Supporting Material to: Force field for hydrogen adsorption in flexible ZIF-11

1   Linker choice [1]

A special property of the X-ray structure file of ZIF-11 is that there are multiple positions for whole or parts of the linkers. In the X-ray structure file it is mentioned that this is due to fact that some of the carbon atoms were found to be disordered over two sites. This means for the force field development that a reasonable combination of those possible linker configurations has to be chosen.

In Figure 1(a) one can see that there are carbon atoms which are very close to each other. In comparison with Figure 2 one can notice that those carbon atoms which are very close to each other are forming two possible configurations of the linkers (please note that there are only halves of the linkers in Figure 1(a)). Therefore one finds that next to one metal node there are 4 linkers where 3 of them do have 2 possible configurations. The choice of those 3 linker configurations will be explained in the following text and each of the linker types will get a separate name to distinguish them.

Wall linker:

Figure 3 shows 4 wall linkers as they were chosen out of the 2 possible configurations. One unit cell of ZIF-11 fits into a cubic box and the face wall linkers are those nearly parallel to the wall of the simulation box as it was chosen in this paper. In Figure 3 the top and the bottom linker are nearly parallel to the box wall while the left and right linker are bent towards the viewer. These are the two possible configurations for those linkers. They can be either straight or bent. This would normally give us a lot of possibilities how the wall linkers can be chosen (not only the ones shown in Figure 3).

(a)
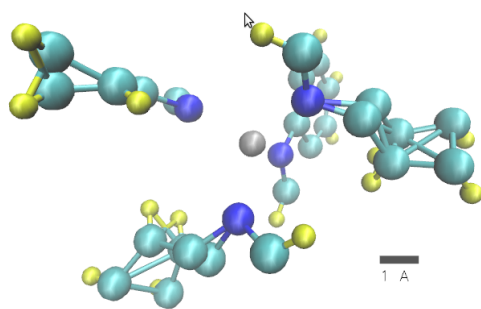
10 A
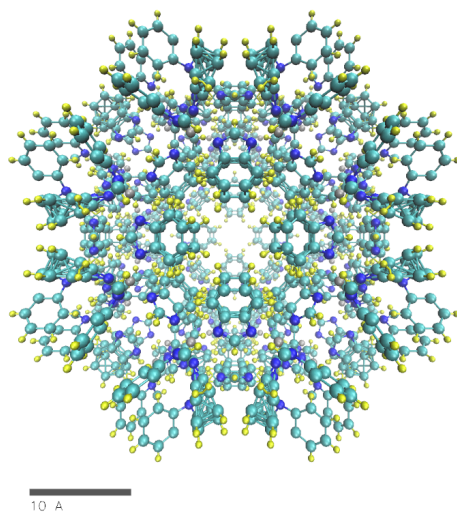
(b)

Figure 1: X-ray structure of ZIF-11. (a) Smallest part of ZIF-11 that can be used to complete one unit cell. (b) One unit cell of ZIF-11.
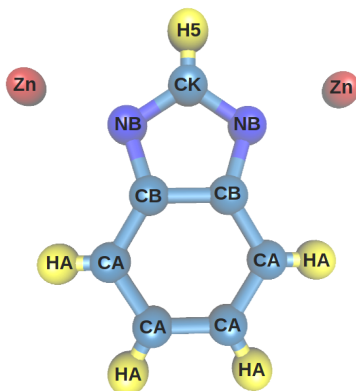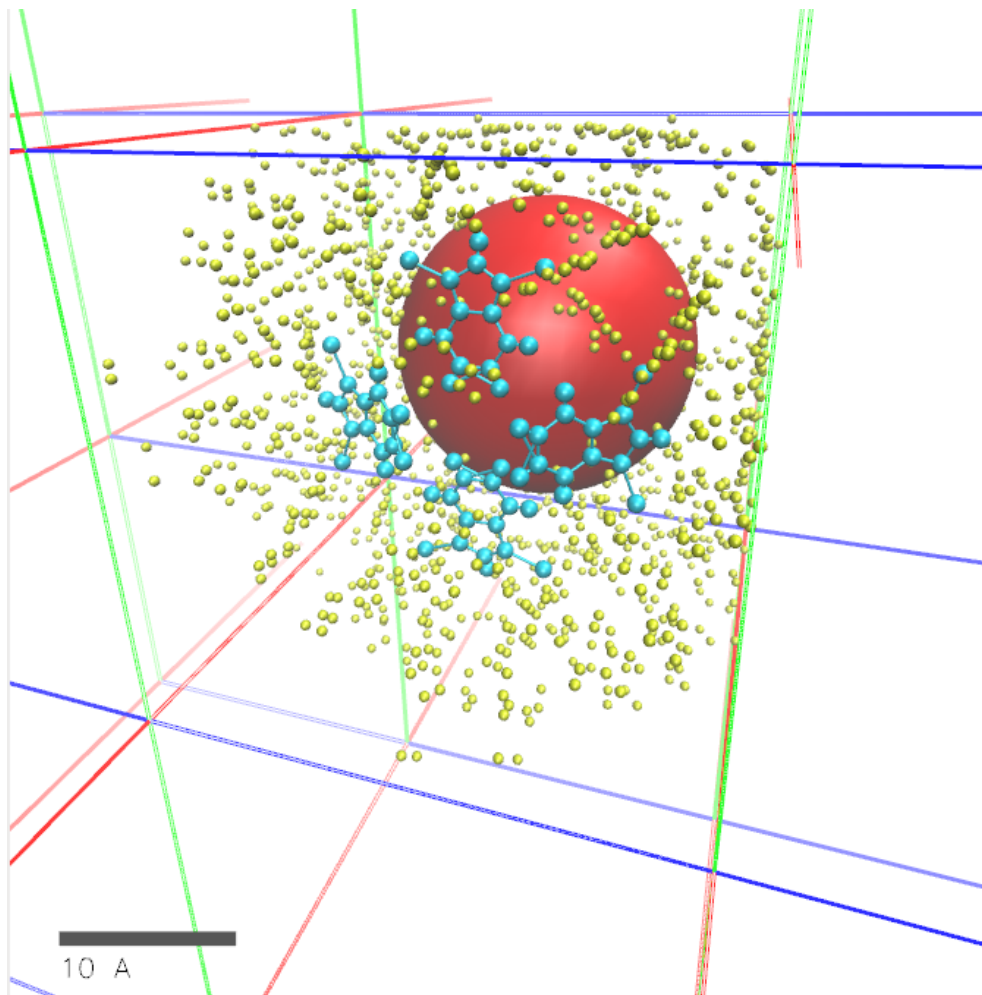

Figure 2: Linker of ZIF-11.

