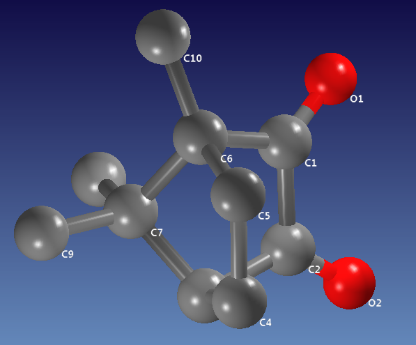
**TUTORIAL EXPO: STRUCTURE MODEL OPTIMIZATION**

The **Structure model optimization** folder contains:

* **COVMAP** folder

It contains: **camphor.exp** [the input file for the default run of *EXPO* in case of 1,7,7-Trimethylbicyclo(2.2.1) hepta-2,3-dione (C10H14O2), after that the cell and the space group have been determined]; **camphor.pow** (the file containing the experimental profile counts); **camphor.fra** (the file of the fractional coordinates and the isotropic thermal parameters of the true model, hydrogen atoms excluded). The structure has not been published yet (courtesy by Dr. Michela Brunelli).



The input file ‘camphor.exp’ consists of the following lines:

|  |
| --- |
| %Structure camphor  %Job 1,7,7-Trimethylbicyclo(2.2.1)hepta-2,3-dione (C10 H14 O2)  %Data  Cell 12.008 11.488 6.631 90 91.613 90  SpaceGroup p 21/n  Content (C10H14O2)4  Range 2.001 26.0  Pattern camphor.pow  filetype double  Wavelenght 0.49002  Synchrotron  %continue |

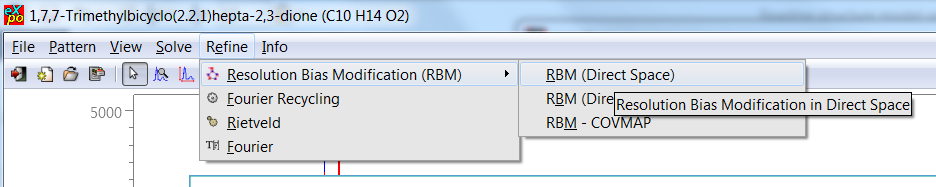
The range has been reduced to 26° because the signal is too noisy beyond that value. The directive ‘Filetype double’ has been introduced because of the format of camphor.pow file.

To run EXPO on camphor in default way:

* Click on EXPO icon
* **File** in the upper Menu
* **Load & Go**
* Use ‘camphor.exp’ as Input File and give the Output Filename you like (camphor.out is the default output file name)
* **Go**
* Click on **Next** to go on continuously until the end of the run.

The structure model obtained at the end of the Direct Methods procedure, executed on the first set of phases (default choice), is not interpretable.

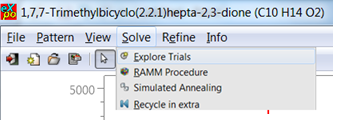
It is so rough and uninterpretable that is not advisable to try to improve it, for example, by cyclic application of RBM (RBM is advisable because the structure is organic). Indeed, by clicking on **Refine > Resolution Bias Modification (RBM)> RBM (Direct Space)** in the upper Menu



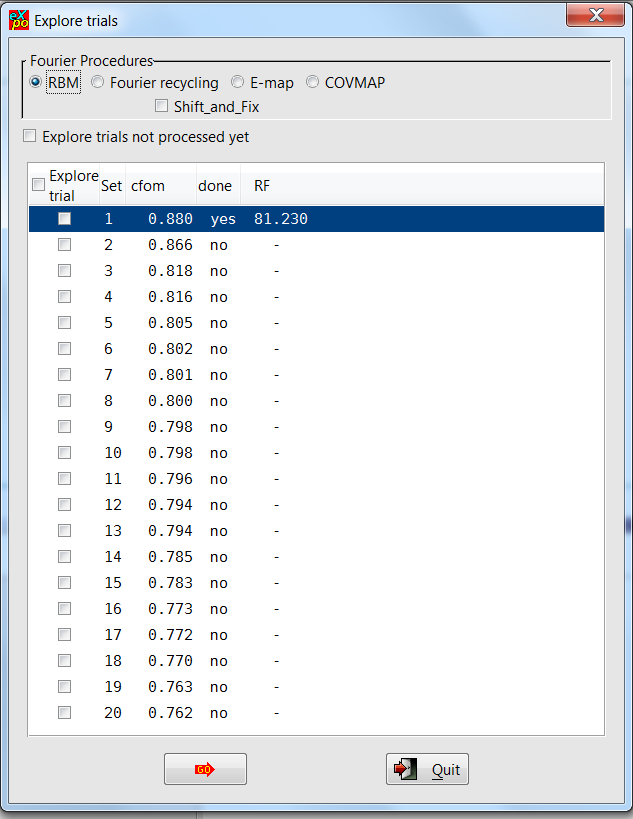
no improvement of the structure model is attained.

