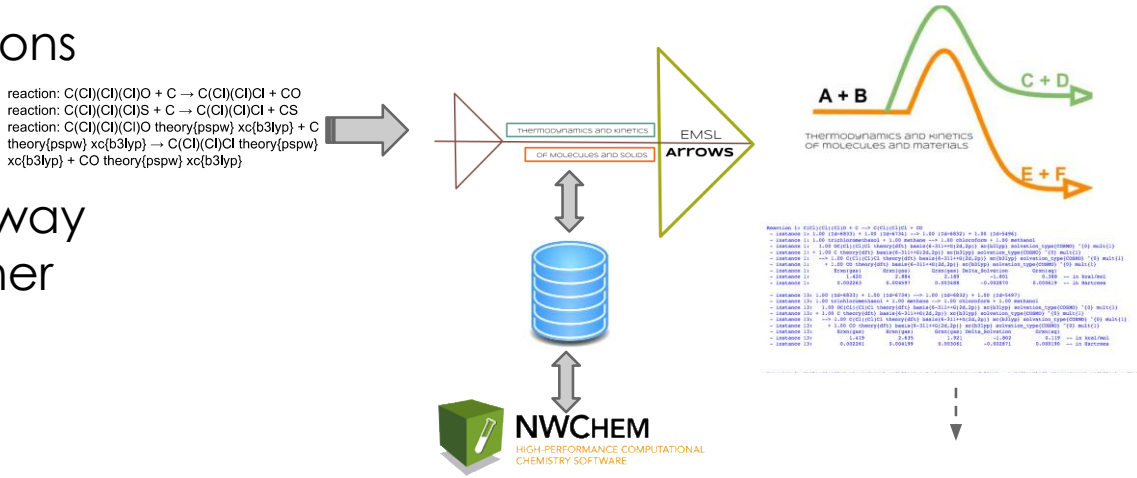
EMSL Arrows: Making molecular modeling accessible by combining NWChem, databases, and email

E. Bylaska

EMSL Arrows is a very simple way to use NWChem.
The user emails chemical reactions to arrows@emsl.pnnl.gov and then an email is sent back with thermodynamic, reaction pathway (kinetic), spectroscopy, and other results.



EMSL Arrows can calculate:

- DFT, PSPW, BAND, HF, MP2, CCSD(T)
- Reaction thermodynamics for molecular systems
- Reaction paths for molecular systems
- IR, Raman spectra, UV-vis for molecular systems, phonon spectra for materials systems
- NMR and EXAFS spectra for molecular and materials systems
- Energetics, structures, and band structures of crystals using the Crystal Open Database
- A variety of datafiles can be returned including XYZ files, CIF files, NWChem output files

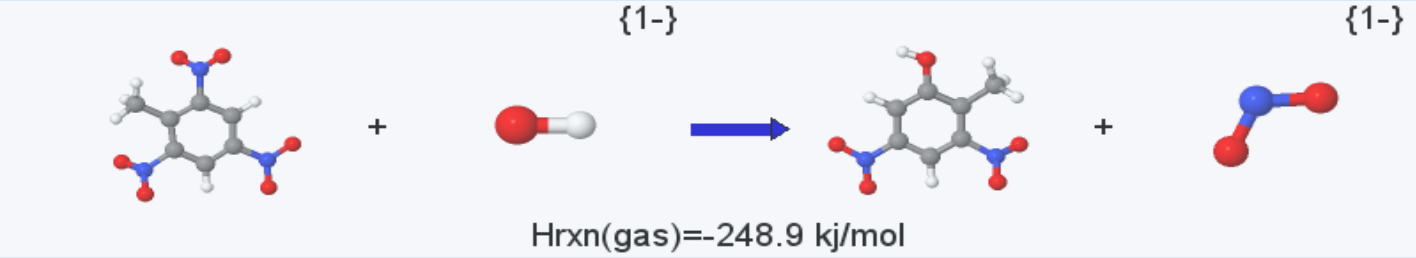
EMSL Arrows: Making molecular modeling accessible by combining NWChem, databases, and email

