COSMORSAverage

Averaging COSMO Profiles from Gaussian/TurboMole/DMOL3 for Usage in

COSMO-SAC and COSMO-RS(Ol)

DDBSP - Dortmund Data Bank Software Package

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Introduction

This program performs the averaging of an electronic charges surface elements profiles obtained from the quantum mechanical chemistry programs Gaussian[i], TurboMole[ii], and DMol3[iii].

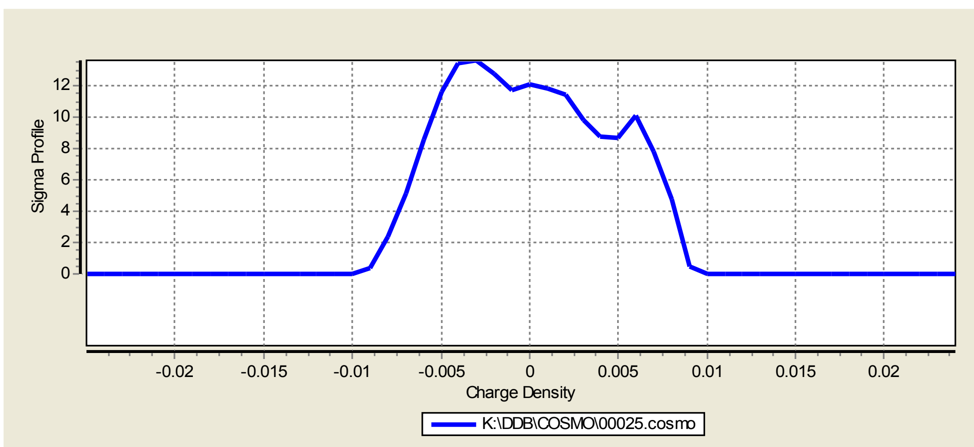


Figure 1: Averaged Profile

The averaged profiles are used in COSMO-SAC[iv] and COSMO-RS(Ol)[v] for the calculation of activity coefficients and the derived phase equilibria VLE, LLE, SLE, gas solubilities, and heats of mixing.

Single File/s Conversion

This mode allows selecting a single COSMO file or multiple COSMO files created by a quantum chemistry

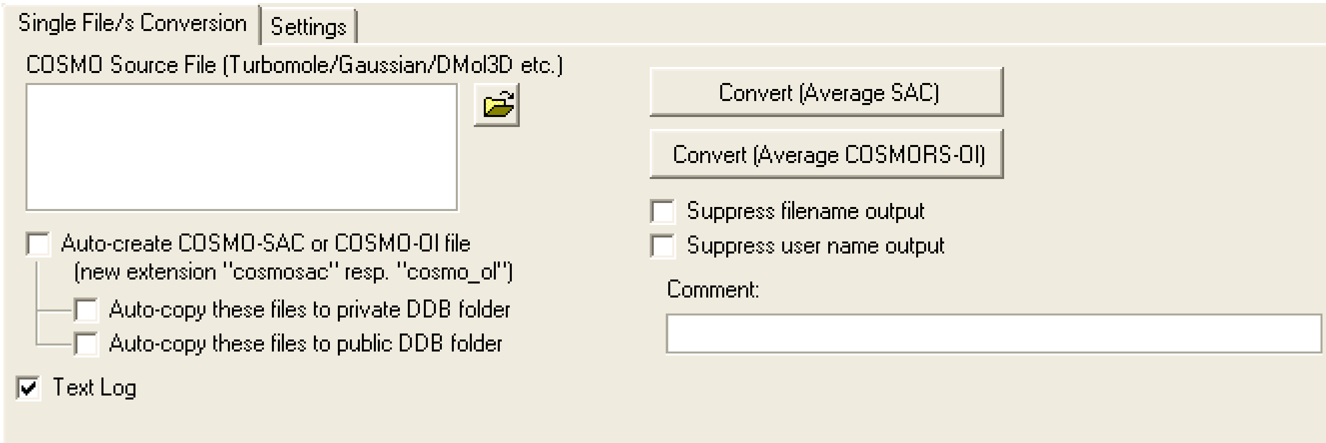
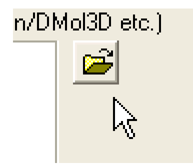


Figure 2: Single File Conversion

program by a standard Windows "Open" dialog. This special dialog allows the selection of multiple files.



