Here are some infos about the new implemetation of COSMO in ricc2.
Especially, for MP2 calculations. In the first part the acronyms
are introduced, followed by a short HOWTO.
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In MP2 computations COSMO can be integrated at different points in
the theory. Usually, these approaches are called PTE, PTD, and PTED.
PTE is a noniterative energy-only scheme. Only the MOs are calculated
with COSMO and MP2 single-point energies integrated with those.
PTD (2) is a density-only scheme. Not available in Turbomole.
PTED (3) is an iterative scheme, where the correlated density is used
to make the reaction field (COSMO) self-consistent.
For single point energies PTE and PTED are quit straightforward.
For gradient calculations COSMO also has to be included in the solution
of CPHF equations for the relaxed densities. We only have that for
PTE. This contribution can be called PTED0.
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1)
Run define; in the cc menu select cbas and frozen core.
Run cosmoprep and say yes to cosmo_correlated.

2a)
A single point energy according to the PTE scheme:
Use in control
```
$ricc2
  mp2
```

Run 'dscf > dscf.out ; ricc2 > ricc2.out'
Find "Final MP2 energy" in ricc2.out

2b)
A geometry optimization according to the PTE scheme:
Use in control
```
$ricc2
  mp2
  geoopt model=mp2       state=(x)
```

Run 'jobex -level cc2'
Find "MP2-PTE energy (with OCC)" in job.last

3)
A single point energy according to the PTED scheme:
Use in control
```
$ricc2
  mp2
$response
 fop relaxed
```

Run 'cc2cosmo'
Find "MP2-PTED energy (with OCC)" in the last ricc2.log.x