To: arrows@emsl.pnnl.gov Subject: Calculate SN2 Aromatic reaction

Arrows::
reaction: TNT + OH- --> TNT-2-OH + nitrite :reaction
::Arrows

Reaction 1: TNT + OH- --> TNT-2-OH + nitrite
- instance 1: 1.00 (Id=12540) + 1.00 (Id=767) --> 1.00 (Id=11836) + 1.00 (Id=1909)
- instance 1: 1.00 2-methyl-1,3,5-trinitrobenzene + 1.00 oxidane anion --> 1.00 2-methyl-3,5-dinitrophenol + 1.00 azonous acid anion
- instance 1: 1.00 C7H5N3O6 + 1.00 H1O1 --> 1.00 C7H6N2O5 + 1.00 N1O2
- instance 1: 1.00 O=N(=O)c1cc(N(=O)=O)c(c(c1)N(=O)=O)C theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{0} mult{1} nf{0}
- instance 1: + 1.00 [OH] theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{-1} mult{1} nf{?}
- instance 1: --> 1.00 O=N(=O)c1cc(O)c(c(c1)N(=O)=O)C theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{0} mult{1} nf{0}
- instance 1: + 1.00 [N]([O])[O] theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{-1} mult{1} nf{?}

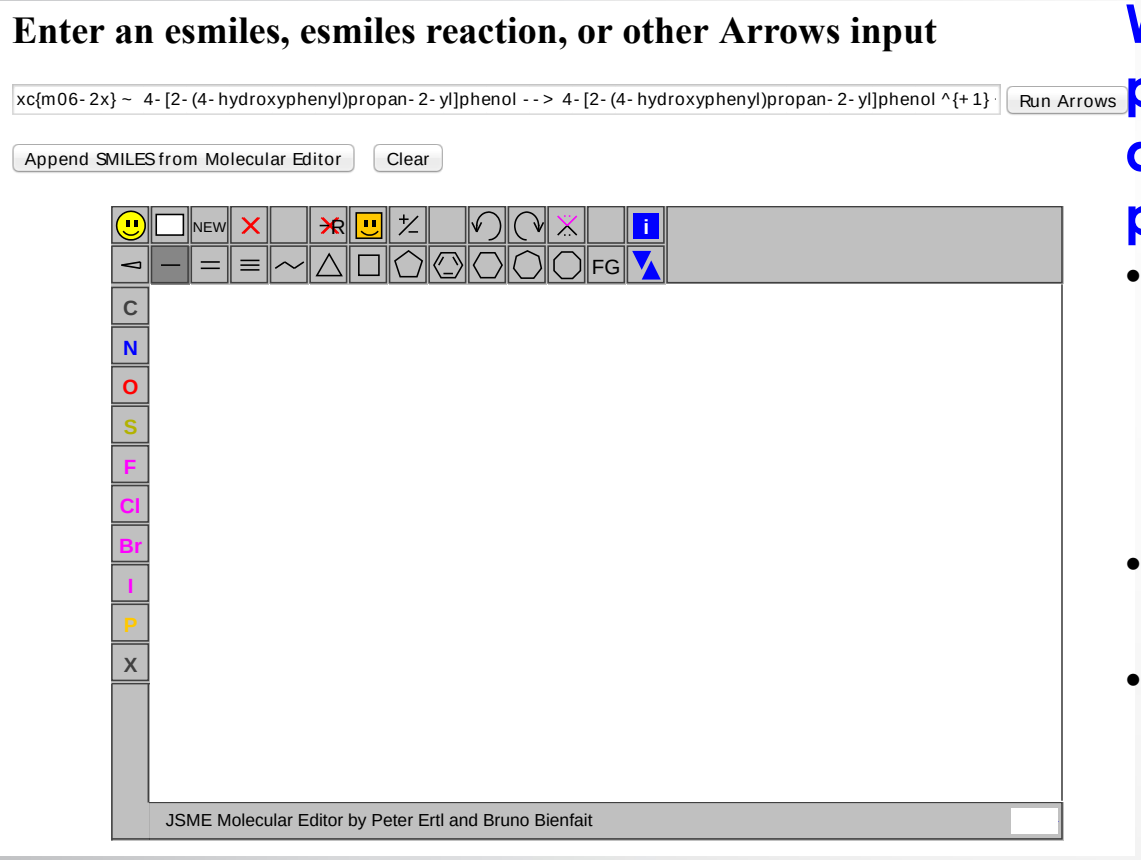
	Erxn(gas)	Hrxn(gas)	Grxn(gas)	Delta_Solvation	Grxn(aq)	
- instance 1:	-59.826	-59.500	-62.091	25.445	-36.645	-- in kcal/mol
- instance 1:	-250.310	-248.949	-259.787	106.463	-153.324	-- in kj/mol
- instance 1:	-0.095338	-0.094820	-0.098948	0.040550	-0.058398	-- in Hartrees