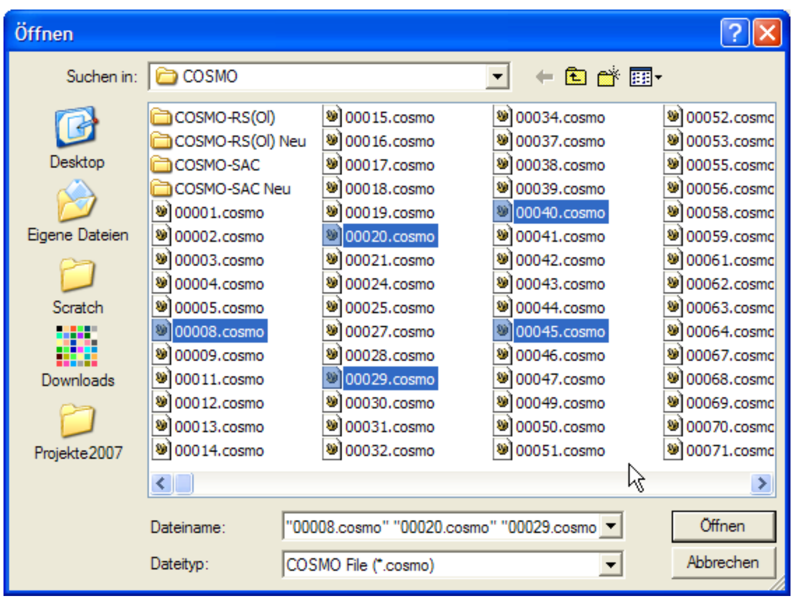


Figure 3: COSMO Files Open Dialog

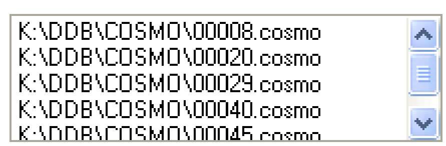


Figure 4: List of Selected Files

The averaging process can be started by the buttons

and

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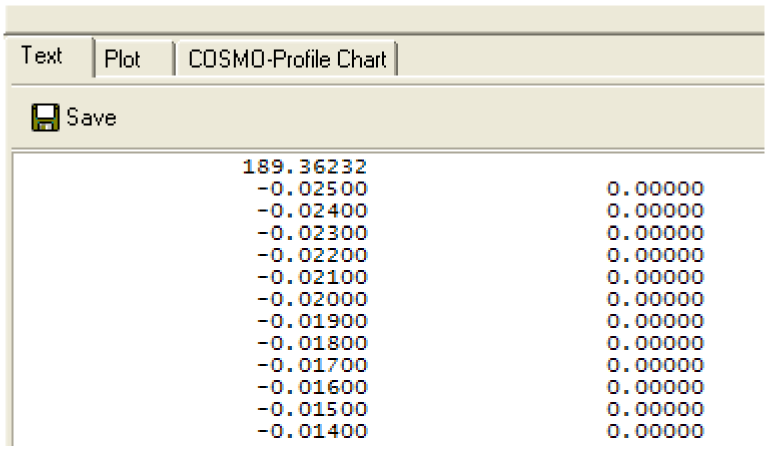
The result of this averaging is displayed in the “Text” page.



189.36232	
-0.02500	0.00000
-0.02400	0.00000
-0.02300	0.00000
-0.02200	0.00000
-0.02100	0.00000
-0.02000	0.00000
-0.01900	0.00000
-0.01800	0.00000
-0.01700	0.00000
-0.01600	0.00000
-0.01500	0.00000
-0.01400	0.00000

Figure 5: Text Output of Averaged Profile

If multiple source files have been selected the COSMORSAverage program appends all averaged tables to this text output.

The result starts with a single number defining the (“total cavity”) volume of the molecule, a value used in all COSMO calculations.

Averaging for COSMO-SAC yields always two columns displaying the charge density ranging from -0.025 to +0.025 and the profile values. For COSMO-RS(Ol) there's always a third column which contains non-zero value only for ethers. COSMO-RS(Ol) uses a correction regarding hydrogen-bonding for ethers. Additionally the charge density (normally) ranges from -0.040 to +0.040 for COSMO-RS(Ol).

The current version of the plot output of the averaged profile shows always the plot of the last file in the list – it does not combine several plots.