Figure 3: The 4 wall linkers are displayed as blue spheres with blue bonds, the yellow spheres represent the remaining ZIF-11 lattice, the big red sphere fills the centre pore volume, the straight lines are the boundaries of the unit cell.

The first possibility would be that all wall linkers would be straight but this leads to the problem that the hydrogen atoms attached to the 6 membered carbon rings would only have a distance of 1.1 Å. This is too tight for non-bonded interactions of the involved atoms and would lead to very strong forces (for example Lennard-Jones forces) which would destroy the lattice shape. The second possibility would be to bend all 4 linkers. Then the distance between their hydrogen atoms would go up to 2.16 Å which is still tight for non-bonded atoms but not as critical as before. However, this possibility is

also ruled out by the fact that the distance to the hydrogen atoms of the neighbouring simulation box image would go down to 0.9 Å which is also much too close for non-bonded atoms.

Therefore the only possible solution is to alternate bent and straight wall linkers to keep them at a reasonable distance. They have to be chosen with respect to the neighbour unit cell in a way that a bent wall linker is always next to a straight one. If then one of the linkers is chosen the others are completely determined.

Corner linker:

The situation for the corner linkers (Figure 4) is very similar to the wall linker case. The linkers can again be straight or bent. They were named corner linkers because of their occurrence in the X-ray structure. They are occurring in the corners of the chosen simulation box.

If all linkers would be straight the hydrogen distance would go down to 1.3 Å which is again too tight. If all linkers would be bent the distance to the linker above would go down to 1.4 Å and therefore this possibility is also rejected. Consequently, the only solution is again to alternate them leading to a reasonable structure as shown in Figure 4. Another hint to the alternating configurations of the corner linkers and the wall linkers is that this can also explain the two measured configurations via X-ray diffraction. Since X-ray measures a lot of unit cells at once it would get a mixed picture like Figure 1(a).

In the publication of Assfour et al. [2] there are also pictures of those configurations which were obtained with density functional theory and showed those alternating configurations of the corner and wall linkers reproduced in Figure 5.
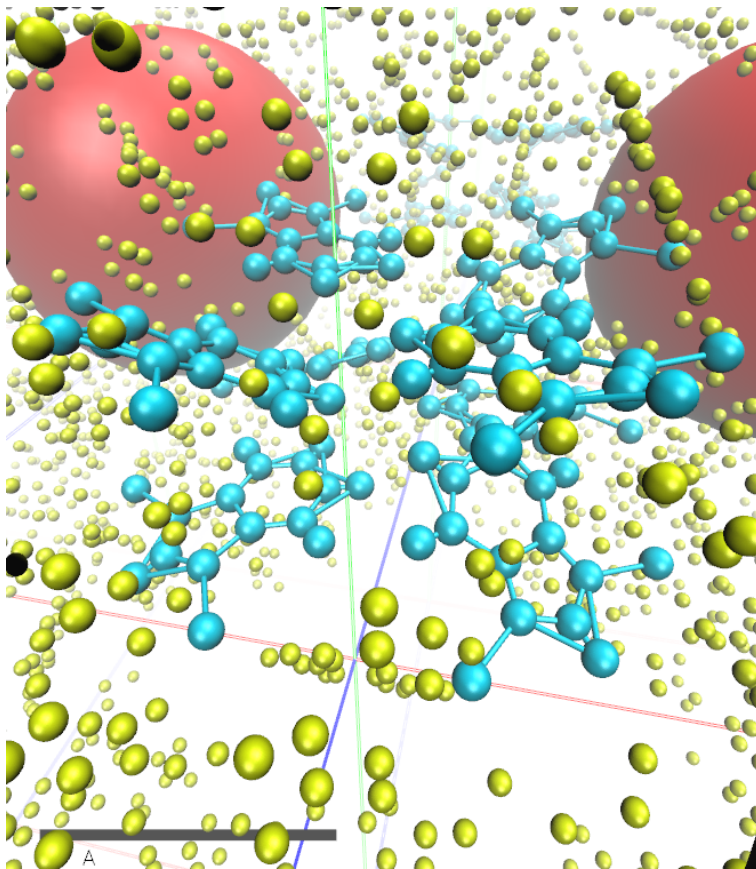
Figure 4: The 8 corner linkers are displayed as blue spheres with blue bonds, the yellow spheres represent the remaining ZIF-11 lattice, the big red sphere fills the centre pore volume, the straight lines are the boundaries of the unit cell.

Window linker:

The window linkers are most important for the diffusion of guest molecules from one pore to another. They are forming the connection between the two different pores and are therefore essential for the question whether guest molecules will diffuse or not.

The choice of the configuration for those linkers is more difficult than for the wall linkers and corner linkers. Only the first possibility where all linkers would be straight can be ruled out because it would lead to a hydrogen distance of 1.88 Å. This leaves the two possibilities that all window linkers could be bent (see Figure 6(a)) or that in each window two linkers could be bent and one straight (see Figure 6(b)).