EMSL Arrow API

There is a Web API for EMSL Arrows

https://arrows.emsl.pnnl.gov/api/



Web API can be used in perform standard calculation and interface with other programs

- Perform standard EMSL Arrows operation such as fetch xyz and nwchem input file, calculate nmr spectra, calculate reaction energies….
- Can be used with speech recognizer
- Can be used with OCR chemical software such as OSRA

Calculate a Molecule

EMSL Arrows: A Revolutionary Approach To Materials and Chemical Simulations

A scientific service that uses NWChem and chemical computational databases to make materials and chemical modeling accessible via a broad spectrum of digital communications including posts to web APIs, social networks, and traditional email.

Click here for more information about EMSL Arrows.

73584 Arrows calculations carried out
44121 Molecular calculations in database

Enter an esmiles, esmiles reaction, or other Arrows input, then push the "Run Arrows" button.

Sc1ccccc1 theory{pspw}

Run Arrows

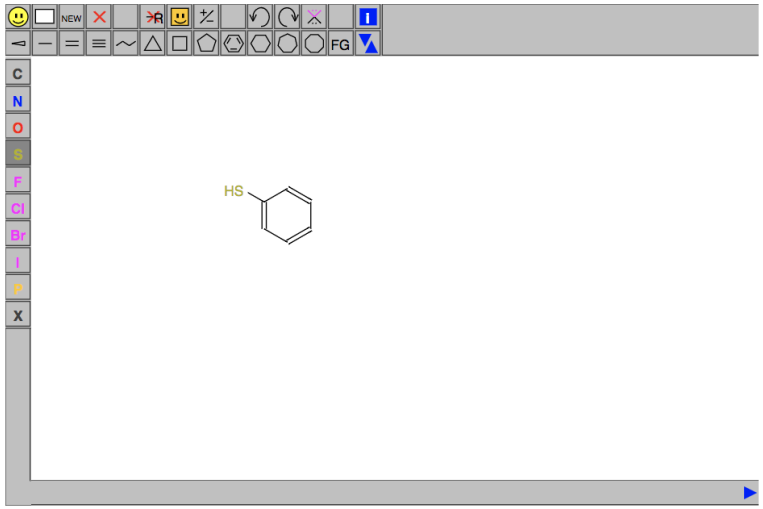
Append SMILES from Molecular Editor | no html5 | Clear | Email Submit

theory{dft} | theory{pspw} | theory{pspw4} | theory{mp2} | theory{ccsd(t)} | theory{pm3}

xc{lda} | xc{pbe} | xc{pbe0} | xc{b3lyp} | xc{m06-2x} | solvation_type{COSMO} | solvation_type{COSMO-SMD} | solvation_type{None}

--> | + | ~ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 0

Switch to Reaction Editor



JSME Editor Citation: B. Bienfait and P. Ertl, JSME: a free molecule editor in JavaScript, J. Cheminformatics 5:24 (2013)

Just enter molecule and then push Run Arrows

Id = 35419

NWOutput = Link to NWChem Output

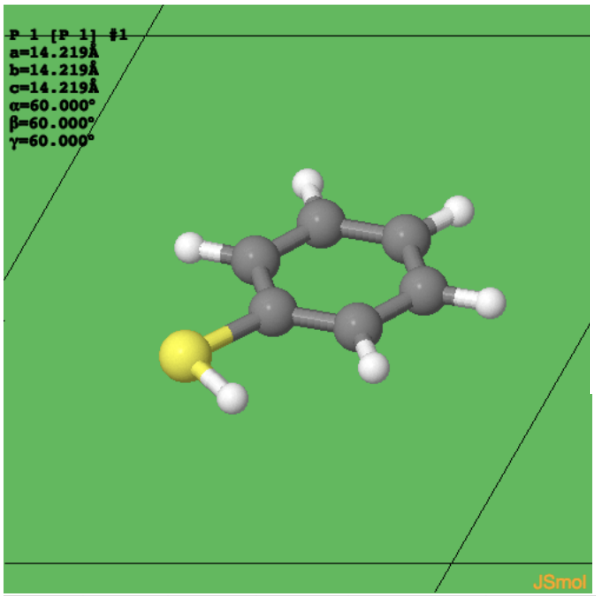
Datafiles:
lumo-restricted.cube-2016-12-1-13:33:21 (download)
homo-restricted.cube-2016-12-1-13:33:21 (download)