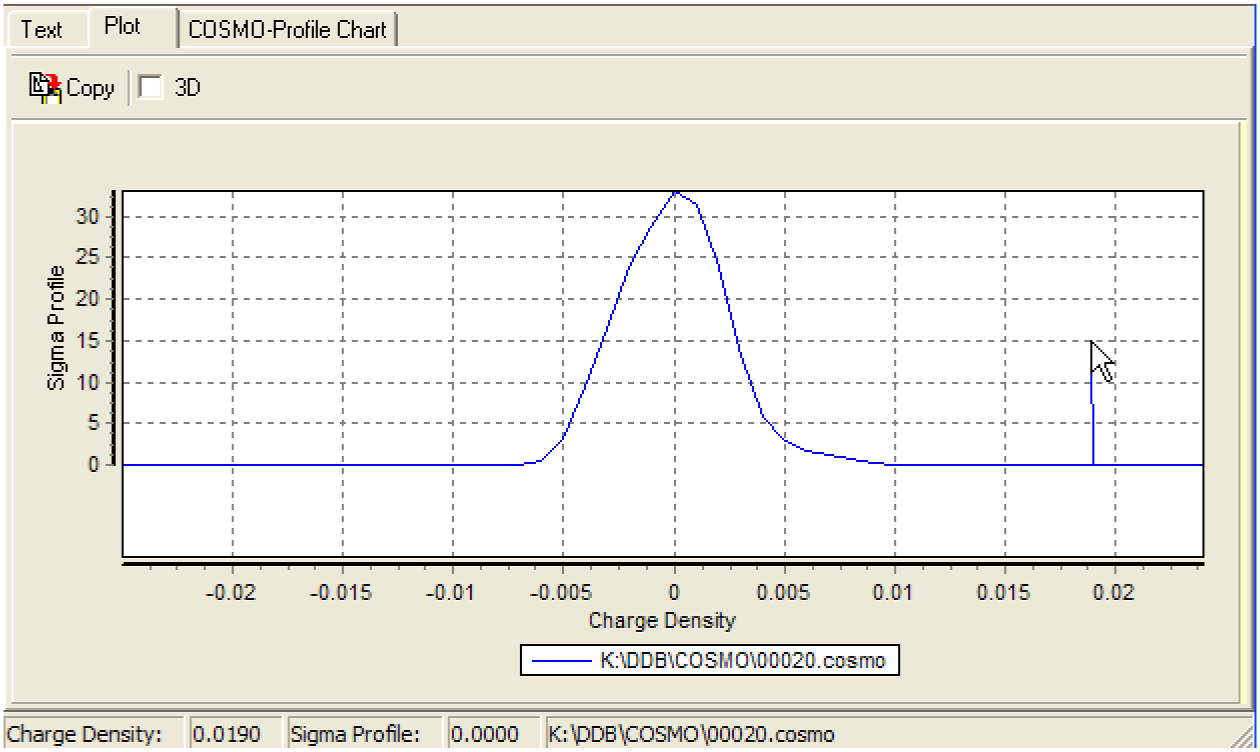
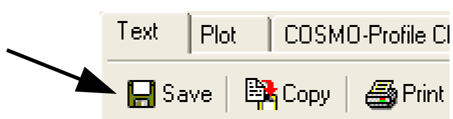


Figure 6: Plot of Averaged Profile

The mouse cursor can be used to display the chart values in the status bar of the dialog.

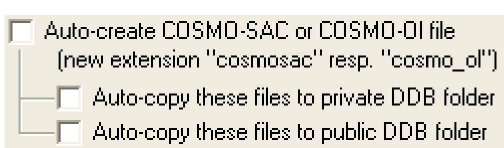
The averaged profile can be saved by the



button in the text output. The standard Windows save dialog allows specifying a path and name for the profile. For saving a profile usable in DDB software it is necessary to use only a single component in the list. A file for COSMO-SAC must have the extension ".cosmo_sac" and a file for COSMO-RS(Ol) must have the extension ".cosmo_ol".

Multiple File Conversion

If multiple averaged files should be saved it is necessary to check the option



This option toggles an automatic creation of files with averaged profiles. These file will have the same name as the source file but the extension will be changed from "*.cosmo" to "*.cosmo_sac" resp. "*.cosmo_ol". The resulting files are stored in the same folder as the source file. For using the produced files in the DDB software it is necessary to move the averaged files to sub folders of the DDB directory. The “Auto-copy” can be used to let the COSMORSAverage program copying the created files to the correct folders.

Suppress File and User Name Output

The created file normally contain additional lines with information about the user (Windows log-in name) and the filename.

```
$Sourcefile: q:\ddb\cosmo-Gaussian-B3LYP\22412.cosmo
$Date: 06-07-14 15:37 $Time: 3:40:38 PM
$User: rarey
```

The output of the additional lines for the source file and user name can be suppressed.

