

```
C:\temp>pip install RASPA2
Collecting RASPA2
  Using cached RASPA2-2.0.3.tar.gz
data_CON

_audit_creation_method RASPA-1.0
_audit_creation_date 2011-12-20
_audit_author_name 'David Dubbeldam'

_citation_author_name      'R. F. Lobo and M. E. Davis'
_citation_title            'CIT-1: A new molecular sieve with intersecting pores bounded by 10- and 12-rings'
_citation_journal_abbrev   'J. Am. Chem. Soc.'
_citation_journal_volume   117
_citation_page_first      3766
_citation_page_last       3779
_citation_year            1994

_cell_length_a    22.6242
_cell_length_b    13.3503
_cell_length_c    12.3642
_cell_angle_alpha 90
_cell_angle_beta  68.913
_cell_angle_gamma 90
_cell_volume      3484.4

_symmetry_cell_setting      monoclinic
_symmetry_space_group_name_Hall '-C 2y'
_symmetry_space_group_name_H-M 'C 1 2/m 1'
_symmetry_Int_Tables_number  12

loop_
_symmetry_equiv_pos_as_xyz
```

```
'x,y,z'  
'-x,y,-z'  
'-x,-y,-z'  
'x,-y,z'  
'x+1/2,y+1/2,z'  
'-x+1/2,y+1/2,-z'  
'-x+1/2,-y+1/2,-z'  
'x+1/2,-y+1/2,z'
```

```
loop_
```

```
_atom_site_label
```

```
_atom_site_type_symbol
```

```
_atom_site_fract_x
```

```
_atom_site_fract_y
```

```
_atom_site_fract_z
```

```
_atom_site_charge
```

Si	Si	0.0677	0.1102	0.4914	0
Si	Si	0.1567	0.1889	0.251	0
Si	Si	0.0734	0.1204	0.739	0
Si	Si	0.2879	0.1171	0.1026	0
Si	Si	0.277	0.1141	0.8607	0
Si	Si	0.0738	0.1195	0.1043	0
Si	Si	0.148	0.1898	0.8835	0
0	0	0.0763	0	0.4256	0
0	0	0.0784	0.138	0.6085	0
0	0	0.1205	0.1669	0.3814	0
0	0	0	0.1458	0.5	0
0	0	0.2185	0.12	0.2009	0
0	0	0.1097	0.1569	0.186	0
0	0	0.1728	0.3005	0.2109	0
0	0	0.0852	0	0.7309	0
0	0	0.0003	0.1379	0.8223	0

```
0      0      0.1271      0.1859      0.7717      0
0      0      0.3045      0          0.1272      0
0      0      0.2721      0.133      0.9904      0
0      0      0.3442      0.1888      0.0983      0
0      0      0.2102      0.1217      0.8382      0
0      0      0.3046      0          0.8219      0
0      0      0.0873      0          0.1087      0
0      0      0.0837      0.1783      0.99        0
```

Exception:

Traceback (most recent call last):

```
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\tarfile.py", line 2257, in utime
    os.utime(targetpath, (tarinfo.mtime, tarinfo.mtime))
OSError: [WinError 87] The parameter is incorrect: 'C:\\Users\\vaesens\\AppData\\Local\\Temp\\pip-build-
k13p02rb\\RASP2\\structures/cif/CON.cif'
```

During handling of the above exception, another exception occurred:

Traceback (most recent call last):

```
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\basecommand.py", line 215,
in main
    status = self.run(options, args)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\commands\install.py", line
310, in run
    wb.build(autobuilding=True)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\wheel.py", line 750, in
build
    self.requirement_set.prepare_files(self.finder)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\req\req_set.py", line 370,
in prepare_files
    ignore_dependencies=self.ignore_dependencies))
```

```
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\req\req_set.py", line 587,
in _prepare_file
    session=self.session, hashes=hashes)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\download.py", line 810, in
unpack_url
    hashes=hashes
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\download.py", line 653, in
unpack_http_url
    unpack_file(from_path, location, content_type, link)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\utils\__init__.py", line
605, in unpack_file
    untar_file(filename, location)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\site-packages\pip\utils\__init__.py", line
581, in untar_file
    tar.utime(member, path)
File "c:\users\vaesens\appdata\local\programs\python\python35-32\lib\tarfile.py", line 2259, in utime
    raise ExtractError("could not change modification time")
tarfile.ExtractError: could not change modification time
```