We can try to explore the other Direct Methods trials:

**Solve > Explore Trials** in the upper Menu



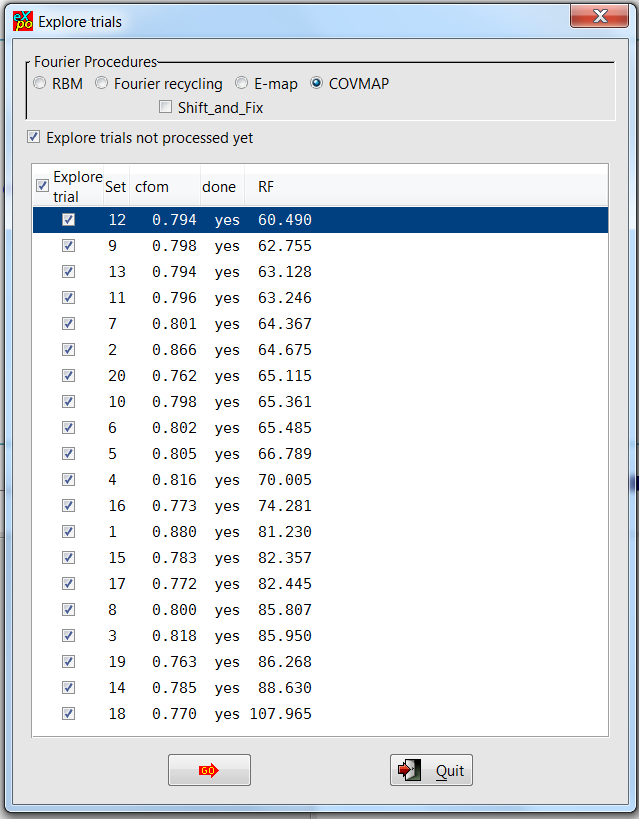
and exploring and ranking all the other 19 trials not processed in the standard run by Direct Methods (only the highest CFOM figure of merit phasing trial is automatically processed)



Click on **GO.**

The model first ranked by RF doesn’t correspond to the correct solution.

The structure solution can be attempted by the optimization of **COVMAP** to be applied to the 20 Direct Methods phasing trials

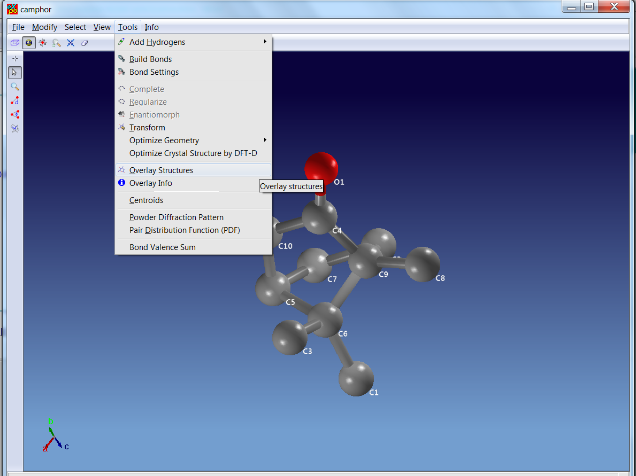
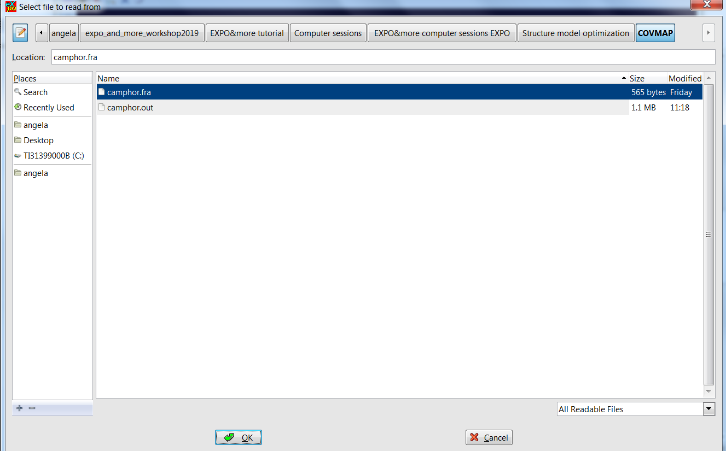


