StrDiscr2 v.1.0

Short User Manual

StrDiscr2 is the program for structural classification and similarity estimation of atomic clusters. It reads the Cartesian coordinates of cluster structures written in different formats along with the cluster energies and frequencies (if they are available) calculated at the quantum chemical or empirical potential levels and applies several algorithms in order to compare the supplied structures with each other and classify them to the classes of identic structures.

Algorithms that are used to classify the clusters

1. Comparison of cluster energies;
2. Comparison of the cluster principal moments of inertia;
3. Comparison of sorted lists of interatomic distances between all atom pairs in the cluster;
4. Comparison of structural "fingerprints" i.e. sorted eigenvalues of the matrix of overlap integrals between the Gaussian functions solid spherical functions (Gaussian atomic pseudo orbitals, pseudo-GAO) centered at all atoms of a cluster;
5. Comparison of canonicalized g6-strings describing the isomorphic graphs corresponding to the cluster connectivity matrix.

Formats of files containing the cluster coordinates

1. ASCII files containing the NXYZ matrices of atom names and Cartesian coordinates of cluster structures (both single and multiple structures per file). The beginning of each structure is marked with a text label at any place of the line preceding the NXYZ matrix. The energy of the structure should be provided as a separate word/value at the line where the text label is present. The calculated frequencies of the cluster (obtained e.g. using quantum chemical calculations) can also be provided at the same file. The end of structure is marked with blank line(s) immediately after NXYZ matrix. Example files are given below.
2. Output file of Gaussian03/09/16 containing Cartesian coordinates (standard orientation), energies and vibrational frequencies (if any) calculated with DFT/HF methods. In the case of successful optimization, only the optimized structure (located by the Gaussian text string 'Stationary point found') will be analyzed. In the case of multiple structures presented in the file without a successful optimization string, only the last structure will be analyzed.

Main input file of the program

The file *StrDiscr2.inp* should be present at the same directory where the program runs. It contains the main keywords and parameters describing the program operations. The first line of the file contains the keywords, the remaining lines describe files where the Cartesian coordinates have to be read from. There can be single or multiple coordinate files, each at the separate line. First blank line appeared in the list of structure files means the end of input stream. Main keywords (placed at the first line of *StrDiscr2.inp*, case insensitive) are:

Keyword	**Example**	**Meaning**	**Default**
FilOut	FilOut=Mg10.out	Output file name	*StrDiscr2.out*
Method=[Str|PMOI|FP]	Method=FP	Main classification algorithm to be used	All algorithms 1-5 at once
Rbond=<Rmax>	Rbond=3.2	Maximum bond length in Angstroems to be used as a threshold for connectivity matrix construction	1.15*(Ra+Rb) where Ra, Rb – valence readii of atoms A and B
EpsE=<value>	EpsE=0.01	Threshold (in the units of energy) for discrimination on the basis of energy (algorithm 1). The structures are considered identic if the relative absolute difference between their energies is within EpsE.	0.1 units of energy (units can be indicated by *Eunits* keywords)
EpsPMOI=<value>	EpsPMOI=0.05	Threshold (dimensionless) for discrimination on the basis of PMI (algorithm 2). The structures are considered identic if the relative absolute difference between each pair of their sorted PMIs is within epsPMOI: $\left\|\frac{PMI_i^A - PMI_i^B}{PMI_i^B}\right\| < EpsPMOI$	0.01
EpsStr=<value>	EpsStr=0.01	Threshold (dimensionless units) for discrimination on the basis of interatomic distances (algorithm 3). The structures are considered identic if the relative absolute deviation for any pair in the lists of sorted interatomic distances of two clusters is within EpsStr: $\left\|\frac{r_{ij}^A - r_{ij}^B}{r_{ij}^B}\right\| < EpsStr$	0.03
EpsFP=<value>	EpsFP=0.01	Threshold (dimensionless) for discrimination on the basis of fingerprints (algorithm 4). Two structures are considered	10^{-4}