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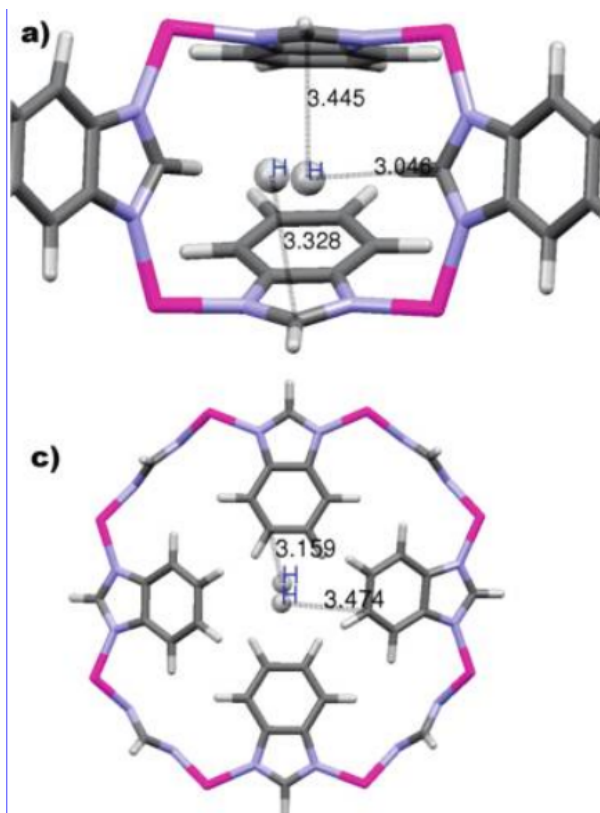
Figure 5: Configurations obtained from density functional theory (taken from [2]). Top: Corner linkers. Bottom: Wall linkers.

Molecular dynamics test simulations were done for both cases and with interaction parameters which were fitted via rigid Monte Carlo simulations to measured adsorption isotherms separately for both cases. In the case in which one of the window linkers was bent there was no diffusion between pores for more than 20 ns and the value of the potential inside the window that is connecting the pores was around 4.7 kJ/mol while at 77 K the kinetic energy for hydrogen treated as a Lennard-Jones particle is only around 1 kJ/mol. Therefore the diffusion from one pore to another one is highly improbable.

Due to the fact that one does only know from the so far measured data that hydrogen is
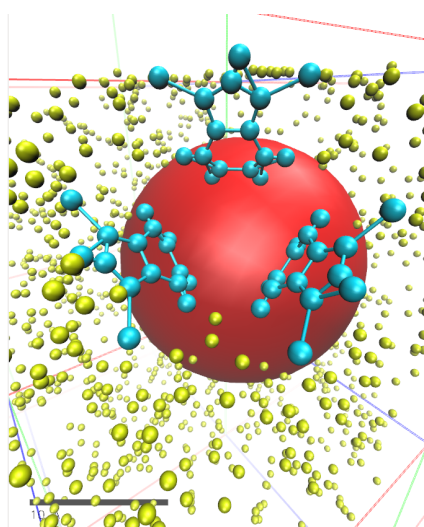
(a) 3 bent window linkers.
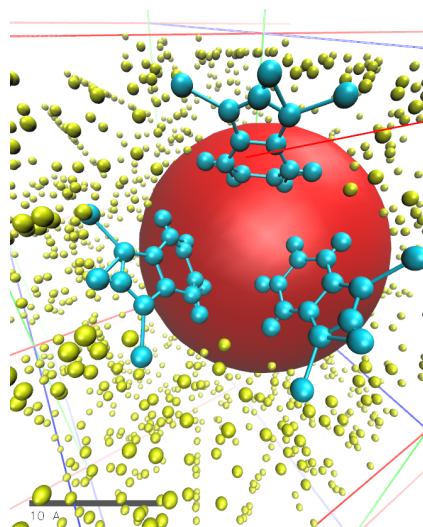
(b) 2 bent and 1 straight window linkers (the lower left one is the straight linker).

Figure 6: The 3 window linkers are displayed as blue spheres with blue bonds, the yellow spheres represent the remaining ZIF-11 lattice, the big red sphere fills the centre pore volume, the straight lines are the boundaries of the unit cell.

diffusing but not how fast, it is not possible to make a strict conclusion that one of the structures can be ruled out. But it is highly probable that one would see no diffusion for the 2 bent, 1 straight window linkers structure or that the diffusion coefficient would be much smaller than the experimental one.

In this paper the window linkers will be treated to be all bent, where the height of the potential for a guest molecule in the window is below 0 kJ/mol and diffusion between pores is very probable.

Straight linker:

It was mentioned that there are 4 different linker types where 3 of them do have 2 possible shapes. Therefore there is 1 linker type left which will only be called the straight linker. Figure 7 shows where those straight linkers are located.
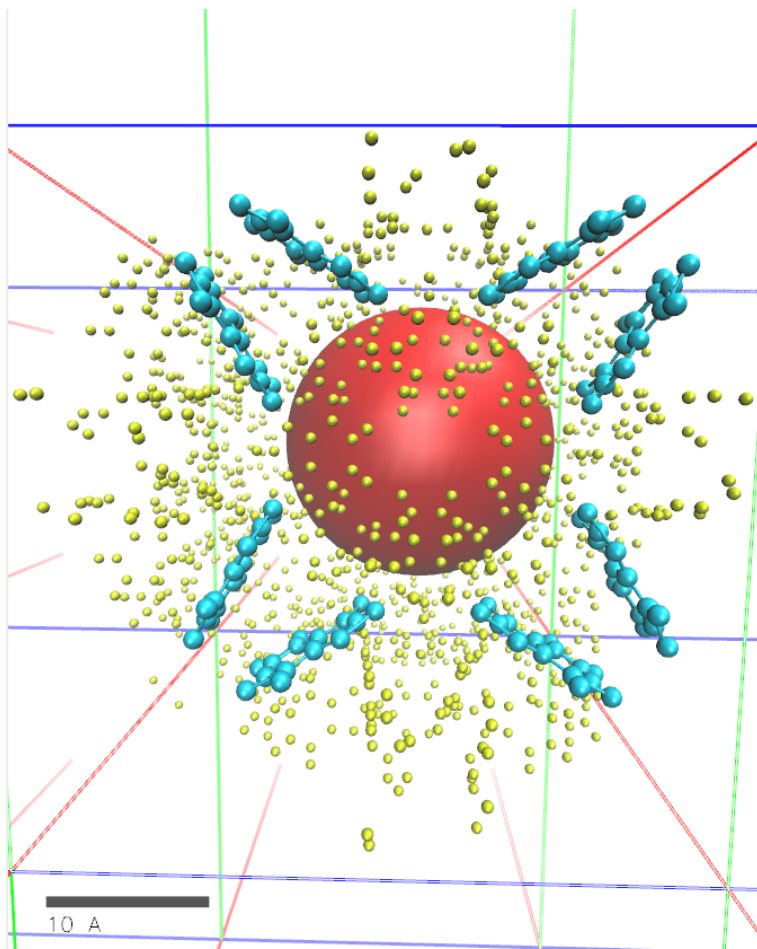
Figure 7: 4 straight linkers (blue), the other colors remain the same as in Figure 4.