Click on **GO**. The execution of COVMAP requires a time longer than the standard RBM process.

Now the COVMAP model first ranked by RF corresponds to the correct solution.

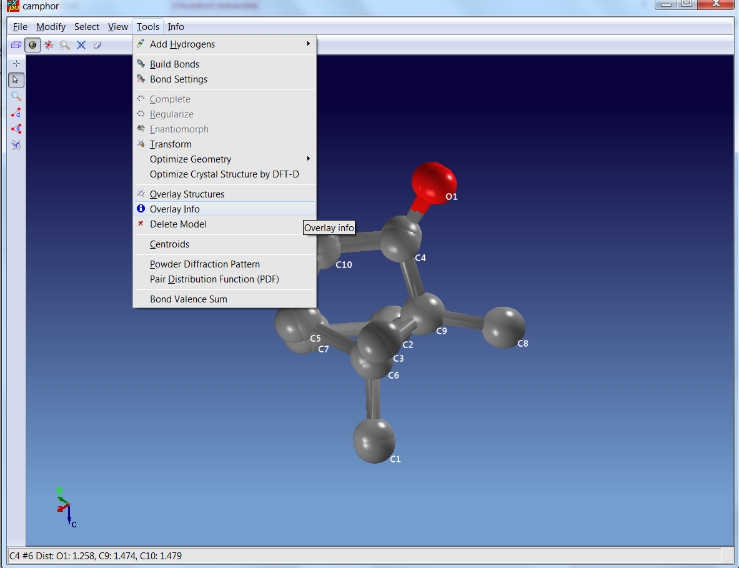
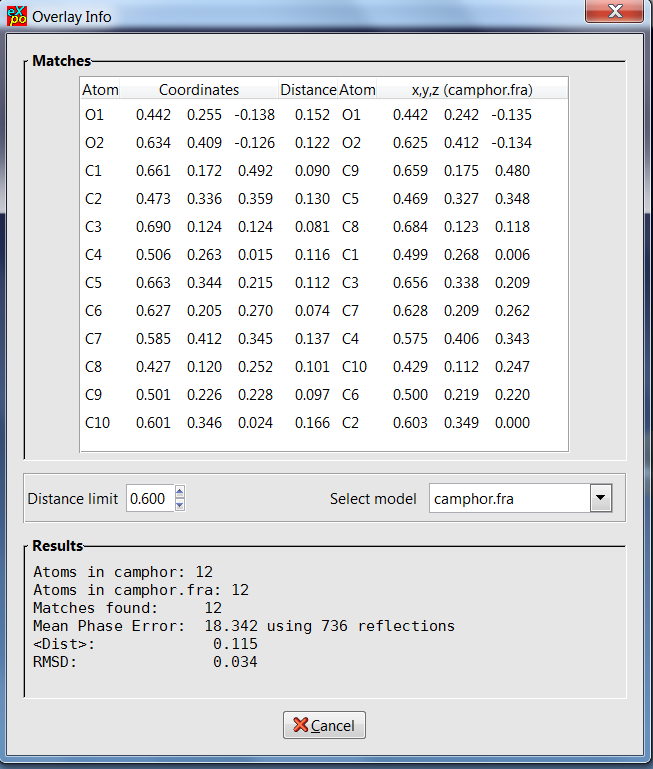
The obtained solution can be compared with the published fractional coordinates contained in the camphor.fra file. It can be done by the following graphic pathway:

**Tools > Overlay structures** in the upper Menu and select camphor.fra and **OK**

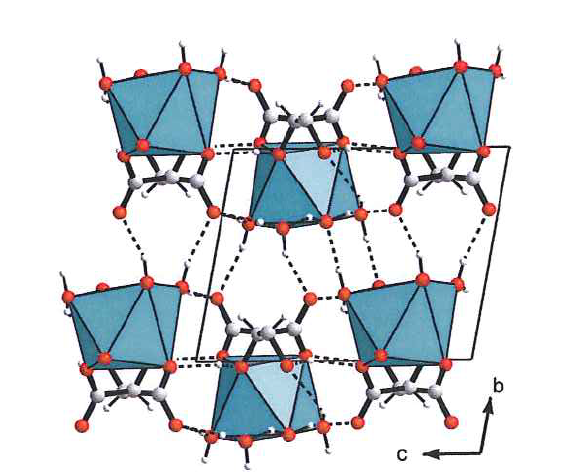
The two models are superimposed and information on comparison can be output:

**Tools > Overlay Info** in the upper Menu

* **SHIFT\_AND\_FIX** folder

It contains: **tartrate.exp** [the input file for the default run of *EXPO* in case of Calcium tartrate tetrahydrate (CaC4H12O10), after that the cell and the space group have been determined]; **tartrate.pow** (the file containing the experimental profile counts); **tartrate.fra** (the file of the fractional coordinates and the isotropic thermal parameters of the true model, hydrogen atoms excluded); **tartrate.pdf** (the article in which the structure is cited).



The input file ‘tartrate.exp’ consists of the following lines:

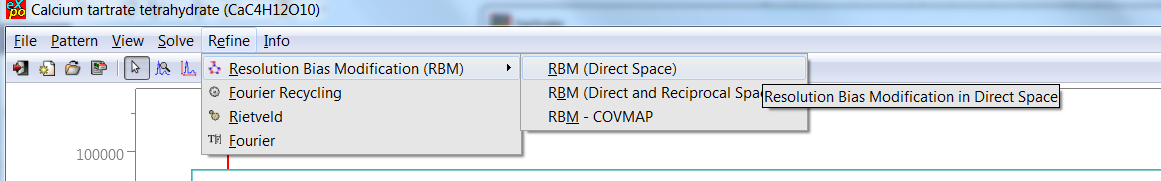
|  |
| --- |
| %Structure tartrate  %Job Calcium tartrate tetrahydrate (CaC4H12O10)  %Data  Cell 8.222 10.473 6.249 105.97 107.51 94.94  SpaceGroup p -1  Content (CaC4H12O10)2  Pattern tartrate.pow  Wavelenght 1.5418  Synchrotron  %continue |

To run EXPO on tartrate in default way:

* Click on EXPO icon
* **File** in the upper Menu
* **Load & Go**
* Use ‘tartrate.exp’ as Input File and give the Output Filename you like (tartrate.out is the default output file name)
* **Go**
* Click on **Next** to go on continuously until the end of the run.

The structure model obtained at the end of the Direct Methods procedure, executed on the first set of phases (default choice), is not interpretable.

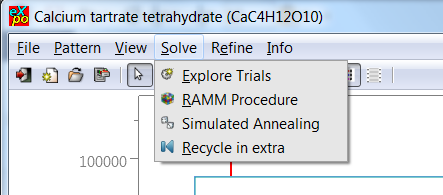
It is so rough and uninterpretable that is not advisable to try to improve it, for example, by cyclic application of RBM (RBM is advisable because the structure is metal-organic). Indeed, by clicking on **Refine > Resolution Bias Modification (RBM)> RBM (Direct Space)** in the upper Menu



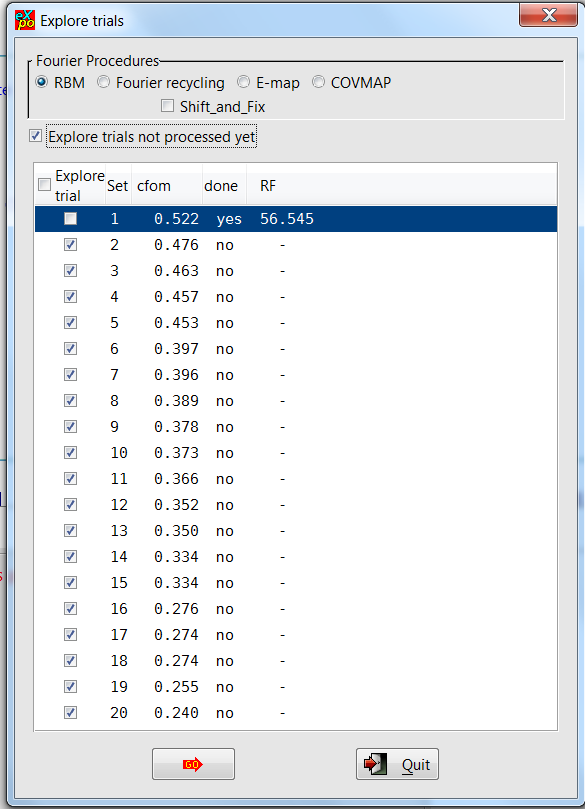
no improvement of the structure model is attained.

