Compound_2_Mat. std_output file

```
Module                          : Sorption
Version                         : 6.1
Build date                      : Oct 12 2012
Host                            : vardha-PC
Operating system                : Windows
Task started                    : Mon Apr 21 11:32:08 2014


Task                            : Adsorption isotherm
Monte Carlo method              : Metropolis
Random number seed              :  337760021


---- Fixed pressure calculation parameters ----

Equilibration steps             :  10000
Production steps                :  100000


---- Energy parameters ----

Forcefield                      : COMPASS27
Electrostatic terms:
  Summation method              : Ewald & Group
  Accuracy                      : 0.0001 kcal/mol
  Charge group cutoff           : 15.5 A
  Buffer width                  : 0.5 A

van der Waals terms:
  Summation method              : Atom based
  Truncation method             : Cubic spline
  Cutoff distance               : 15.5 A
  Spline width                  : 1 A
  Buffer width                  : 0.5 A

Sample interval                 : 50 steps


---- Metropolis Monte Carlo method parameters ----

 |               | Ratio       | Maximum     |
 |               |             | amplitude   |
 |_____________________________________________
 | Exchange      |       2.000 |             |
 | Rotate        |       1.000 | 5 deg       |
 | Translate     |       1.000 | 1 A         |
 | Regrowth      |       0.100 |             |


---- Fugacity point 1 of 26 ----



---- Fixed pressure calculation ----

Framework charge                :  1.600 e per cell

 | Sorbate      | Charge      | Fugacity    |
 |              |             | kPa         |
 |_____________________________________________
 | 3D Atomistic |       0.000 |       0.144 |

Temperature                     :  298.000 K
Total Fugacity                  :  0.144 kPa



---- Monte Carlo steps ----
```

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps |
| 3D Atomistic | 3 | | | | | | |
| Accepted | | 1 | 0 | 0 | 17025 | 1956 | 0 |
| Attempted | | 24456 | 24431 | 2460 | 24239 | 24414 | 0 |
| Ratio | | 4.089e-005 | 0.000 | 0.000 | 0.702 | 0.080 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 2.837 | 2 | 3 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 41.013 | 9.492 | 71.992 |

---- Overall system energies ----

Average total energy : 2683.807 kcal/mol

---- Fugacity point 2 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.257 |

Temperature : 298.000 K
Total Fugacity : 0.257 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps |
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 1 | 0 | 0 | | | |

```
15649 |        1673 |           0 |
  |  Attempted    |             |       24260 |       24539 |        2361 |
24638 |       24202 |           0 |
  |  Ratio        |             |  4.122e-005 |       0.000 |       0.000 |
0.635 |       0.069 |             |
```

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 3.584 | 3 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 53.238 | 16.692 | 73.292 |

---- Overall system energies ----

Average total energy : 3376.114 kcal/mol

---- Fugacity point 3 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.371 |

Temperature : 298.000 K
Total Fugacity : 0.371 kPa

---- Monte Carlo steps ----

```
 | Sorbate      | Loading     | Creation    | Destruction | Regrowth    |
Rotation    | Translation | C/D Ratio   |
 |              |             | steps       | steps       | steps       | steps
    | steps       |             |
|_____________________________________________________________________________
_____________________________________
 | 3D Atomistic |           4 |             |             |             |
    |              |             |
 |  Accepted    |             |           0 |           0 |           0 |
14576 |        1346 |           0 |
 |  Attempted   |             |       24427 |       24256 |        2348 |
24370 |       24599 |           0 |
 |  Ratio       |             |       0.000 |       0.000 |       0.000 |
0.598 |       0.055 |             |
```

---- Loading ----

```
 | Sorbate      | Average     | Minimum     | Maximum     |
```

| | loading | loading | loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.020 | 39.592 | 73.892 |

---- Overall system energies ----

Average total energy : 3757.294 kcal/mol

---- Fugacity point 4 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.484 |

Temperature : 298.000 K
Total Fugacity : 0.484 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio steps |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14375 | 1373 | 0 |
| Attempted | | 24334 | 24511 | 2404 | 24418 | 24333 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.589 | 0.056 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 59.569 | 41.992 | 73.092 |

---- Overall system energies ----

Average total energy : 3758.703 kcal/mol

---- Fugacity point 5 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.597 |

Temperature : 298.000 K
Total Fugacity : 0.597 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14678 | 1366 | 0 |
| Attempted | | 24491 | 24394 | 2323 | 24403 | 24389 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.601 | 0.056 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.189 | 40.592 | 73.292 |

---- Overall system energies ----

Average total energy : 3757.616 kcal/mol

---- Fugacity point 6 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.711 |

Temperature : 298.000 K
Total Fugacity : 0.711 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14983 | 1471 | 0 |
| Attempted | | 24504 | 24217 | 2430 | 24534 | 24315 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.611 | 0.060 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.670 | 39.292 | 73.992 |

---- Overall system energies ----

Average total energy : 3758.416 kcal/mol

---- Fugacity point 7 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.824 |