		identic if the relative absolute deviation for any pair in the lists of their sorted fingerprints is within EpsFP: $\left\|\frac{p_i^A - p_i^B}{p_i^B}\right\| < EpsStr$	
StrLabel=<string>	StrLabel=*Geo	Label to read the Cartesian coordinates from the ASCII file with structures(s). It is case insensitive.	no defaults
Eword=<string>	Eword=9	Ordering number of the word (i.e. separate value) on the line with StrLabel containing the value of structure energy	no defaults
E1value=<value>	E1value=-2605.354678	Single atom energy for the atoms forming the cluster. It is needed to calculate the binding energy and energies per atom.	no default. Units are regulated by the Eunits keyword.
Einput=<integer>	Einput=2	Type of energy on input (total energy (1), binding energy (2), per atom binding energy (3))	1
Eanalysis=<integer>	Eanalysis=3	Type of energy to be analyzed (total energy (1), binding energy (2), per atom binding energy (3))	1
Eunits=[au|ev|kcal|kj]	Eunits=kcal	Units ot the energy that is read in (Hartee(au), electron-volts(ev), kcal/mol(kcal), kJ/mol(kj)	au
SymEps=<value>	SymEps=0.05	Threshold (Angstroems) to recognize the symmetry group. Atoms are considered equivalent if they are within SymEps after symmetry transformation.	0.1
Freq1min=<value>	Fre1min=5	Minimum frequency allowed. Structure will be discarded from the further analysis if it has the frequencies lower Freq1min	0.
ShowAll(nr,ud,hs,vs,np)	ShowAll(5,1,19.,15.,30)	Combine all the clusters as a single structure (for drawing on a single page). Nr – number of structures	nr=1 ud=1 hs=15 vs=15

		in a row; ud=1|-1 – numeration up to down or vice versa; hs,vs – horizontal and vertical shifts; np – number of clusters on a page.	np= <all structures>
NoGraph	Present | Not present	Do not carry out the graph isomorphism calculations	Not present
GeoTemp=<file>	GeoTemp=g.gjf	Generate the additional input file(s) with the corrected structures in case the imaginary frequencies were found on input. The structures will be corrected by the addition of the imaginary vibration vector to the input coordinates.	no defaults

Output files

After the calculations finished, the main output file *StrDiscr2.out* will be created. Its name can be changed by the keyword *FilOut.* It contains all the comments on the calculations and the final table with classified structures.

Along with *StrDiscr2.out*, additional files will be created:

File	**Description**
Structures-original.xyz	Original structures to be analyzed (all coordinates extracted from all input files, some structures discarded due to negative frequencies and other restrictions, as described in file *StrDiscr2.out*)
Structures-rotated.xyz	Original structures reduced to the principal axes
Structures-classes.xyz	Classified structures: 1st structures of each class
Structures-graphs.g6	g6 strings corresponding to each structure to be analyzed. This file is used for further graph isomorphism analysis

Graph isomorphism analysis

To perform classification based on the graph isomorphism algorithm (algorithm 5), the generated file *Structures-graphs.g6* should be processed with the separate program *labelg* from the program suite *Traces/Nauty* of B.D. McKay and A. Piperno. This program is freely available on the *Traces/Nauty* site https://pallini.di.uniroma1.it/ . Unfortunately, it operates under LINUX only. Once *labelg* is downloaded and compiled, the generated file *Structures-graphs.g6* should be processed with it using the command

```
./labelg Structures-graphs.g6 Structures-canonic.g6
```

This produces the file *Structures-canonic.g6* containing the canonicalized g6 strings corresponding to the clusters under analysis. The file *Structures-canonic.g6* should be transferred to your working directory and *StrDiscr2.exe* should be run once more with the same input files (no input file modifications are required). Once *StrDiscr2* finds the *Structures-canonic.g6* it compares the canonic strings of the connectivity graphs and classifies the structures based on the graph isomorphism. The results will be printed at the end of main output file *StrDiscr2.out*.

Analysis of results

Some additional information on the input and results can be found in the example files described below.