We can try to explore the other Direct Methods trials:

**Solve > Explore Trials** in the upper Menu



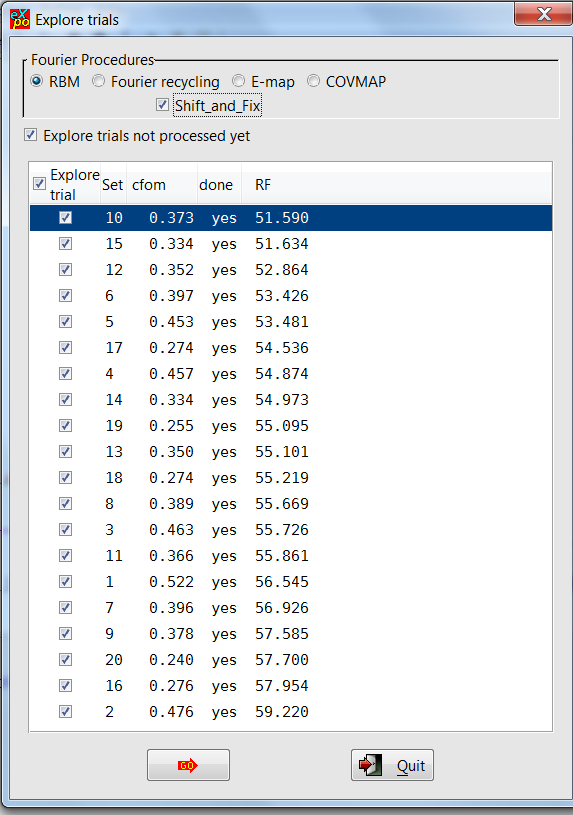
and exploring and ranking all the other 19 trials not processed in the standard run by Direct Methods (only the highest CFOM figure of merit phasing trial is automatically processed)



Click on **GO.**

The model first ranked by RF doesn’t correspond to the correct solution.

The structure solution can be attempted by the optimization of **SHIFT\_AND\_FIX** to be applied to the 20 Direct Methods phasing trials

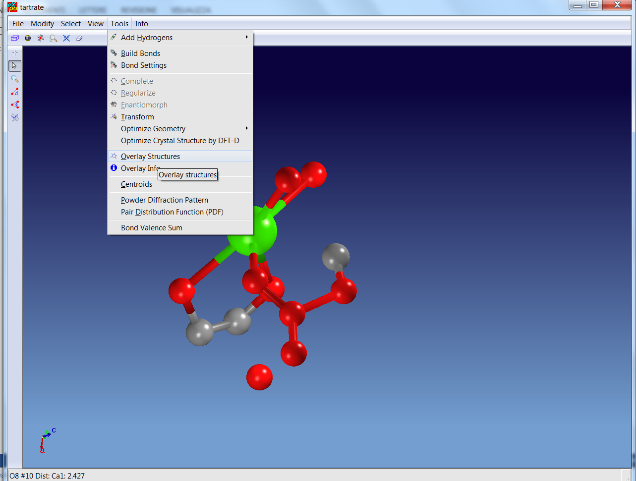
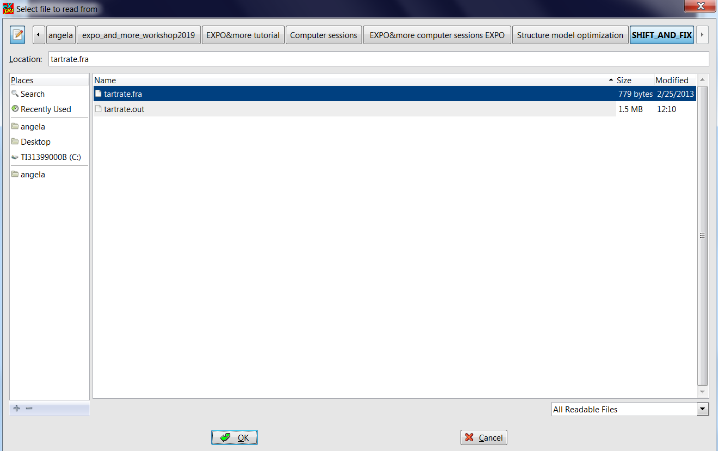