File Name Conventions

The program COSMORSAverage expects the extension “*.cosmo” for output files of the quantum mechanical programs. You have to rename the files if they have, for some reason, another extension.

The output files (averaged files) have to have the extensions “*.cosmo_sac” for the COSMO-SAC model resp. “*.cosmo_ol” for the COSMO-RS(Ol) model.

For using these files in the DDB system the files need to have the DDB number as file name with five digits. Leading zeros have to be inserted if the DDB number is shorter. Valid names are

00011.cosmo_sac
00121.cosmo_ol
04321.cosmo_sac
12345.cosmo_ol

Private components have negative numbers.

The files have to be copied to the sub folder “COSMO” of the public or private (customer's) DDB folder. The original “*.cosmo” files are in the root (“`somewhere\DDB\COSMO`”) whereas the “*.cosmo_sac” files have to be in the
“`somewhere\DDB\COSMO\COSMO-SAC`”
and the “*.cosmo_ol” files have to be in the
“`somewhere\DDB\COSMO\COSMO-RS(Ol)`”
folder. If files with the same names exist in both the private and public folder the file in the private folder will be preferred.

Settings

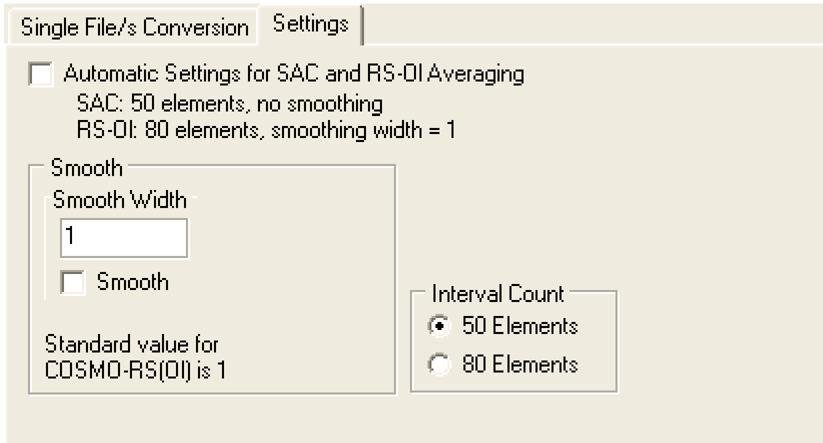


Figure 7: Settings

Smooth Width

This value affects the resulting averaged profile.

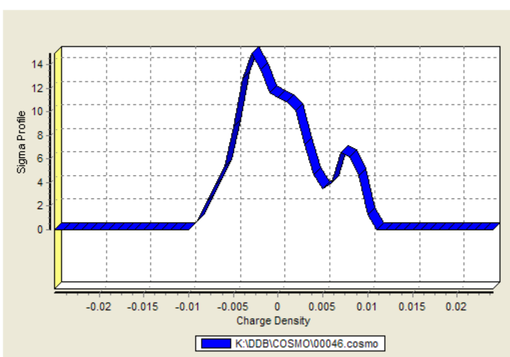


Figure 8: Smoothed Averaged Profile

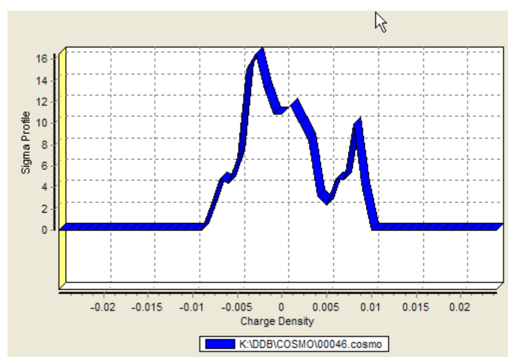


*Figure 9: Averaged Profile **Without** Smoothing*

Smoothing is used for COSMO-RS(Ol) with step width 1. This means that a value at position x is the mean value of the values at x-1, x+1, and x. Smoothing must not be used for COSMO-SAC.

Interval Count

This value only determines the width of the averaged profile but it does not change the shape of the profile or alter any values. It simply broadens the scale. The COSMO-RS(Ol) normally uses a 80 (+1 for the 0) elements scale because its average procedure results in slightly broader profiles than the averaging procedure of COSMO-SAC does where 50 elements are standard and sufficient.

Automatic Settings for SAC and RS(Ol)

If this options is checked the setting in smooth width and interval count are automatically set for both models.