Temperature : 298.000 K
Total Fugacity : 0.824 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps |
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14703 | 1470 | 0 |
| Attempted | | 24346 | 24273 | 2438 | 24663 | 24280 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.596 | 0.061 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.242 | 39.392 | 73.792 |

---- Overall system energies ----

Average total energy : 3757.825 kcal/mol

---- Fugacity point 8 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 0.937 |

Temperature : 298.000 K
Total Fugacity : 0.937 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps |

| 3D Atomistic | 4 | | | | |
|---|---|---|---|---|---|
| Accepted | | 0 | 0 | 0 | 14541 | 1410 | 0 |
| Attempted | | 24626 | 24404 | 2403 | 24193 | 24374 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.601 | 0.058 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.238 | 40.492 | 74.092 |

---- Overall system energies ----

Average total energy : 3757.565 kcal/mol

---- Fugacity point 9 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.050 |

Temperature : 298.000 K
Total Fugacity : 1.050 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 15730 | 1636 | 0 |
| Attempted | | 24583 | 24116 | 2455 | 24409 | 24437 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.644 | 0.067 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 58.406 | 37.992 | 73.492 |

---- Overall system energies ----

Average total energy : 3759.892 kcal/mol

---- Fugacity point 10 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.164 |

Temperature : 298.000 K
Total Fugacity : 1.164 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 15487 | 1494 | 0 |
| Attempted | | 24331 | 24245 | 2406 | 24456 | 24562 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.633 | 0.061 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average | Minimum | Maximum |
|---|---|---|---|

| | kcal/mol | kcal/mol | kcal/mol |
|---|---|---|---|
| 3D Atomistic | 58.472 | 40.992 | 75.292 |

---- Overall system energies ----

Average total energy : 3760.088 kcal/mol

---- Fugacity point 11 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.277 |

Temperature : 298.000 K
Total Fugacity : 1.277 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14715 | 1424 | 0 |
| Attempted | | 24190 | 24703 | 2456 | 24372 | 24279 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.604 | 0.059 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.551 | 41.192 | 73.292 |

---- Overall system energies ----

Average total energy : 3758.159 kcal/mol

---- Fugacity point 12 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.390 |

Temperature : 298.000 K
Total Fugacity : 1.390 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation steps | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14173 | 1349 | 0 |
| Attempted | | 24281 | 24659 | 2526 | 24279 | 24255 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.584 | 0.056 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.166 | 38.392 | 74.092 |

---- Overall system energies ----

Average total energy : 3757.340 kcal/mol

---- Fugacity point 13 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.503 |

Temperature : 298.000 K
Total Fugacity : 1.503 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps |
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14694 | 1415 | 0 |
| Attempted | | 24424 | 24310 | 2422 | 24407 | 24437 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.602 | 0.058 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.068 | 40.092 | 73.392 |

---- Overall system energies ----

Average total energy : 3757.684 kcal/mol

---- Fugacity point 14 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.617 |

Temperature : 298.000 K
Total Fugacity : 1.617 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | | |
| Accepted | | 0 | 0 | 0 | 14534 | 1405 | 0 | |
| Attempted | | 24442 | 24359 | 2531 | 24253 | 24415 | 0 | |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.599 | 0.058 | | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.669 | 40.292 | 73.292 |

---- Overall system energies ----

Average total energy : 3756.983 kcal/mol

---- Fugacity point 15 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.730 |

Temperature : 298.000 K
Total Fugacity : 1.730 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio steps |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14717 | 1396 | 0 | |
| Attempted | | 24261 | 24554 | 2368 | 24603 | 24214 | 0 | |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.598 | 0.058 | | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.403 | 39.492 | 74.292 |

---- Overall system energies ----

Average total energy : 3757.604 kcal/mol

---- Fugacity point 16 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.843 |

Temperature : 298.000 K
Total Fugacity : 1.843 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14501 | 1418 | 0 |
| Attempted | | 24449 | 24552 | 2415 | 24205 | 24379 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.599 | 0.058 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.074 | 40.492 | 73.692 |

---- Overall system energies ----

Average total energy : 3757.335 kcal/mol

---- Fugacity point 17 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 1.957 |

Temperature : 298.000 K
Total Fugacity : 1.957 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14437 | 1411 | 0 |
| Attempted | | 24312 | 24373 | 2454 | 24288 | 24573 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.594 | 0.057 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.315 | 41.192 | 73.692 |

---- Overall system energies ----

Average total energy : 3756.544 kcal/mol

---- Fugacity point 18 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.070 |

Temperature : 298.000 K
Total Fugacity : 2.070 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation steps | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14407 | 1448 | 0 |
| Attempted | | 24310 | 24630 | 2374 | 24217 | 24469 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.595 | 0.059 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.530 | 39.792 | 73.792 |

---- Overall system energies ----

Average total energy : 3757.472 kcal/mol

---- Fugacity point 19 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|

| 3D Atomistic | 0.000 | 2.183 |

Temperature : 298.000 K
Total Fugacity : 2.183 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14637 | 1341 | 0 |
| Attempted | | 24423 | 24230 | 2425 | 24381 | 24541 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.600 | 0.055 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.219 | 40.592 | 73.992 |