Click on **GO**. The execution of SHIFT\_AND\_FIX requires a time longer than the standard RBM process.

Now the model first ranked by RF corresponds to the correct solution (the chemical label should be corrected: left-click on the wrongly labelled atom position, right-click, Change Species, select the label ).

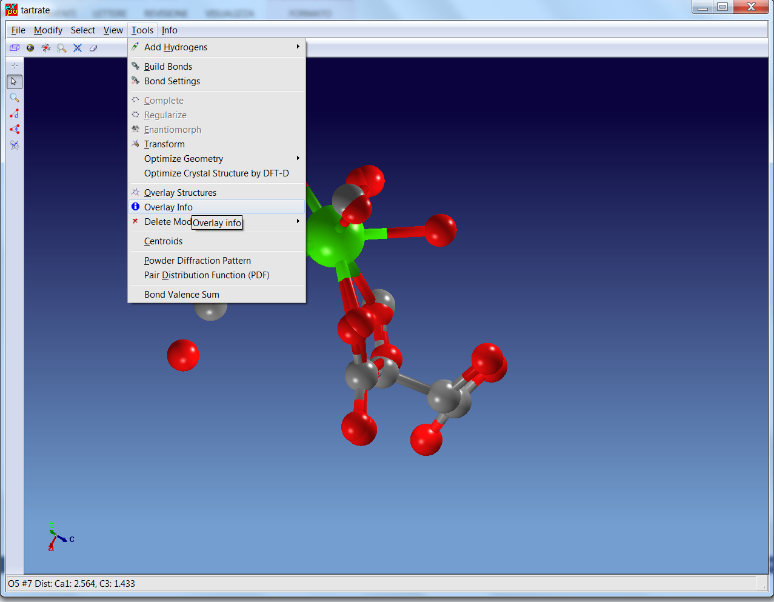
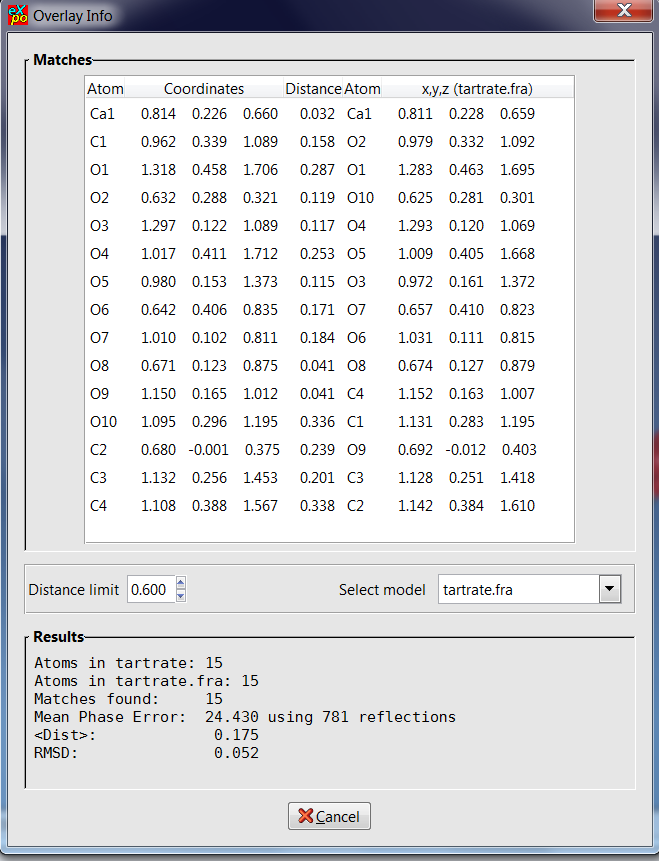
The obtained solution can be compared with the published fractional coordinates contained in the tartrate.fra file. It can be done by the following graphic pathway:

**Tools > Overlay structures** in the upper Menu and select tartrate.fra and **OK**

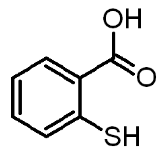
The two models are superimposed and information on comparison can be output:

**Tools > Overlay Info** in the upper Menu

* **RAMM** folder.