2   Torsion interaction parameters for the Zn-N bond

The parameters for the torsion of the Zn-N bond are set to zero in the paper of Sant et al. [3] to guarantee a high flexibility of the linkers. But it was not mentioned in this paper why this interaction potential should be completely neglected. In this work we will use a small torsion potential instead and the necessary parameters were obtained from the paper of Ryde [4]. This paper is providing torsion interaction parameters for several neighbour atoms of the Zn-N bond (see Table 1). Because it did not include the exact neighbours NB-Zn-NB-CK and NB-Zn-NB-CB, the X-Zn-NB-X torsion potential value was obtained by averaging over the given parameters for the given neighbours.

The $\gamma_{X-Zn-NB-X}$ value of the torsion potential

$$E_{\text{torsion}} = \gamma_o \left[1 + \cos(p_o \theta_{i,j,k,l} - \theta_o)\right] \tag{1}$$

is therefore set to 2.038 kJ/mol which still is very low in comparison to all other torsion interaction parameters in the ZIF-11 lattice. The $p_{X-Zn-NB-X}$ parameter was set to 3 according to Table 1 and the $\theta_{X-Zn-NB-X}$ value was calculated from the structure determined from the X-ray diffraction analysis.

Table 1: Zn-N torsion parameters $E_{\text{torsion}} = C_{in} \left[\cos(n\theta_i) + 1\right]$ [4].

Atom types				n	Zn4 C_{in} (kJ/mol)
HC	C	OC$^-$	Zn	3	0.27
C	C	OC$^-$	Zn	3	0.27
HC	C	S$^-$	Zn	3	0.76
C	C	S$^-$	Zn	3	0.76
HC	Ca	Na	Zn	1	−196.8
C	Ca	Na	Zn	1	73.8
Na	Ca	Na	Zn	1	80.0
HO	N	Zn	O=C	3	−1.03
HO	N	Zn	OH	3^a	−0.75
HO	N	Zn	OH2	3^a	−0.19
HO	N	Zn	OH$^-$	3	−5.45
HO	N	Zn	OC$^-$	3	−4.02
HO	N	Zn	S$^-$	3	−0.79
Ca	Na	Zn	O=C	2	11.8
Ca	Na	Zn	OH	2	11.8

3   Equipotential surface

Due to the interactions with the lattice atoms a guest atom in the structure has different potential energies depending on its position. If the surface is drawn where a guest molecule would have one special interaction energy with all lattice atoms we will get an equipotential surface for this certain energy (see Figure 8).

Those pictures are helpful for determining whether a set of interaction parameters could in principle lead to a diffusion between the pores. The equipotential surface picture
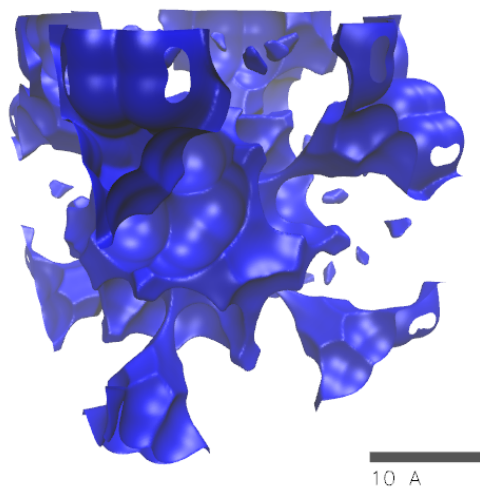
Figure 8: Equipotential surface for 0 kJ/mol of hydrogen in ZIF-11.

can be used to see the height of the potential walls between the pores. When this value is compared to the average kinetic energy, due to the temperature, it is possible to conclude how likely the travelling from one pore to another is.

Application to an example case:

A guest molecule at 77 K has an average one-particle kinetic energy of 0.96 kJ/mol. In Figure 9(a) we see an equipotential surface picture for hydrogen in ZIF-11 at 3 kJ/mol. With an average kinetic energy of 0.96 kJ/mol some particles will in some cases also have a higher kinetic energy and will be able to enter regions with a higher potential energy. But the surface with a potential energy that is 3 times the kinetic energy is a boundary that the particle can only cross with a low probability. In Figure 9(a) we see the centre pore and the edge pore parts with the equipotential surface as their boundary. We compare Figures 9(b) and 9(a) to draw some conclusions.
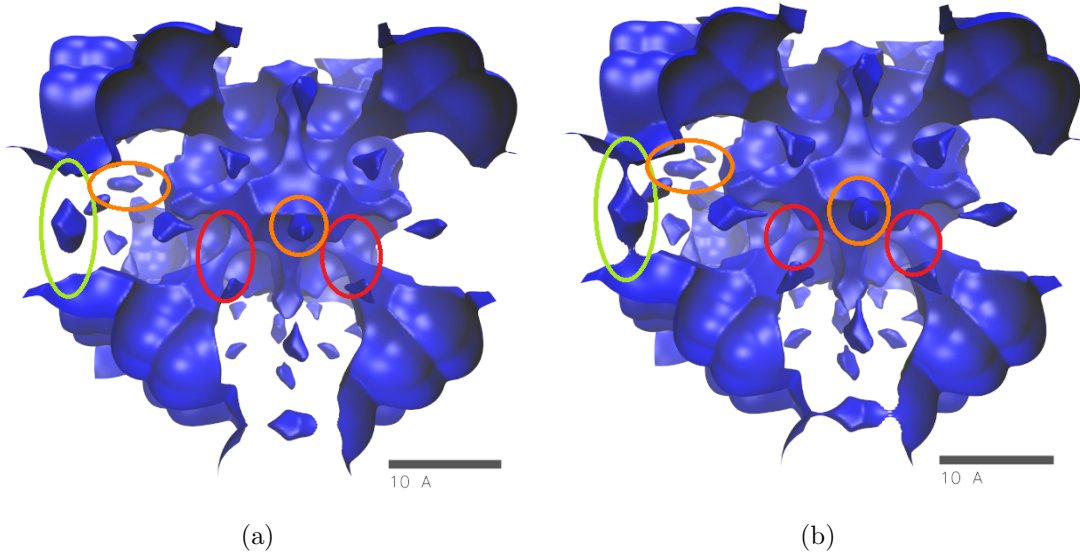
Figure 9: Equipotential surface at (a) 3 kJ/mol and (b) 12 kJ/mol.

