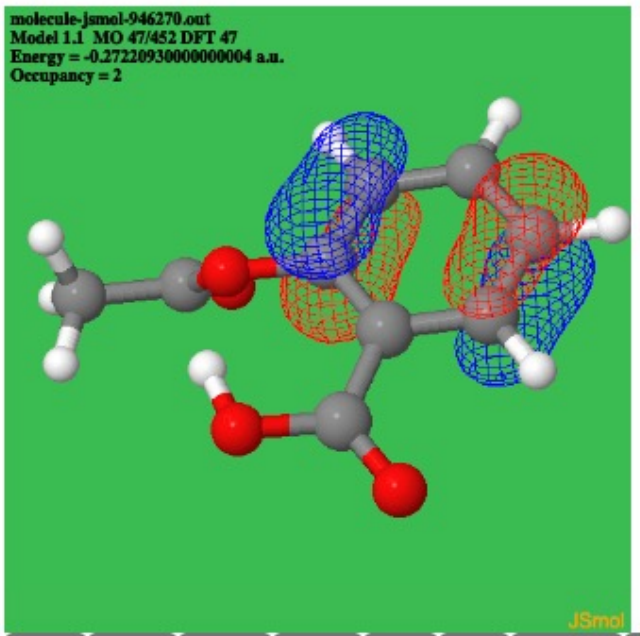
```
+=================================================+
||              Molecular Calculation              ||
+=================================================+

Id      = 33587

NWOutput = Link to NWChem Output (download)

Datafiles:
lumo-restricted.cube-2016-8-3-3:59:10 (download)
homo-restricted.cube-2016-8-3-3:59:10 (download)
mo_orbital_nwchemarrows.out-754304-2017-12-4-21:37:12 (download)

image_resset: api/image_reset/33587

Calculation performed by orbital
Numbers of cpus used for calculation = 4
Calculation walltime = 147398.600000 seconds (1 days 16 hours 56 minutes 38

+----------------+
| Energetic Data |
+----------------+

Id          = 33587
iupac       = 2-acetyloxybenzoic acid
mformula    = C9H8O4
inchi       = InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,
inchikey    = BSYNRYMUTXBXSQ-UHFFFAOYSA-N
esmiles     = CC(=O)Oc1ccccc1C(=O)O theory(dft) xc(b3lyp) basis(6-311++G(2d,2p)
calculation_type = ovcn
theory           = dft
xc               = b3lyp
basis            = 6-311++G(2d,2p)
charge,mult      = 0 1
energy           =    -648.912781 Hartrees
enthalpy correct.=       0.169439 Hartrees
entropy          =        109.438 cal/mol-K
solvation energy =       -14.463 kcal/mol  solvation_type = COSMO
Sitkoff cavity dispersion          =          2.657 kcal/mol
Honig cavity dispersion            =          8.986 kcal/mol
ASA solvent accesible surface area =        359.433 Angstrom2
ASA solvent accesible volume       =        337.193 Angstrom3

+-----------------+
| Structural Data |
+-----------------+
```



spin ON | spin OFF | labels On | labels Off | HOMO | LUMO | mo previous | mo next

JSmol: an open-source HTML5 viewer for chemical structures in 3D