It contains: **merca.exp** [the input file for the default run of *EXPO* in case of 2-Mercaptobenzoic acid (C7H6O2S), after that the cell and the space group have been determined]; **merca.pow** (the file containing the experimental profile counts); **merca.fra** (the file of the fractional coordinates and the isotropic thermal parameters of the true model, hydrogen atoms excluded); **merca.pdf** (the structure publication).



The input file ‘merca.exp’ consists of the following lines:

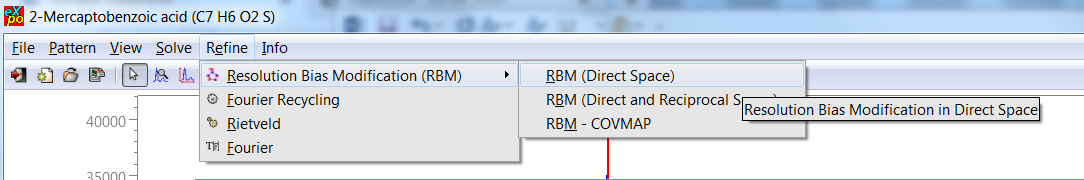
|  |
| --- |
| %Structure merca  %Job 2-Mercaptobenzoic acid (C7 H6 O2 S)  %Data  Cell 7.885 5.976 14.949 90.0 100.48 90  SpaceGroup p 21/c  Content (C7 H6 O2 S)4  Pattern merca.pow  Wavelength 1.54056  %continue |

To run EXPO on merca in default way:

* Click on EXPO icon
* **File** in the upper Menu
* **Load & Go**
* Use ‘merca.exp’ as Input File and give the Output Filename you like (merca.out is the default output file name)
* **Go**
* Click on **Next** to go on continuously until the end of the run.

The structure model obtained at the end of the Direct Methods procedure, executed on the first set of phases (default choice), is not interpretable.

You can apply RBM cycling (RBM is advisable because the structure is metal-organic) by iterated clicking on **Refine > Resolution Bias Modification (RBM)> RBM (Direct Space)** in the upper Menu



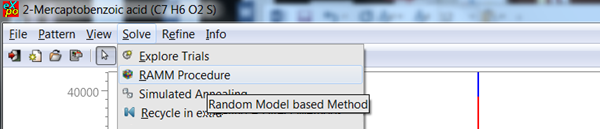
At the end of the RBM application, the model is improved in some way but the complete and correct solution is not attained.

The structure solution can be obtained by one of the two following strategies:

* **the RAMM procedure**:

(The RAMM method which usually requires quite long execution time can be attempted as first non-default choice because the structure is small and RAMM execution time is not expected to be long).

**Solve > RAMM Procedure** in the upper Menu

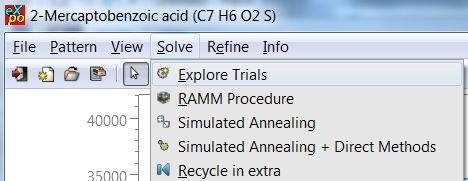


The procedure provides only one model that corresponds to the correct solution.

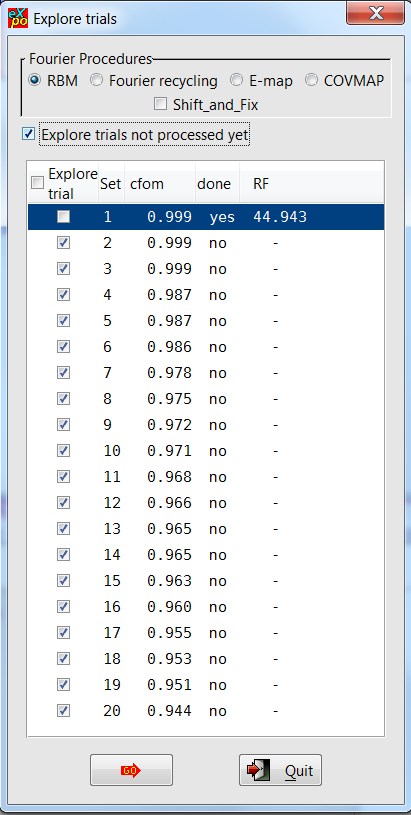
.