There is a window (a connected equipotential surface marked by a red ellipse) between the edge and the centre pore even at 3 kJ/mol. By varying the energy value one finds that the potential wall between the edge and the centre pore is lower than 0 kJ/mol. This means that hydrogen has the ability to travel from the centre to the edge pores for all temperatures.

In contrast, the connection between the edge pores (marked by a green ellipse in Figure 9(a)) is closed at 3 kJ/mol and only slightly open for hydrogen at 12 kJ/mol. With such a big difference between the mean kinetic energy of a particle and the height of the potential wall the particle should not be able to travel from one edge pore to another because it is very unlikely to have the necessary kinetic energy at 77 K.

In addition, the connection between the centre pores is not even open for 12 kJ/mol (orange circles in Figures 9(a) and 9(b)). Therefore the only type of connections of adjacent cavities that is open for hydrogen is the one in the red circles in Figures 9(a) and 9(b) which is connecting the centre pore and the edge pore. This explains the conclusion that there was no 8-ring window (as it was suggested in [5]) found in this

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work since the red circles are corresponding to a 6-ring window.

4   Ideal gas approximation for hydrogen

The conditions for the surrounding hydrogen in this work are ranging from 77 K up to 298 K in a pressure range of up to 10 bar. It has been checked that the assumption to treat hydrogen as an ideal gas is justified under those conditions.

Figure 10(a) shows an isotherm of free hydrogen gas at 77 K. The agreement of the hydrogen data obtained from NIST Chemistry WebBook [6], the ideal gas equation and the van der Waals equation is good enough to accept the ideal gas approximation. In fact the hydrogen van der Waals parameters are amongst the smallest that a gas can have. Zero van der Waals parameters would mean a perfect ideal gas and since the hydrogen parameters are very small [7] it is reasonable that the ideal gas equation approximates hydrogen behaviour in a wide range compared to other gases.

If we plot again the adsorption isotherm for 298 K (see Figure 10(b)) and again for a pressure up to 10 bar we get a very similar picture that also shows a good agreement of hydrogen data, the ideal gas equation and the van der Waals equation. Therefore we have looked at the limits of the conditions that this work will be dealing with. We assume that in the regions between those limits the ideal gas approximation also holds.

5 Tables of parameters

List of linker types:

1. Straight linker

2. Wall linker

   (a) straight

   (b) bent

3. Corner linker

   (a) straight

   (b) bent

4. Window linker

Table 2: Lennard-Jones parameters $E_{\mathrm{LJ}} = 4\epsilon_e \left[\left(\frac{\sigma_e}{r} \right)^{12} - \left(\frac{\sigma_e}{r} \right)^6 \right]$.
The atom types are referring to Figure 13.

atom type e	$\epsilon_e (\mathrm{kJ \cdot mol^{-1}})$	σ_e (Å)
H5	0.063	2.42
CK	0.360	3.40
NB	0.712	3.25
CB	0.360	3.40
CA	0.360	3.40
HA	0.063	2.60
Zn	0.052	1.96

Table 3: Parameters of the bond potential $E_{\mathrm{bond}} = \alpha_b(r - r_{0b})^2$.
The subscripts of the bonds are corresponding to the numbers in Figure 12.

