the minimal distortion interconversion path between two given polyhedra as well as the generalized coordinate. Two and only two reference polyhedra should be coded in 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	<i>file</i>	Points to a <i>file.ref</i> 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 <b>SHAPE</b> , but the program can properly handle input files with the old keyword.
%select	<i>label</i>	Performs shape measures only for the set of coordinates under the structure label specified and places the results in a file with the name <i>label</i> .
%stop	<i>N</i>	Calculates the shape measures for the first <i>N</i> 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	<i>x</i>	This option is replaced in <b>SHAPE 2.1</b> 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	15
Example 2: Atomic coordinates from a .cor file generated by CSD's ConQuest	16
Example 3: Input with external coordinates	17
Example 4: Use of the %fullout keyword	17
Example 5: Deviation from minimal distortion pathways	19
Example 6: Use of the %maxdev keyword	21
Example 7: Use of the %maxgco and %mingco keywords	23
Example 8: Use of a user-defined reference polyhedron	24
Example 9. Large polyhedra: specifying a vertex pairing with the %fixperm option	25
Example 10: Truncated Icosahedron	29
Examples 11 and 12: Other %fixperm options	31
Example 13: Getting coordinates of internally defined ideal shapes	34
Example 14: Generating coordinates of structures along a minimal distortion path	34

## 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 distortion 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
Cl       3.11326    4.57241    0.99635    1555002
ADUVOL  **FRAG**           1
Ni1      6.37726    3.85616   10.65061    1555001
Cl       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 distortion 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 distortion 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, %mingco and %maxgco options
!           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, %mingco and %maxgco options

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

Minimal distortion 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

*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, %mingco and %maxgco options

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

Minimal distortion 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 Nil ,	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 distortion 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*

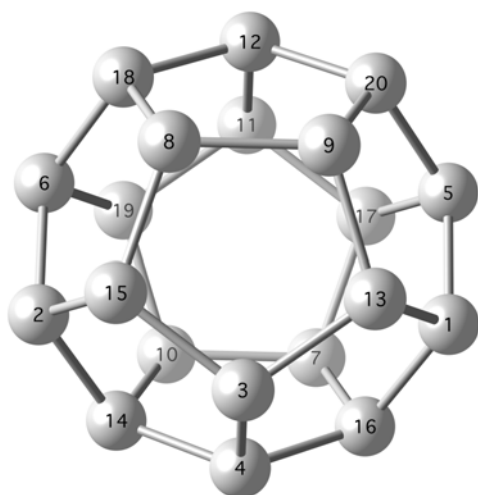
DD-20

Dodecahedron

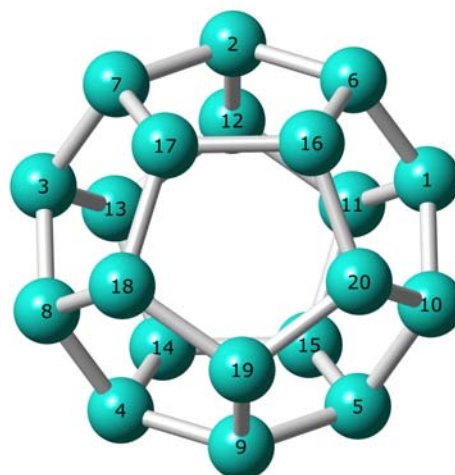
Ih

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<sub>20</sub>H<sub>20</sub>)



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
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                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
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                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
Dinhf
      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 Dinhf 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
OCAZIA	1	,	0.310
OCAZIA01	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.