Author, licenses and reviews

The author of the program:
Prof. Dr. Stanislav K. Ignatov
Theoretical Chemistry Group, Chair of Physical Chemistry, Department of Chemistry
N.I. Lobachevsky State University of Nizhny Novgorod,
Nizhny Novgorod, Russia, 2020-2021.
skignatov@gmail.com , ignatov@ichem.unn.ru , http://qchem.unn.ru

Questions about program usage, messages about possible bugs, feedback and wishes should be sent to skignatov@gmail.com

Example of the main input file *StrDiscr2.inp:*

```
EpsE=1.0 EpsFP=0.0001 EpsStr=0.05 EpsPMOI=0.01 StrLabel=*lm Eword=9 E1value=-200.069705900  Eanalysis=2 Einput=1 Eunits=au
mg13.sbas_
mg13-nneg.sbas_
mg13-coh-cont2-tight.log
```

EOF

Example of NXYZ coordinate file *mg13.bas_* .

The file was generated by the program of global optimization RUNNER. It contains some comments (marked with ! sign at the beginning of lines) , NXYZ matrices of Cartesian coordinates (columns 1-4 after line marked with the label `*lm` requested in the main input file). It also contains the vibrational frequencies (columns 5-7) and some other information which does not matter for calculations. There are 2 clusters in the example file. Energy of each structure is the 9th word on the line being recognized by the label *lm.

<Beginning of the file *mg13.bas_*>

```
!ShortBase file :01/09/2020  15:44:45 RunCode 200901-154445-520791
!Stoichiometry  :Mg13
@geo-000204-00 icyc    17 iStrGeo    9246 nStrProc   201 Etot         -2601.109823     *end *opt *freq *lm        5.73      6.84     21.31
Mg1       -1.185901    0.543332   -1.453378            5.731       6.841      21.315            0.070      -0.080       0.030
Mg2       -3.879159    2.218442   -1.393885           30.533      36.669      48.376            0.190       0.110      -0.040
Mg3        1.173944   -1.639323   -0.413771           54.834      56.936      64.652           -0.100      -0.230       0.080
Mg4        3.596972   -0.000321   -0.000226           72.703      74.014      87.110            0.000      -0.390       0.070
Mg5        6.672047   -0.000150   -0.000018          101.373     109.702     115.677            0.000      -0.120      -0.010
Mg6        9.983393    0.000214    0.000270          117.781     117.981     129.687            0.000       0.670      -0.140
Mg7       -4.440231    0.856101    1.281450          136.375     142.187     143.393            0.020       0.150      -0.060
Mg8        1.174258    1.639130    0.413412          155.242     159.932     169.756            0.100      -0.230       0.080
Mg9       -1.794660    2.465461    0.854672          170.772     176.764     178.432            0.150      -0.040       0.020
Mg10      -1.185850   -0.543261    1.453155          184.709     194.204     200.804           -0.070      -0.080       0.030
Mg11      -3.879064   -2.218366    1.394173          204.182     229.342     264.488           -0.190       0.110      -0.040
Mg12      -1.795042   -2.465327   -0.854886            0.000       0.000       0.000           -0.150      -0.040       0.020
Mg13      -4.440706   -0.855932   -1.280969            0.000       0.000       0.000           -0.020       0.150      -0.060

@geo-000205-00 icyc    37 iStrGeo    9283 nStrProc   202 Etot         -2601.108000     *end *opt *freq *lm        9.30     18.78     29.86
Mg1        2.114945   -0.884675    1.126934            9.299      18.777      29.859            0.130      -0.030       0.140
Mg2        0.483242    1.479274   -0.130703           35.288      39.799      48.216            0.000       0.000       0.340
Mg3        5.020322   -1.491294   -0.769086           54.032      63.310      71.094           -0.050       0.030      -0.200
Mg4        3.683349    1.378816   -0.209598           76.591      85.146      91.449           -0.010       0.010       0.050
Mg5        1.793634   -0.684518   -1.854895          105.329     106.139     113.147           -0.160       0.050       0.170
Mg6       -2.601103    1.441255   -0.089957          127.802     138.840     139.326            0.000      -0.010       0.210
Mg7       -5.379175    1.011108    1.604629          149.100     151.333     152.721           -0.260       0.090      -0.210
Mg8       -0.793330   -1.345701   -0.173120          154.978     161.054     167.424            0.010       0.000       0.410
```

```
Mg9       -3.886129   -1.341362    0.010285          170.126     172.885     181.337           -0.010      -0.010       0.150
Mg10      -5.588968    1.002911   -1.354144          185.042     196.588     202.502            0.200      -0.080      -0.240
Mg11       5.361970   -0.326498    1.967783          206.055     217.554     241.921            0.230      -0.090      -0.190
Mg12       6.783953    0.971355   -0.368403            0.000       0.000       0.000           -0.030       0.030      -0.290
Mg13      -6.992710   -1.210670    0.240275            0.000       0.000       0.000           -0.050       0.010      -0.330
```

<EOF>

Example of NXYZ coordinate file *mg13-nneg.bas_* .