bond type b	$\alpha_b(\mathrm{kcal \cdot mol^{-1} \mathring{A}^2})$	r_{0b} ($\mathring{A}$)					
		1.	2.a)	2.b)	3.a)	3.b)	4.
$(\mathrm{CK\text{-}H5})_1$	367.0	0.932	0.932	0.932	0.928	0.928	0.928
$(\mathrm{CK\text{-}NB})_{3,4}$	529.0	1.316	1.339	1.339	1.315	1.315	1.289
$(\mathrm{NB\text{-}CB})_{6,7}$	414.0	1.366	1.391	1.389	1.537	1.283	1.383
$(\mathrm{CB\text{-}CB})_8$	520.0	1.472	1.455	1.323	1.428	1.472	1.452
$(\mathrm{CB\text{-}CA})_{9,10}$	469.0	1.409	1.403	1.444	1.383	1.454	1.397
$(\mathrm{CA\text{-}HA})_{11,12}$	367.0	0.929	0.929	0.929	0.930	0.929	0.959
$(\mathrm{CA\text{-}HA})_{16,17}$	367.0	0.931	0.930	0.931	0.929	0.928	0.929
$(\mathrm{CA\text{-}CA})_{13,14}$	469.0	1.340	1.399	1.414	1.367	1.350	1.282
$(\mathrm{CA\text{-}CA})_{15}$	469.0	1.421	1.369	1.329	1.358	1.362	1.521
$(\mathrm{Zn\text{-}NB})_{2,5}$	78.50	1.976	1.988	1.988	1.986	1.986	1.966
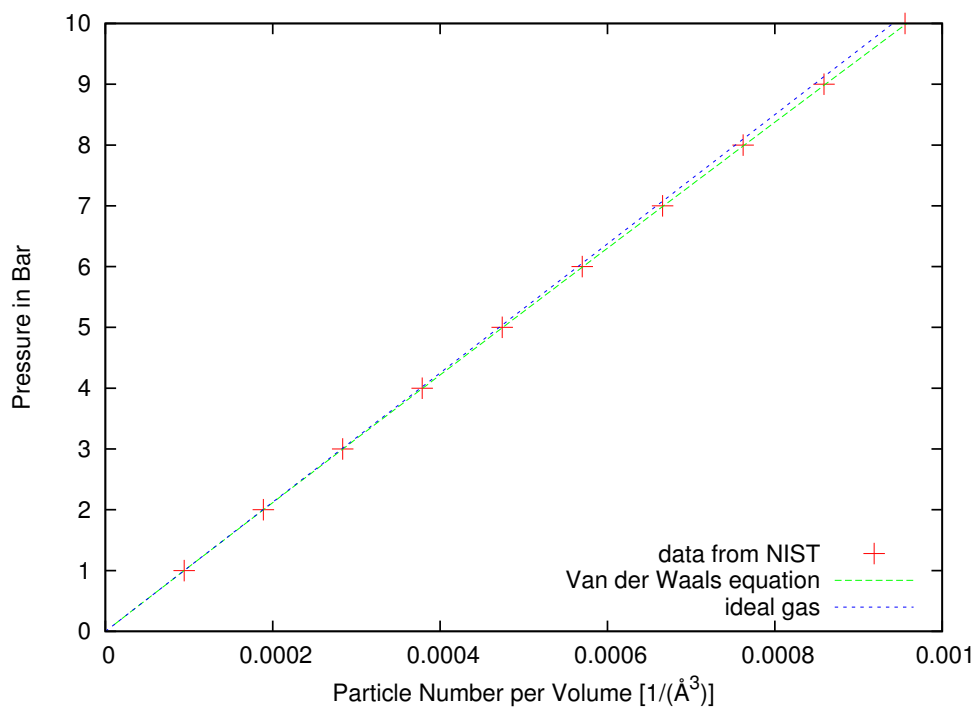
(a)
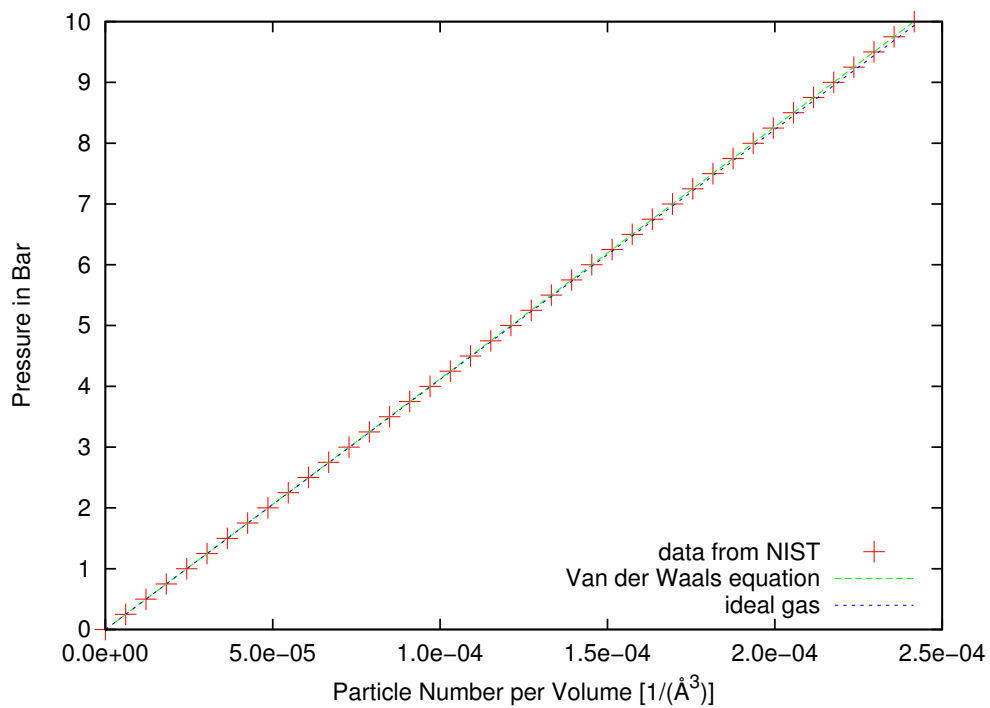
(b)

Figure 10: Free hydrogen isotherm at: (a) 77 K; (b) 298 K.

Figure 11: A zinc knot with the surrounding hydrogen. The numbers with dots next to the N's are referring to the attached linker types listed at the beginning of section 5. The numbers without dots are defining names for the bonds.

Figure 12: Numbering of the bonds.

Figure 13: Atom types of the linker.
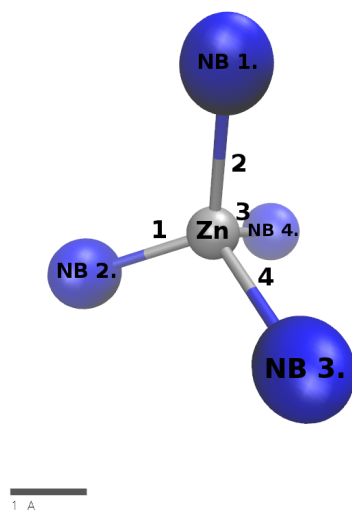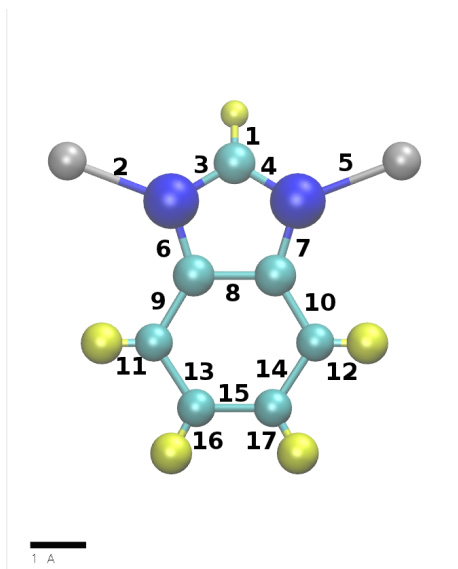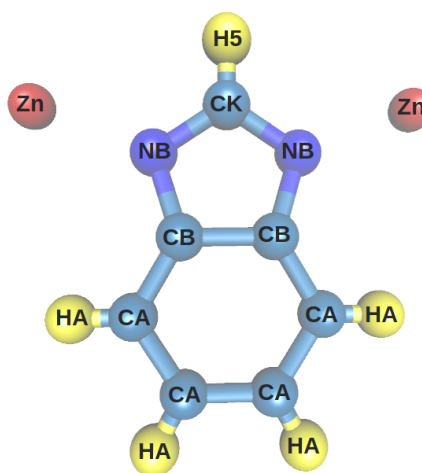
Table 4: Parameters of the valence angle potential $E_{\text{bend}} = \beta_c(\Phi - \Phi_{0c})^2$.
The subscripts of the 3 atom types are related to the numbers of the bonds (Figure 11 or Figure 12) that are forming the group of 3 atoms.