Calculation performed by we16124
Numbers of cpus used for calculation = 2
Calculation walltime = 10220.900000 seconds (0 days 2 hours 5(

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

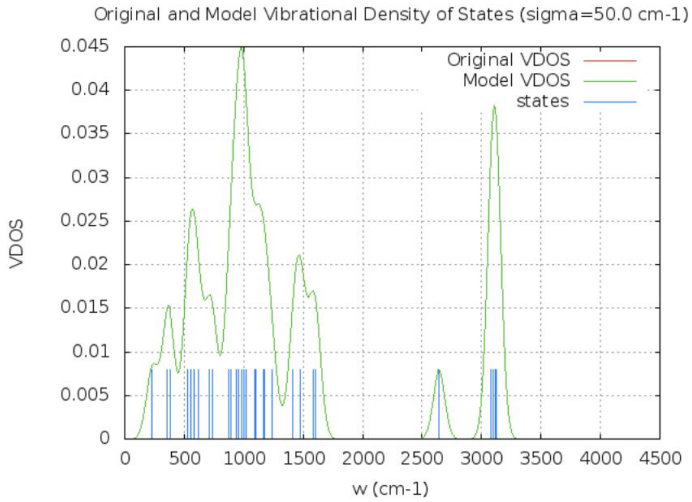
```
Id          = 35419
iupac       = benzenethiol
mformula    = C6H6S1
inchi       = InChI=1S/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H
inchikey    = RMVRSNDYEFQCLF-UHFFFAOYSA-N
esmiles     = Sc1ccccc1 theory{pspw} xc{pbe} basis{100.0 Ry} solv
calculation_type = ov
theory           = pspw
xc               = pbe
basis            = 100.0 Ry
charge,mult      = 0 1
energy           =     -48.010690 Hartrees
enthalpy correct.=       0.106271 Hartrees
entropy          =         75.570 cal/mol-K
solvation energy =          0.000 kcal/mol  solvation_type = 1
Sitkoff cavity dispersion          =          2.220 kcal/mol
Honig cavity dispersion            =          6.798 kcal/mol
ASA solvent accesible surface area =        271.902 Angstrom2
ASA solvent accesible volume       =        259.163 Angstrom3
```

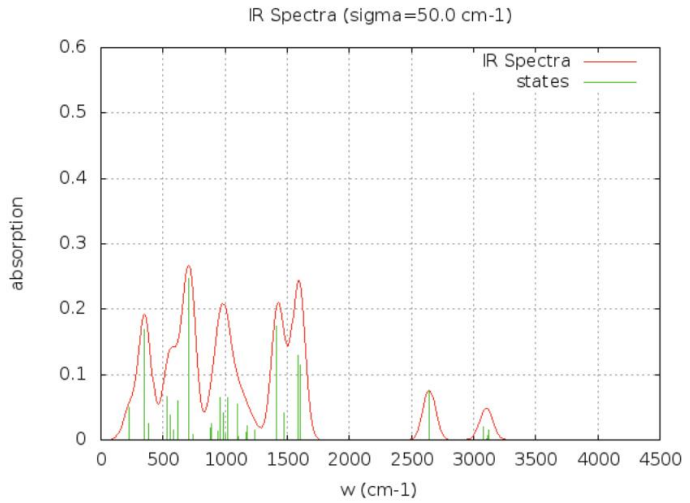
+-----------------+
| Structural Data |
+-----------------+



spin ON | spin OFF | labels On | labels Off | unitcell/axes On | unitcell/axes Off

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





NWOutput = Link to NWChem Output

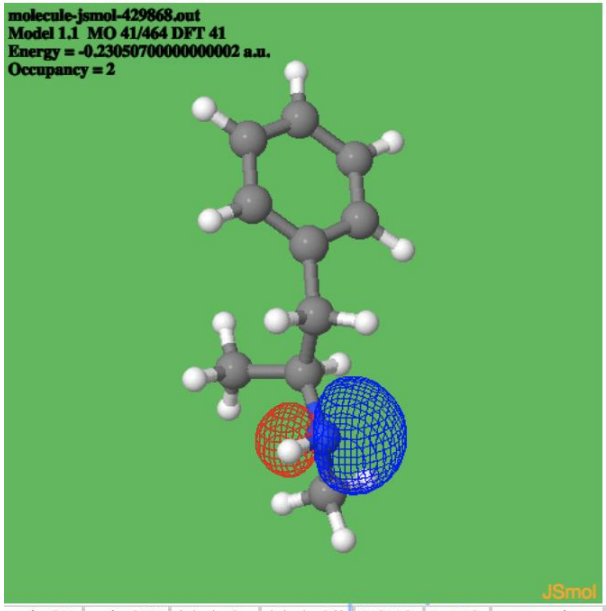
Datafiles:
homo-restricted.cube-984065-2017-6-8-22:37:2 (download)
lumo-restricted.cube-984065-2017-6-8-22:37:2 (download)
mo_orbital_nwchemarrows.out-389786-2017-12-4-22:37:55 (download)