It contains NXYZ matrices of Cartesian coordinates (columns 1-4) after the line marked with the requested label `*lm`. No frequencies, no other information except for Cartesian coordinates. There is only 1 cluster in a single file. Energy of the structure is a 9th word on the line labeled ***lm* (`-2601.157248`)

Example of NXYZ coordinate file *mg13-nneg.sbas_*

```
@geo-000001-00 icyc    68 iStrGeo      68 nStrProc     1 Etot         -2601.157248     *end *opt *freq *lm       33.81     57.41     59.40
Mg1       -0.798616   -1.521954   -2.127490
Mg2       -0.798656    1.520814   -2.128293
Mg3       -2.122554   -2.004816    0.508246
Mg4        0.807039   -2.144862    0.447859
Mg5       -0.580600    0.000610    2.221105
Mg6       -2.122684    2.005108    0.507151
Mg7       -3.462261   -0.000431   -1.447479
Mg8        3.973031    1.507641   -0.179525
Mg9        1.752717   -0.000398   -1.642894
Mg10      -3.952499    0.000351    1.606679
Mg11       3.973074   -1.507728   -0.178693
Mg12       0.806940    2.145111    0.446782
Mg13       2.525069    0.000553    1.966552
```

<EOF>

Example of output file StrDiscr2.out (shown only partially)

