

StrDiscriminator2 v.1.0

Short User Manual

StrDiscriminator2 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 the 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 present in the file without successful optimization string, only the last structure will be analyzed.

Main input file of the program

The file *StrDiscriminator2.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 *StrDiscriminator2.inp*, case insensitive) are:

Keyword	Example	Meaning	Default
FilOut	FilOut=Mg10.out	Output file name	<i>StrDiscriminator2.out</i>
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 Angstroms to be used as a threshold for connectivity matrix construction	$1.15 \cdot (R_a + R_b)$ where R_a , R_b – valence radii 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 are within EpsE.	0.1 units of energy (units can be indicated by <i>Eunits</i> 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 are 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 identic if the relative absolute deviation for any pair in the lists of their sorted fingerprints are within EpsFP: $\left \frac{p_i^A - p_i^B}{p_i^B} \right < EpsStr$	10 ⁻⁴
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 of the energy that is read in (Hartree(au), electron-volts(ev), kcal/mol(kcal), kJ/mol(kj))	au
SymEps=<value>	SymEps=0.05	Threshold (Angstroems) to recognize the symmetry group. Atoms 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 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.	nr=1 ud=1 hs=15 vs=15 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 the 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 *StrDiscrimintaor2.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 *StrDiscrimintaor2.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 <i>StrDiscrimintaor2.out</i>)
Structures-rotated.xyz	Original structures reduced to the principal axes
Structures-classes.xyz	Classified structures: 1 st 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 J. McKay and M. Piperno. This program is freely available on the *Traces/Nauty* site. 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 *StrDiscriminator2.exe* should be run once more with the same input files (no input file modifications are required). Once *StrDiscriminator2* 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 *StrDiscriminator2.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

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The program is experimental, distributed on the “as is” basis, under the BSD2 license.

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

Example of the main input file *StrDiscriminator2.inp*:

```
EpsE=1.0 EpsFP=0.0001 EpsStr=0.05 EpsPMOI=0.01 StrLabel=*lm Eword=9 Elvalue=-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 a 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 of 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 StrDiscriminator2.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: ELVALUE=-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 mgl3.sbas_
2 mgl3-nneg.sbas_
3 mgl3-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 correposnding standard deviations.
 *** If SD is too large, there ar 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	lStr	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	lStr	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>