* **Exploring the other Direct Methods trials:**

**Solve > Explore Trials** in the upper Menu



and exploring and ranking all the other 19 trials not processed in the standard run by Direct Methods (only the highest CFOM figure of merit phasing trial is automatically processed)

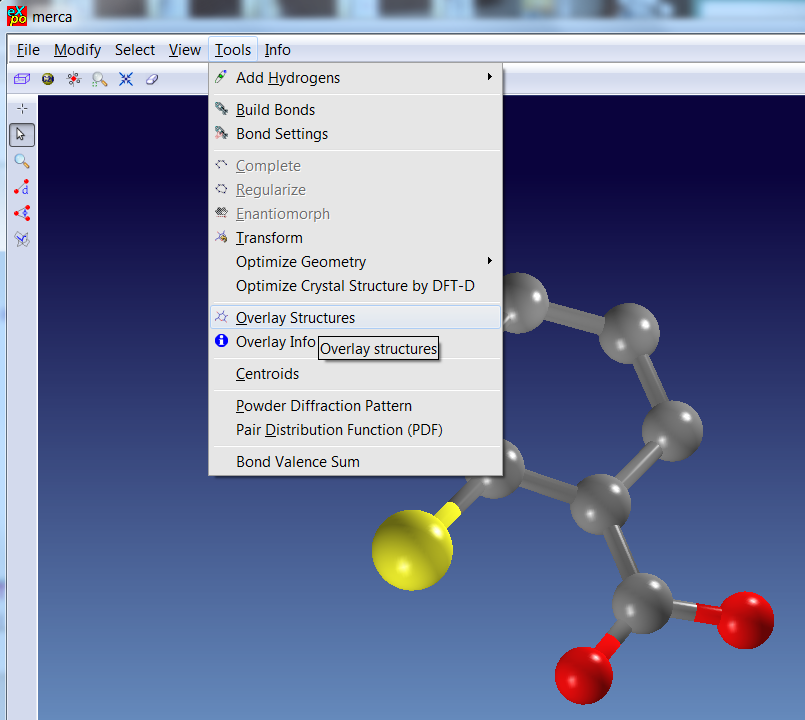
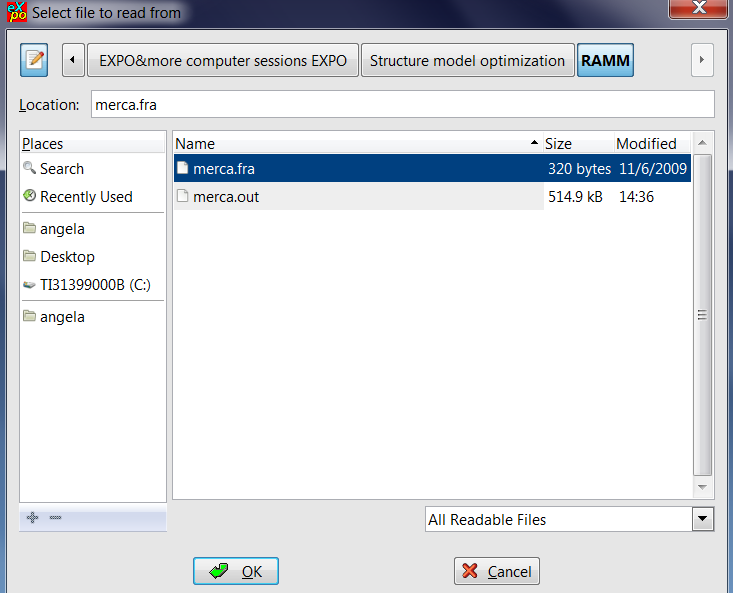


Click on **GO.**

The model first ranked by RF corresponds to the correct solution.

The obtained solution can be compared with the published fractional coordinates contained in the merca.fra file. It can be done by the following graphic pathway:

**Tools > Overlay structures** in the upper Menu and select merca.fra and **OK**

The two models are superimposed and information on comparison can be output:

**Tools > Overlay Info** in the upper Menu