Calculation performed by Eric Bylaska - arrow1.emsl.pnl.gov
Numbers of cpus used for calculation = 32
Calculation walltime = 90576.800000 seconds (1 days 1 hours 9 minutes 36 seconds)

Energetic Data

Id = 42995
iupac = (2S)-N-methyl-1-phenylpropan-2-amine
mformula = C10H15N1
inchi = InChI=1S/C10H15N/c1-9(11-2)8-10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3/t9-/m0/s1
inchikey = MYWUZJCMWCOHBA-VIFPVBQESA-N
esmiles = CN[C@H](Cc1ccccc1)C theory{dft} xc{b3lyp} basis{6-311++G(2d,2p)} solvation_type{COSMO} ^{0}
calculation_type = ovc
theory = dft
xc = b3lyp
basis = 6-311++G(2d,2p)
charge,mult = 0 1
energy = -444.991100 Hartrees
enthalpy correct.= 0.242309 Hartrees
entropy = 104.886 cal/mol-K
solvation energy = -3.141 kcal/mol solvation_type = COSMO
Sitkoff cavity dispersion = 2.729 kcal/mol
Honig cavity dispersion = 9.347 kcal/mol
ASA solvent accesible surface area = 373.892 Angstrom2
ASA solvent accesible volume = 337.171 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

NMR example

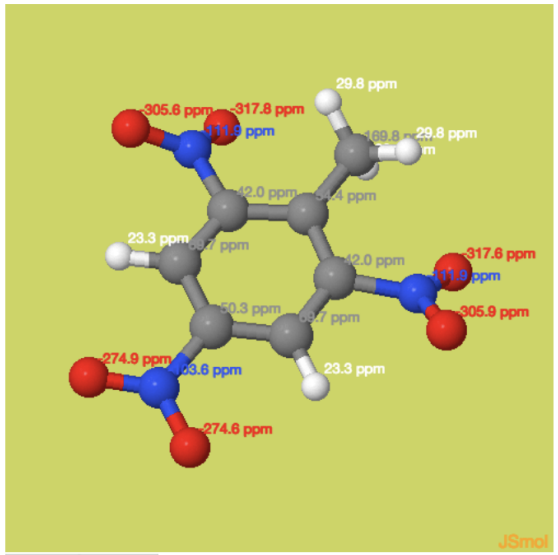
nmr for O=N(=O)c1cc(N(=O)=O)c(c(c1)N(=O)=O)C basis{6-31G*} solvation_type{None}

Run Arrows

Append SMILES from Molecular Editor | no html5 | Clear | Email Submit

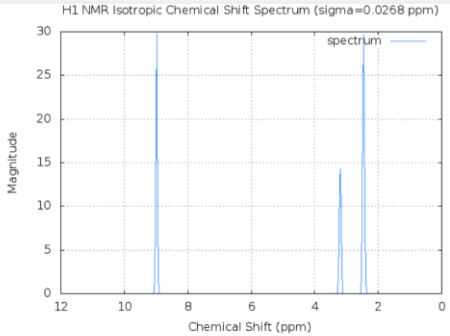
```
+----------------------------------------+
| NMR Shielding and Chemical Shift Data |
+----------------------------------------+

Id              = 33438
iupac           = 2-methyl-1,3,5-trinitrobenzene
mformula        = C7H5N3O6
InChI           = InChI=1S/C7H5N3O6/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10(15)16/h2-3H,1H3
smiles          = O=N(=O)c1cc(N(=O)=O)c(c(c1)N(=O)=O)C
esmiles         = O=N(=O)c1cc(N(=O)=O)c(c(c1)N(=O)=O)C theory{dft} xc{b3lyp} basis{6-31G*} solvation_type{None} ^{0} property{nmr}
theory          = dft
xc              = b3lyp
basis           = 6-31G*
theory_property = dft
xc_property     = b3lyp
basis_property  = 6-31G*
charge          = 0
mult            = 1
solvation_type  = None
```