bond type c	$\beta_c(\text{kcal}\cdot\text{mol}^{-1}\text{rad}^{-2})$	$\Phi_{0c}(1°)$					
		1.	2.a)	2.b)	3.a)	3.b)	4.
$(\text{H5-CK-NB})_{1,3}$	50.0	120.53	122.41	122.42	122.06	122.06	139.48
$(\text{H5-CK-NB})_{1,4}$	50.0	120.53	122.42	122.41	122.06	122.06	98.714
$(\text{NB-CK-NB})_{3,4}$	70.0	118.94	115.17	115.17	115.88	115.88	121.8
$(\text{CK-NB-Zn})_{3,2;4,5}$	48.7	130.49	126.92	126.91	130.23	130.23	128.59
$(\text{CK-NB-CB})_{3,6;4,7}$	70.0	103.64	103.97	102.37	106.34	104.05	102.26
$(\text{Zn-NB-CB})_{2,4;5,7}$	32.5	125.8	127.89	128.8	123.09	123.08	128.53
$(\text{CB-CB-NB})_{6,8;7,8}$	70.0	106.89	106.82	109.73	105.11	107.15	106.83
$(\text{NB-CB-CA})_{6,9;7,10}$	70.0	133.22	132.13	127.75	134.06	132.03	134.53
$(\text{CB-CB-CA})_{8,9;8,10}$	63.0	119.88	120.56	122.39	120.78	120.24	118.61
$(\text{CB-CA-CA})_{9,13;10,12}$	63.0	117.21	116.7	114.39	116.29	114.02	115.59
$(\text{CA-CA-HA})_{11,13;12,14}$	50.0	121.33	121.67	122.73	121.83	123.02	110.74
$(\text{CA-CA-HA})_{13,16;14,17}$	50.0	118.51	118.63	118.59	118.76	117.05	120.24
$(\text{CA-CA-HA})_{16,15;15,17}$	50.0	118.59	118.65	118.4	118.36	117.27	120.1
$(\text{CA-CA-CA})_{13,15;14,15}$	63.0	122.9	122.72	123.02	122.88	125.67	119.66
$(\text{HA-CA-CB})_{11,9;10,12}$	50.0	121.46	121.62	122.88	121.89	122.97	124.29
bond type c	$\beta_c(\text{kcal}\cdot\text{mol}^{-1}\text{rad}^{-2})$	$\Phi_{0c}(1°)$					
$(\text{NB-Zn-NB})_{1,2}$	35.2	107.46					
$(\text{NB-Zn-NB})_{1,3}$	35.2	111.33					
$(\text{NB-Zn-NB})_{1,4}$	35.2	107.04					
$(\text{NB-Zn-NB})_{2,3}$	35.2	104.72					
$(\text{NB-Zn-NB})_{2,4}$	35.2	109.95					
$(\text{NB-Zn-NB})_{4,3}$	35.2	116.07					

Table 5: Parameters of the dihedral potential $E_{\text{dih}} = \gamma_d[1 + \cos(n_d\phi - \phi_{0d})]$.
The subscripts of the 4 atom types are related to the numbers of the bonds (Figure 12) that are forming the group of 4 atoms.

bond type d	$\gamma_d(\text{kcal}\cdot\text{mol}^{-1})$	n_d	$\phi_{0d}(1°)$					
			1.	2.a)	2.b)	3.a)	3.b)	4.
(H5-CK-NB-Zn)$_{(1,3,2)}$	20.00	2	170.68	166.73	189.98	189.98	189.98	198.17
(H5-CK-NB-Zn)$_{(1,4,5)}$	20.00	2	189.32	193.27	170.02	170.02	170.02	160.98
(H5-CK-NB-CB)$_{(1,3,6)}$	20.00	2	176.85	142.93	153.16	203.16	153.16	181.11
(H5-CK-NB-CB)$_{(1,4,7)}$	20.00	2	183.15	217.07	206.84	156.84	206.84	178.04
(NB-CK-NB-Zn)$_{(3,4,5)}$	20.00	2	188.97	193.28	170.16	170.16	170.16	159.35
(NB-CK-NB-Zn)$_{(4,3,2)}$	20.00	2	171.03	166.72	189.84	189.84	189.84	200.65
(NB-CK-NB-CB)$_{(3,4,7)}$	20.00	2	182.8	217.08	206.97	156.97	206.97	176.41
(NB-CK-NB-CB)$_{(4,3,6)}$	20.00	2	177.2	142.92	153.03	203.03	153.03	183.59
(CK-NB-CB-CB)$_{(3,6,8)}$	5.10	2	181.49	200.52	194.89	167.4	194.89	178.18
(CK-NB-CB-CB)$_{(4,7,8)}$	5.10	2	178.51	159.48	165.11	192.6	165.11	181.82
(CK-NB-CB-CA)$_{(3,6,9)}$	5.10	2	178.95	184.08	176.91	162.63	176.91	174.21
(CK-NB-CB-CA)$_{(4,7,10)}$	5.10	2	181.05	175.92	183.09	197.37	183.09	185.79
(Zn-NB-CB-CB)$_{(2,6,8)}$	5.10	2	187.27	176.4	161.45	179.41	161.45	161.13
(Zn-NB-CB-CB)$_{(5,7,8)}$	5.10	2	172.73	183.6	198.55	180.59	198.55	198.87
(Zn-NB-CB-CA)$_{(2,6,9)}$	5.10	2	184.73	159.96	143.46	174.64	143.46	157.17
(Zn-NB-CB-CA)$_{(5,7,10)}$	5.10	2	175.27	200.04	216.54	185.36	216.54	202.83
(NB-CB-CB-NB)$_{(6,8,7)}$	21.80	4	180	180	180	180	180	180
(NB-CB-CB-CA)$_{(6,8,10)}$	21.80	4	175.73	151.71	149.11	172.02	149.11	173.56
(NB-CB-CB-CA)$_{(7,8,9)}$	21.80	4	175.73	151.71	210.89	187.98	210.89	186.44
(CA-CB-CB-CA)$_{(9,8,10)}$	21.80	4	180	180	180	180	180	180
(NB-CB-CA-HA)$_{(6,9,11)}$	14.00	4	181.32	210.55	208.62	200.18	208.62	225.07
(NB-CB-CA-HA)$_{(7,10,12)}$	14.00	4	178.68	149.45	151.38	159.82	151.38	134.93
(NB-CB-CA-CA)$_{(6,9,13)}$	14.00	4	182.48	209.93	207.99	200.1	207.99	78.27
(NB-CB-CA-CA)$_{(7,10,14)}$	14.00	4	177.52	150.07	152.01	159.9	152.01	281.73
(CB-CB-CA-HA)$_{(8,9,11)}$	14.00	4	175.72	173.98	168.8	189.45	168.8	216.43
(CB-CB-CA-HA)$_{(8,10,12)}$	14.00	4	184.28	186.02	191.2	170.55	191.2	143.57
(CB-CB-CA-CA)$_{(8,9,13)}$	14.00	4	176.88	173.36	168.18	189.37	168.18	69.625
(CB-CB-CA-CA)$_{(8,10,14)}$	14.00	4	183.12	186.64	191.82	170.63	191.82	290.37
(CB-CA-CA-CA)$_{(9,13,15)}$	14.50	4	183.23	186.8	192.58	170.41	192.58	291.61
(CB-CA-CA-CA)$_{(10,14,15)}$	14.50	4	176.77	173.2	167.42	189.59	167.42	68.391
(CB-CA-CA-HA)$_{(9,13,16)}$	14.50	4	183.97	186.41	192.23	170.11	192.23	292.41
(CB-CA-CA-HA)$_{(10,14,17)}$	14.50	4	176.03	173.59	167.77	189.89	167.77	67.593
(CA-CA-CA-HA)$_{(11,13,15)}$	14.50	4	184.38	186.18	191.95	170.33	191.95	164.12
(CA-CA-CA-HA)$_{(12,14,15)}$	14.50	4	175.62	173.82	168.05	189.67	168.05	195.88
(HA-CA-CA-HA)$_{(11,13,16)}$	14.50	4	185.12	185.79	191.6	170.03	191.6	164.92
(HA-CA-CA-HA)$_{(17,14,12)}$	14.50	4	174.88	174.21	168.4	189.97	168.4	195.08
(CA-CA-CA-CA)$_{(13,15,14)}$	14.50	4	180	180	180	180	180	180
(CA-CA-CA-HA)$_{(17,15,13)}$	14.50	4	179.26	179.61	179.65	179.7	179.65	180.8
(CA-CA-CA-HA)$_{(16,15,14)}$	14.50	4	179.26	179.61	180.35	180.3	180.35	179.2
(HA-CA-CA-HA)$_{(16,15,17)}$	14.50	4	180	180	180	180	180	180