Displaying Electronic Charges Surface Elements Profiles Obtained from Quantum Mechanics Programs

This is only a rather simple chart for displaying the "*.cosmo" files obtained from, e. g., Gaussian.

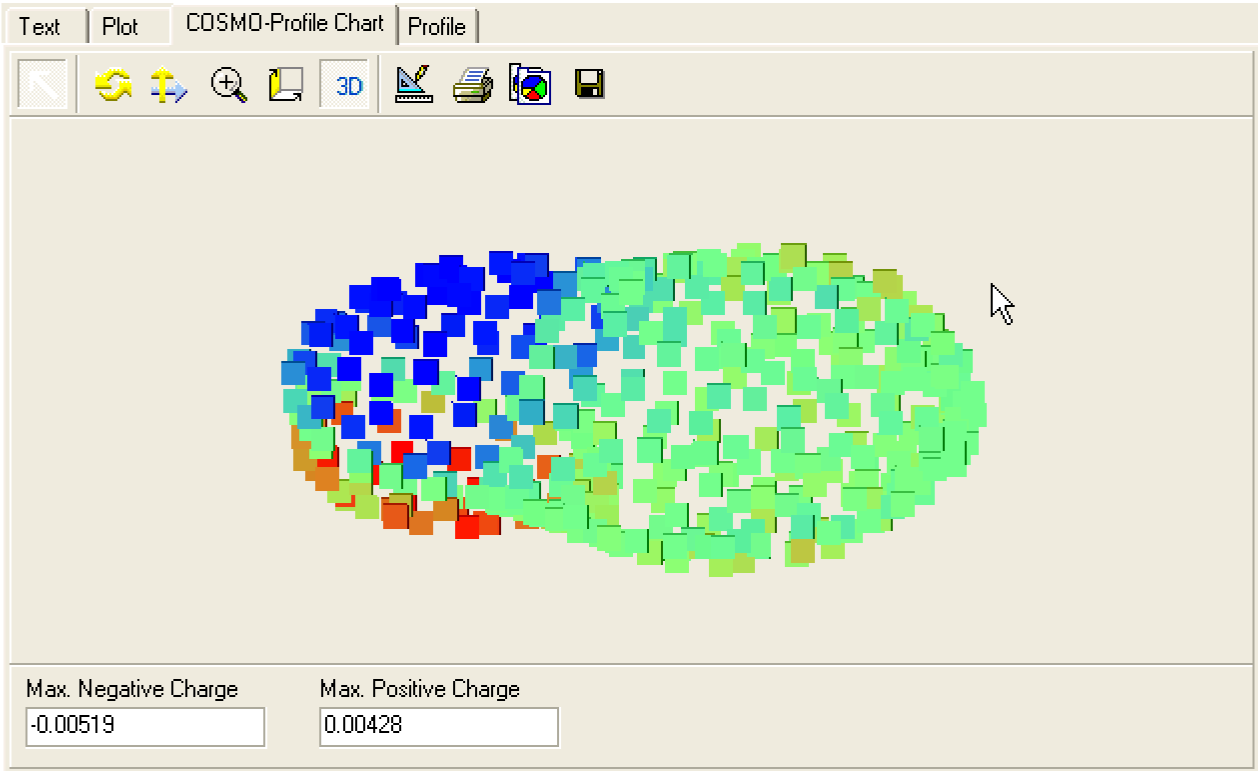
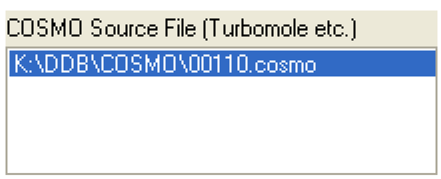


Figure 10: Methanol

The single elements are drawn as squares. Blue squares are positively charged, red squares are negatively charged and green denotes neutrality.

These charts are displayed if an entry in the files list



is left-clicked with the mouse.

i Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.
http://www.gaussian.com

ii http://www.cosmologic.de/QuantumChemistry/main_turbomole.html

iii http://www.accelrys.com/products/mstudio/modeling/quantumandcatalysis/dmol3.html

iv Oldland R.J., "Predicting Phase Equilibria Using COSMO-Based Thermodynamic Models and the VT-2004 Sigma-Profile Database", Thesis, Virginia Polytechnic Institute and State University, p1-68, 2004

v Grensemann H., "Weiterentwicklung thermodynamischer Vorhersagemodelle durch Einsatz von quantenchemischen Methode ", Thesis, Carl-von-Ossietzky-Universität Oldenburg, p1-235, 2005