Some comments on the information in the file are given with *** labels.

```
<beginning of file>

 *****  STRUCTURE DISCRIMINATOR II v.1.0 *****
Keyword found:  EPSE=1.0
Keyword found:  EPSFP=0.0001
Keyword found:  EPSSTR=0.05
Keyword found:  EPSPMOI=0.01
Keyword found:  STRLABEL=*LM
Keyword found:  EWORD=9
Keyword found:  E1VALUE=-200.069705900
Keyword found:  EINPUT=1
Keyword found:  EUNITS=AU
Keyword found:  SHOWALL(5,1,20.,15.,30)


Discrimination thresholds:
Energy         1.00000
Structure      0.05000
PMOI           0.01000
Fingerprints   0.00010
SymGroup eps   0.10000 A
RbondMax not set -- will be used by default as 1.15*(Ra+Rb)


Structures will be read in from files:
  1  mg13.sbas_
  2  mg13-nneg.sbas_
  3  mg13-coh-cont2-tight.log
*** Comments for the information above: Here are the keywords found in the main input file and the main options in effect.
*** Then, the information on the structures read-in from 3 structure input files follows:

Structures will be selected from file using the label (case-insensitive): *LM


   i Fil FilStr Str         Energy(1)           Energy(2)           Energy(3)  StrDiam  Connect       Graph    Graph No.  SymGrp      StrLabel in fil
   1   1   1    1      -2601.16097400      -159.87577633       -12.29813664    7.85    1           Lyf\Re_EpD      -1  C1          @geo-000002-00
   2   1   2    2      -2601.16372600      -161.60255341       -12.43096565    8.19    1           LqBG^W\``U      -1  C1          @geo-000001-00
   3   1   3    3      -2601.15886200      -158.55057532       -12.19619810    7.86    1           L~_uBEI?{w      -1  C1          @geo-000005-00
   4   1   4    4      -2601.16097400      -159.87577633       -12.29813664    7.85    1           LJPLC`g|te      -1  C1          @geo-000003-00
   5   1   5    5      -2601.16097400      -159.87577633       -12.29813664    7.85    1           L^IkjoNCyA      -1  C1          @geo-000004-01
   6   1   6    6      -2601.15803400      -158.03103629       -12.15623356    7.82    1           LVUY^e`_GE      -1  Cs          @geo-000009-00
   7   1   7    7      -2601.16372600      -161.60255341       -12.43096565    8.19    1           Lm}BcG\EHO      -1  C1          @geo-000006-00
```

```
    8   1   8    8      -2601.15791900       -157.95887809       -12.15068293    8.12    1           Ln?^`yUBHE      -1  C1          @geo-000010-00
    9   1   9    9      -2601.15724800       -157.53785068       -12.11829621    8.26    1           LcCLfD`XGw      -1  Cs          @geo-000012-00
   10   1  10   10      -2601.15700600       -157.38600473       -12.10661575    8.23    1           LcwhEiqiIY      -1  C2          @geo-000014-00
   11   1  11   11      -2601.15617800       -156.86646570       -12.06665121    7.80    1           L}iZ_OaJwA      -1  Cs          @geo-000016-00
   12   1  12   12      -2601.16097400       -159.87577633       -12.29813664    7.85    1           LzBAhql@GP      -1  C1          @geo-000007-00
   13   1  13   13      -2601.16097400       -159.87577633       -12.29813664    7.85    1           LZlFgtOaqH      -1  C1          @geo-000013-00
   14   1  14   14      -2601.15616900       -156.86081854       -12.06621681    7.81    1           LqalMRBbx?      -1  Cs          @geo-000015-00
   15   1  15   15      -2601.15602300       -156.76920900       -12.05916992    7.62    1           LqjokRVAT]      -1  C2          @geo-000017-00
   16   1  16   16      -2601.15571200       -156.57406813       -12.04415909    8.26    1           Lz@NH`TGoN      -1  Cs          @geo-000020-00
   17   1  17   17      -2601.16372600       -161.60255341       -12.43096565    8.19    1           LAjLOhdSPD      -1  C1          @geo-000008-01
   18   1  18   18      -2601.15537300       -156.36135831       -12.02779679    8.30    1           LK}WysUSVO      -1  Cs          @geo-000022-00
   19   1  19   19      -2601.15519600       -156.25029743       -12.01925365    8.26    1           LUd_tJwXIG      -1  C1          @geo-000023-00
   20   1  20   20      -2601.15517800       -156.23900310       -12.01838485    7.98    1           L\PkbcChwX      -1  C1          @geo-000024-00
<continued for 208 structures found in 3 structure input files>