Link to 1H NMR prediction from nmrdb
Link to 13C NMR prediction from nmrdb
Link to COSY prediction from nmrdb
Link to HSQC/HMBC prediction from nmrdb

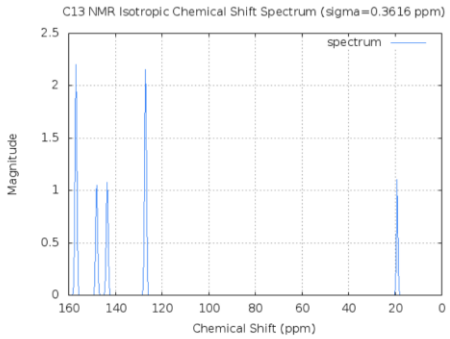


spin ON | spin OFF

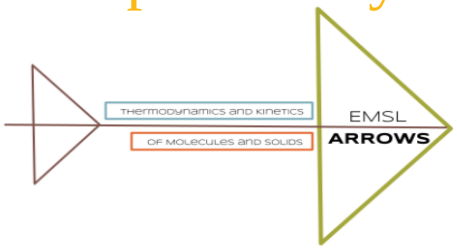
JSmol: an open-source HTML5 viewer for chemical structures in 3D




```
C13 - slope = -0.926900  intersept = 187.474300  - RMSD=2.358100 R2=0.998300
  - theory{dft} xc{b3lyp} basis{6-31G*}
  - theory_property{dft} xc_property{b3lyp} basis_property{6-31G*}
  - solvation_type{None} solvation_dielectric{0.000000}
  - reference{http://cheshirenmr.info/ScalingFactors.htm#tablelaheading}

C13 NMR chemical shifts:
     2   C ppm=   127.078326
     3   C ppm=   147.975726
     4   C ppm=   127.077678
     6   C ppm=   156.925019
     7   C ppm=   143.533175
     8   C ppm=   156.921135
     9   C ppm=    19.101845
```



Other Examples to Try



EMSL Arrows: A Revolutionary Approach To Materials and Chemical Simulations

A scientific service that uses NWChem and chemical computational databases to make materials and chemical modeling accessible via a broad spectrum of digital communications including posts to web APIs, social networks, and traditional email.

Click here for more information about EMSL Arrows.

73581 Arrows calculations carried out
44121 Molecular calculations in database

Enter an esmiles, esmiles reaction, or other Arrows input, then push the "Run Arrows" button.

TNT + hydroxide --> TNT-2-OH + nitrite — Run Arrows
Append SMILES from Molecular Editor | no html5 | Clear — Email Submit

TNT + hydroxide --> TNT-2-OH + nitrite ~ basis{6-31G*} — Run Arrows
Append SMILES from Molecular Editor | no html5 | Clear — Email Submit

TNT + hydroxide --> TNT-2-OH + nitrite ~ theory{ccsd(t)} — Run Arrows
Append SMILES from Molecular Editor | no html5 | Clear — Email Submit

input deck for CCI — Run Arrows
Append SMILES from Molecular Editor | no html5 | Clear — Email Submit

input deck for CCI theory{aimd-mm} property{henry} — Run Arrows
Append SMILES from Molecular Editor | no html5 | Clear — Email Submit

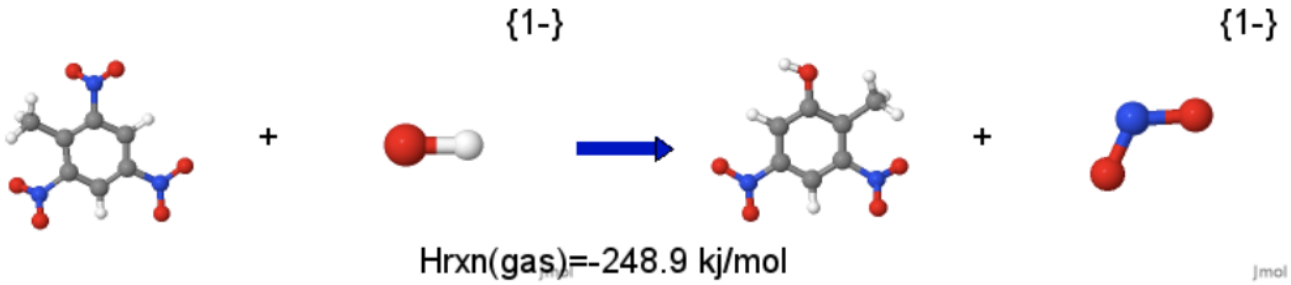
input deck for valium — Run Arrows
Append SMILES from Molecular Editor | no html5 | Clear — Email Submit

A scientific service that uses NWChem and chemical computational databases to make materials and chemical modeling accessible via a broad spectrum of digital communications including posts to web APIs, social networks, and traditional email.