---- Overall system energies ----

Average total energy : 3756.978 kcal/mol

---- Fugacity point 20 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.296 |

Temperature : 298.000 K
Total Fugacity : 2.296 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth |
|---|---|---|---|---|

| Rotation | Translation | C/D Ratio | | | | |
|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps |
| 3D Atomistic | 4 | | | | | |
| Accepted | | 0 | 0 | 0 | 14837 | 1461 |
| | | 0 | | | | |
| Attempted | | 24441 | 24283 | 2431 | 24484 | 24361 |
| | | 0 | | | | |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.606 | 0.060 |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.031 | 40.292 | 73.292 |

---- Overall system energies ----

Average total energy : 3757.684 kcal/mol

---- Fugacity point 21 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.410 |

Temperature : 298.000 K
Total Fugacity : 2.410 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | steps | | | | |
| 3D Atomistic | 4 | | | | | | | | | | |
| Accepted | | 0 | 0 | 0 | 13968 | 1370 | 0 | | | | |
| Attempted | | 24415 | 24332 | 2467 | | | | | | | |

```
24254 |       24532 |           0 |
  |  Ratio       |              |       0.000 |       0.000 |       0.000 |
0.576 |       0.056 |              |
```

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.385 | 40.592 | 73.592 |

---- Overall system energies ----

Average total energy : 3756.832 kcal/mol

---- Fugacity point 22 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.523 |

Temperature : 298.000 K
Total Fugacity : 2.523 kPa

---- Monte Carlo steps ----

```
 | Sorbate      | Loading     | Creation    | Destruction | Regrowth    |
Rotation    | Translation | C/D Ratio   |
 |              |             | steps       | steps       | steps       | steps
    | steps       |             |
|_____________________________________________________________________________
_____________________________________
 | 3D Atomistic |           4 |             |             |             |
    |              |             |
 |  Accepted    |             |           0 |           0 |           0 |
14632 |        1435 |           0 |
 |  Attempted   |             |       24199 |       24418 |        2468 |
24282 |       24633 |           0 |
 |  Ratio       |             |       0.000 |       0.000 |       0.000 |
0.603 |       0.058 |             |
```

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|

| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 59.859 | 40.292 | 72.892 |

---- Overall system energies ----

Average total energy : 3757.151 kcal/mol

---- Fugacity point 23 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.636 |

Temperature : 298.000 K
Total Fugacity : 2.636 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation steps | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 1 | 0 | 14598 | 1336 | 0.000 |
| Attempted | | 24373 | 24416 | 2360 | 24349 | 24502 | 0.998 |
| Ratio | | 0.000 | 4.096e-005 | 0.000 | 0.600 | 0.055 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.099 | 4 | 5 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 59.293 | 8.192 | 74.292 |

---- Overall system energies ----

Average total energy : 3852.421 kcal/mol

---- Fugacity point 24 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.749 |

Temperature : 298.000 K
Total Fugacity : 2.749 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation steps | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14624 | 1338 | 0 |
| Attempted | | 24318 | 24397 | 2363 | 24516 | 24406 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.597 | 0.055 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.502 | 40.092 | 73.892 |

---- Overall system energies ----

Average total energy : 3757.810 kcal/mol

---- Fugacity point 25 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.863 |

Temperature : 298.000 K
Total Fugacity : 2.863 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation steps | Destruction steps | Regrowth steps | Rotation steps | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14848 | 1396 | 0 |
| Attempted | | 24134 | 24607 | 2451 | 24486 | 24322 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.606 | 0.057 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.718 | 38.992 | 73.292 |

---- Overall system energies ----

Average total energy : 3757.463 kcal/mol

---- Fugacity point 26 of 26 ----

---- Fixed pressure calculation ----

Framework charge : 1.600 e per cell

| Sorbate | Charge | Fugacity kPa |
|---|---|---|
| 3D Atomistic | 0.000 | 2.976 |

Temperature : 298.000 K
Total Fugacity : 2.976 kPa

---- Monte Carlo steps ----

| Sorbate | Loading | Creation | Destruction | Regrowth | Rotation | Translation | C/D Ratio |
|---|---|---|---|---|---|---|---|
| | | steps | steps | steps | steps | steps | |
| 3D Atomistic | 4 | | | | | | |
| Accepted | | 0 | 0 | 0 | 14699 | 1430 | 0 |
| Attempted | | 24069 | 24567 | 2403 | 24759 | 24202 | 0 |
| Ratio | | 0.000 | 0.000 | 0.000 | 0.594 | 0.059 | |

---- Loading ----

| Sorbate | Average loading | Minimum loading | Maximum loading |
|---|---|---|---|
| 3D Atomistic | 4.000 | 4 | 4 |

---- Isosteric heats ----

| Sorbate | Average kcal/mol | Minimum kcal/mol | Maximum kcal/mol |
|---|---|---|---|
| 3D Atomistic | 60.416 | 40.492 | 73.492 |

---- Overall system energies ----

Average total energy : 3757.102 kcal/mol

Task terminated : Mon Apr 21 11:46:18 2014

Total CPU time used : 14:09 minutes

Termination status : Normal