*** Here, i numerates the structures found in file(s), Str is the number of the structures to be analyzed (some structures can be omitted during primary check)
*** E.g. if the connectivity > 1 (disconnected graph) the structure will be discarded
*** Graph strings means that the file Structures-canonical.g96 (generated by labelg program) is present in the work directory.
*** Energies 1, 2, 3 are the total energy, binding energy and binding energy per atom

< Detailed information on calculations - not shown here>

*** Final part (below) gives the most reliable classifications by algorithms 4 and 5. 165 structural classes were found among 208 structures
*** Classification is identic in the cases of both algorithms:

 Structure classes, discriminated by fingerprints. Nstr:  208  Ntypes:  165
 Threshold for discrimination:    0.01000% of each compared value.
 Classes with large energy scatter (SD) are marked with ? sign.
 Classes are sorted by energy.  SymGroup eps:    0.1000 A

Class iTyp Nstr Nbeg Nend    Eaver(1)    SD        Eaver(2)    SD        Eaver(3)    SD    IsoGraph   SymGrp   Structures:
    1    2    9    1    9  -2601.1637  0.0000     -161.6026  0.0000     -12.4310  0.0000         2   C1       2   7  17  22  48  64 119 120 205
    2    1    8   10   17  -2601.1610  0.0000     -159.8758  0.0001     -12.2981  0.0000         1   C1       1   4   5  12  13  76 145 208
    3    3    3   18   20  -2601.1589  0.0000     -158.5506  0.0000     -12.1962  0.0000         3   C1       3  27  30
    4    4    1   21   21  -2601.1580  0.0000     -158.0310  0.0000     -12.1562  0.0000         4   Cs       6
    5    5    1   22   22  -2601.1579  0.0000     -157.9589  0.0000     -12.1507  0.0000         5   C1       8
    6    6    5   23   27  -2601.1572  0.0000     -157.5379  0.0000     -12.1183  0.0000         6   Cs       9  23  47 206 207
    7    7    2   28   29  -2601.1570  0.0000     -157.3860  0.0000     -12.1066  0.0000         7   C2      10  99
    8    8    2   30   31  -2601.1562  0.0000     -156.8665  0.0000     -12.0667  0.0000         8   Cs      11  53
    9    9    1   32   32  -2601.1562  0.0000     -156.8608  0.0000     -12.0662  0.0000         9   Cs      14
   10   10    2   33   34  -2601.1560  0.0000     -156.7692  0.0000     -12.0592  0.0000        10   C2      15 156
   11   11    4   35   38  -2601.1557  0.0000     -156.5741  0.0000     -12.0442  0.0000        11   Cs      16  36 125 129
   12   12    1   39   39  -2601.1554  0.0000     -156.3614  0.0000     -12.0278  0.0000        12   Cs      18
   13   13    1   40   40  -2601.1552  0.0000     -156.2503  0.0000     -12.0193  0.0000        13   C1      19
   14   14    1   41   41  -2601.1552  0.0000     -156.2390  0.0000     -12.0184  0.0000        14   C1      20
   15   15    8   42   49  -2601.1552  0.0000     -156.2265  0.0000     -12.0174  0.0000        15   C1      21  39  46  49 107 114 118 139
   16   20    1   50   50  -2601.1550  0.0000     -156.0959  0.0000     -12.0074  0.0000        20   C1      29
   17   16    1   51   51  -2601.1548  0.0000     -156.0137  0.0000     -12.0011  0.0000        16   Cs      24
   18   18    1   52   52  -2601.1548  0.0000     -155.9736  0.0000     -11.9980  0.0000        18   C2      26
```

```
   19   17    1   53   53  -2601.1547  0.0000     -155.9654  0.0000      -11.9973  0.0000        17   C1      25
   20   19    1   54   54  -2601.1544  0.0000     -155.7577  0.0000      -11.9814  0.0000        19   C1      28
… <continued for 165 classes>
*** In the table above, Class is the number of unique class (its internal number iTyp), Nstr is number of structures within the class,
*** column Structures gives the number of structures (Str column in the first table of the file) belonging to the class.
*** Eaver 1, 2, 3 are the averaged energies of the structures within the class, and SD and the corresponding standard deviations.
*** If SD is too large, there are some doubts on the proper assignment of structures to the same class. In this case, SD value is marked with '?' sign
*** Isograph is the number of isomorphic graph corresponding to the fingerprint class (isographs are listed below)
***
*** Additional information on classes follows. It contains label strings taken from the structure input files, energies, and lowest frequencies (if any):

Class 1Str  SymGrp  Structure label in file.   SymGroup eps:    0.1000 A
    1    2  C1      @geo-000001-00 icyc    51 iStrGeo      83 nStrProc     2 Etot         -2601.163726     *end *opt *freq *lm       12.40     42.45     52.87