Molecular modeling software has previously been extremely complex, making it prohibative to all but experts in the field, yet even experts can struggle to perform calculations. This service is designed to be used by experts and non-experts alike. Experts can carry out and keep track of large numbers of complex calculations with diverse levels of theories present in their workflows. Additionally, due to a streamlined and easy-to-use input, non-experts can carry out a wide variety of molecular modeling calculations previously not accessible to them.

Link back to EMSL Arrows API

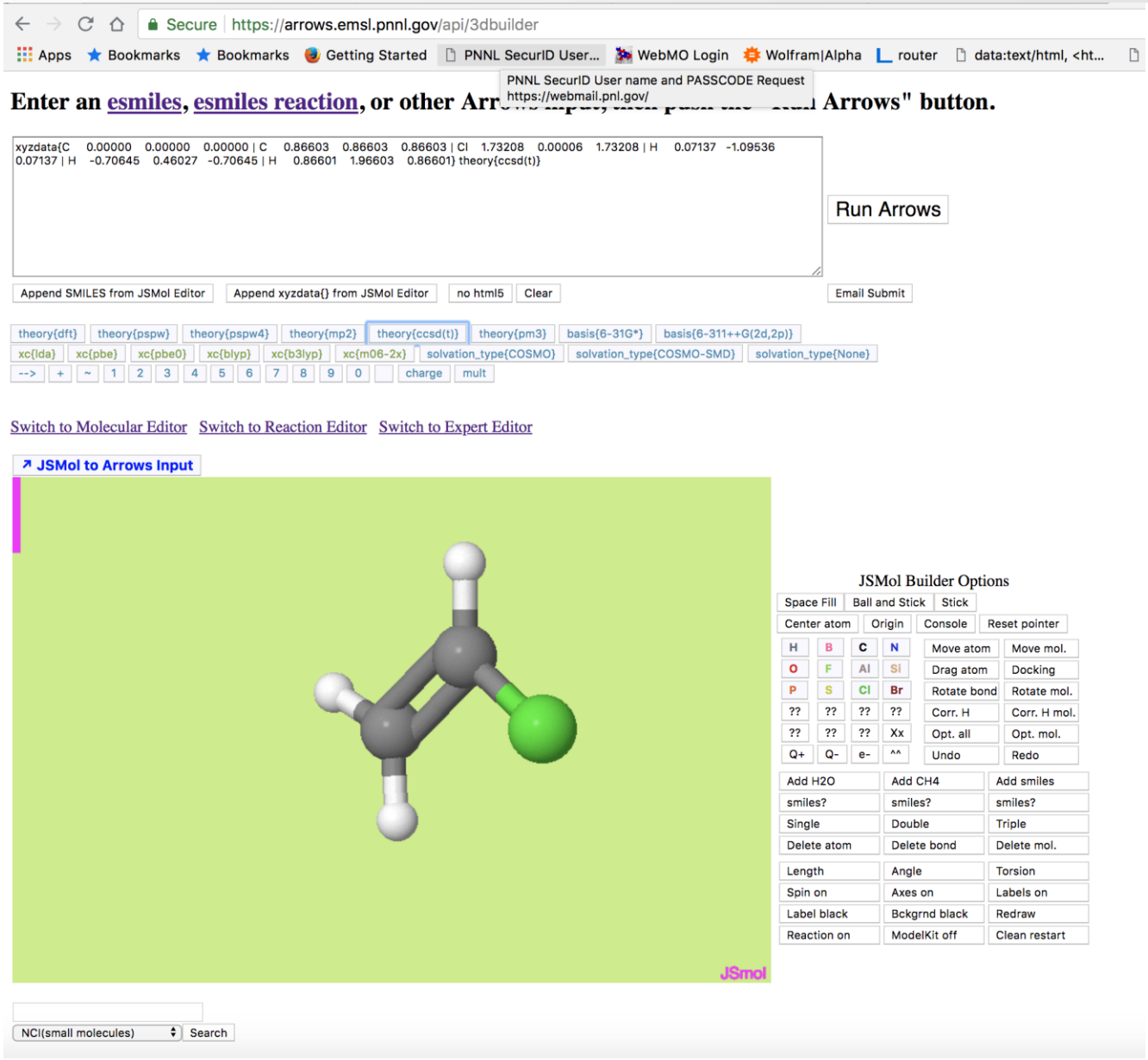
```
Reaction 1: TNT + hydroxide --> TNT-2-OH + nitrite
 - instance 1: 1.00 (Id=12540) + 1.00 (Id=34191) --> 1.00 (Id=11836) + 1.00 (Id=1909)
 - instance 1: 1.00 2-methyl-1,3,5-trinitrobenzene + 1.00 oxidane anion --> 1.00 2-methyl-3,5-dinitrophenol + 1.00 azonous acid anion
 - instance 1: 1.00 C7H5N3O6 + 1.00 H1O1 --> 1.00 C7H6N2O5 + 1.00 N1O2
 - instance 1:   1.00 O=N(=O)c1cc(N(=O)=O)c(c(c1)N(=O)=O)C theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{0} mult
 - instance 1: + 1.00 [OH] theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{-1} mult{1} nf{0}
 - instance 1:   --> 1.00 O=N(=O)c1cc(O)c(c(c1)N(=O)=O)C theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{0} mult{1
 - instance 1:     + 1.00 [N]([O])[O] theory{dft} basis{6-311++G(2d,2p)} xc{b3lyp} solvation_type{COSMO} ^{-1} mult{1} nf{?}
 - instance 1:        Erxn(gas)       Hrxn(gas)       Grxn(gas) Delta_Solvation        Grxn(aq)
 - instance 1:          -59.826         -59.501         -62.091          25.365         -36.726  -- in kcal/mol
 - instance 1:          -250.310        -248.952        -259.790         106.128        -153.662  -- in kj/mol
 - instance 1:         -0.095338       -0.094821       -0.098949        0.040422       -0.058527  -- in Hartrees
```




```
All requests to Arrows were successful.
```

Link back to EMSL Arrows API
More information about EMSL Arrows

3D Builder


Secure https://arrows.emsl.pnnl.gov/api/3dbuilder
Apps Bookmarks Bookmarks Getting Started PNNL SecurID User... WebMO Login Wolfram|Alpha router data:text/html, <ht...
PNNL SecurID User name and PASSCODE Request
https://webmail.pnl.gov/
Enter an esmiles, esmiles reaction, or other Arr Arrows" button.
xyzdata{C 0.00000 0.00000 0.00000 | C 0.86603 0.86603 0.86603 | Cl 1.73208 0.00006 1.73208 | H 0.07137 -1.09536
0.07137 | H -0.70645 0.46027 -0.70645 | H 0.86601 1.96603 0.86601} theory{ccsd(t)}
Run Arrows
Append SMILES from JSMol Editor
Append xyzdata{} from JSMol Editor
no html5
Clear
Email Submit
theory{dft} theory{pspw} theory{pspw4} theory{mp2} theory{ccsd(t)} theory{pm3} basis{6-31G*} basis{6-311++G(2d,2p)}
xc{lda} xc{pbe} xc{pbe0} xc{blyp} xc{b3lyp} xc{m06-2x} solvation_type{COSMO} solvation_type{COSMO-SMD} solvation_type{None}
--> + ~ 1 2 3 4 5 6 7 8 9 0 charge mult
Switch to Molecular Editor
Switch to Reaction Editor
Switch to Expert Editor
↗ JSMol to Arrows Input
JSMol
JSMol Builder Options
Space Fill
Ball and Stick
Stick
Center atom
Origin
Console
Reset pointer
H B C N Move atom Move mol.
O F Al Si Drag atom Docking
P S Cl Br Rotate bond Rotate mol.
?? ?? ?? ?? Corr. H Corr. H mol.
?? ?? ?? Xx Opt. all Opt. mol.
Q+ Q- e- ^^ Undo Redo
Add H2O
Add CH4
Add smiles
smiles?
smiles?
smiles?
Single
Double
Triple
Delete atom
Delete bond
Delete mol.
Length
Angle
Torsion
Spin on
Axes on
Labels on
Label black
Bckgrnd black
Redraw
Reaction on
ModelKit off
Clean restart
NCI(small molecules)
Search