    2    1  C1      @geo-000002-00 icyc    32 iStrGeo      32 nStrProc     1 Etot         -2601.160974     *end *opt *freq *lm       29.89     34.39     54.63
    3    3  C1      @geo-000005-00 icyc    32 iStrGeo     115 nStrProc     3 Etot         -2601.158862     *end *opt *freq *lm       48.80     50.28     62.17
    4    6  Cs      @geo-000009-00 icyc    38 iStrGeo     337 nStrProc     6 Etot         -2601.158034     *end *opt *freq *lm       21.75     46.48     50.84
    5    8  C1      @geo-000010-00 icyc    15 iStrGeo     444 nStrProc     8 Etot         -2601.157919     *end *opt *freq *lm       35.26     58.10     62.73
    6    9  Cs      @geo-000012-00 icyc    49 iStrGeo     493 nStrProc     9 Etot         -2601.157248     *end *opt *freq *lm       33.80     57.41     59.40
    7   10  C2      @geo-000014-00 icyc    42 iStrGeo     535 nStrProc    10 Etot         -2601.157006     *end *opt *freq *lm       33.81     42.17     61.37
    8   11  Cs      @geo-000016-00 icyc    23 iStrGeo     558 nStrProc    11 Etot         -2601.156178     *end *opt *freq *lm       31.38     35.31     38.56
    9   14  Cs      @geo-000015-00 icyc    19 iStrGeo     767 nStrProc    14 Etot         -2601.156169     *end *opt *freq *lm       40.20     52.96     63.35
   10   15  C2      @geo-000017-00 icyc    30 iStrGeo     797 nStrProc    15 Etot         -2601.156023     *end *opt *freq *lm       43.44     56.73     70.76
   11   16  Cs      @geo-000020-00 icyc    30 iStrGeo     927 nStrProc    16 Etot         -2601.155712     *end *opt *freq *lm       27.48     46.09     50.04
   12   18  Cs      @geo-000022-00 icyc    37 iStrGeo     968 nStrProc    18 Etot         -2601.155373     *end *opt *freq *lm       21.17     29.42     40.66
   13   19  C1      @geo-000023-00 icyc    28 iStrGeo     996 nStrProc    19 Etot         -2601.155196     *end *opt *freq *lm       24.25     36.45     42.40
   14   20  C1      @geo-000024-00 icyc    39 iStrGeo    1035 nStrProc    20 Etot         -2601.155178     *end *opt *freq *lm       28.71     34.33     43.60
   15   21  C1      @geo-000025-00 icyc    21 iStrGeo    1056 nStrProc    21 Etot         -2601.155158     *end *opt *freq *lm       37.00     44.63     56.11
   16   29  C1      @geo-000026-00 icyc    49 iStrGeo    1431 nStrProc    29 Etot         -2601.154950     *end *opt *freq *lm       13.33     34.21     45.68
   17   24  Cs      @geo-000027-00 icyc    32 iStrGeo    1247 nStrProc    24 Etot         -2601.154819     *end *opt *freq *lm       40.52     55.59     62.56
   18   26  C2      @geo-000029-00 icyc    34 iStrGeo    1301 nStrProc    26 Etot         -2601.154755     *end *opt *freq *lm       39.33     51.75     57.44
   19   25  C1      @geo-000030-00 icyc    20 iStrGeo    1267 nStrProc    25 Etot         -2601.154742     *end *opt *freq *lm       27.19     48.89     50.62
   20   28  C1      @geo-000031-00 icyc    42 iStrGeo    1382 nStrProc    28 Etot         -2601.154411     *end *opt *freq *lm       19.80     32.13     39.59
… <continued for 165 classes>
*** Finally, information on classes found in the basis of isomorphic graphs follows.
*** It appears only if the file Structures-canonic.g6 is present in the work directory
*** This table gives the canonic g6 strings for each class. If the classifications by algorithms 4 and 5 is different,
*** the corresponding warnings will be given describing relationships between fingerprint and isograph assignments.

Class 1Str  SymGrp  Graph No. Canonic graph g6 string
    1    2  C1          2     L_N@OsBoHwCvD^
    2    1  C1          1     LOO_qucTSTAvzF
    3    3  C1          3     LE@XPS`gm`hlff
    4    6  Cs          4     LC@HWbPkQZDZxn
    5    8  C1          5     LGESKwgaykKV]J
    6    9  Cs          6     LGESS|_THTOv]E
    7   10  C2          7     LAGGeIaTp\y[jW
    8   11  Cs          8     Lt?__KLAyXHR|r
    9   14  Cs          9     L@GOX}SQe@wvN~
```

```
   10   15  C2          10     L?hUCTEMPht^T}
   11   16  Cs          11     LP?CATFFAZfYLl
   12   18  Cs          12     L@MCGgI[RPg~fx
   13   19  C1          13     L?_sOl_SZhd{a|
   14   20  C1          14     LG@g_uQeZDDxrN
   15   21  C1          15     L@GAGnE`XqxF]r
   16   29  C1          20     L?aiacPKiRTfZf
   17   24  Cs          16     L@P?cUFrZWFXLj
   18   26  C2          18     L?ddQiaSP}REXL
   19   25  C1          17     L?AKHdgUJbbyjx
   20   28  C1          19     L?_PkPS[h]KNbZ
… <continued for 165 classes>
```

<EOF>