Table 6: Parameters of the dihedral potential $E_{\text{dih}} = \gamma_d[1 + \cos(n_d\phi - \phi_{0d})]$. The numbers in brackets $(\dots)$ are related to the numbers of the linker types (Figure 11 and list of linker types) that are forming the group of 4 atoms.

bond type d	$\gamma_d(\text{kcal}\cdot\text{mol}^{-1})$	n_d	$\phi_{0d}(1°)$
([CB(1.)]-[NB(1.)]-[Zn]-[NB(2.a)])	0.49	3	329.34
([CB(1.)]-[NB(1.)]-[Zn]-[NB(2.b)])	0.49	3	30.661
([CB(1.)]-[NB(1.)]-[Zn]-[NB(3.a))])	0.49	3	19.13
([CB(1.)]-[NB(1.)]-[Zn]-[NB(3.b))])	0.49	3	19.13
([CB(1.)]-[NB(1.)]-[Zn]-[NB(4.)])	0.49	3	35.215
([CB(2.a)]-[NB(2.a)]-[Zn]-[NB(1.))])	0.49	3	90.485
([CB(2.a)]-[NB(2.a)]-[Zn]-[NB(3.a))])	0.49	3	84.658
([CB(2.a)]-[NB(2.a)]-[Zn]-[NB(3.b))])	0.49	3	275.34
([CB(2.a)]-[NB(2.a)]-[Zn]-[NB(4.)])	0.49	3	108.12
([CB(2.b)]-[NB(2.b)]-[Zn]-[NB(1.))])	0.49	3	9.3948
([CB(2.b)]-[NB(2.b)]-[Zn]-[NB(3.a))])	0.49	3	15.223
([CB(2.b)]-[NB(2.b)]-[Zn]-[NB(3.b))])	0.49	3	344.78
([CB(2.b)]-[NB(2.b)]-[Zn]-[NB(4.)])	0.49	3	351.76
([CB(3.a)]-[NB(3.a)]-[Zn]-[NB(1.)])	0.49	3	99.857
([CB(3.a)]-[NB(3.a)]-[Zn]-[NB(2.a))])	0.49	3	270.88
([CB(3.a)]-[NB(3.a)]-[Zn]-[NB(2.b))])	0.49	3	89.118
([CB(3.a)]-[NB(3.a)]-[Zn]-[NB(4.)])	0.49	3	104.11
([CB(3.b)]-[NB(3.b)]-[Zn]-[NB(1.)])	0.49	3	12.856
([CB(3.b)]-[NB(3.b)]-[Zn]-[NB(2.a))])	0.49	3	2.1174
([CB(3.b)]-[NB(3.b)]-[Zn]-[NB(2.b))])	0.49	3	357.88
([CB(3.b)]-[NB(3.b)]-[Zn]-[NB(4.)])	0.49	3	17.107
([CB(4.)]-[NB(4.)]-[Zn]-[NB(1.)])	0.49	3	333.57
([CB(4.)]-[NB(4.)]-[Zn]-[NB(2.a))])	0.49	3	13.891
([CB(4.)]-[NB(4.)]-[Zn]-[NB(2.b))])	0.49	3	346.11
([CB(4.)]-[NB(4.)]-[Zn]-[NB(3.a))])	0.49	3	337.8
([CB(4.)]-[NB(4.)]-[Zn]-[NB(3.b))])	0.49	3	337.8
([CK(1.)]-[NB(1.)]-[Zn]-[NB(2.a)])	0.49	3	160.43
([CK(1.)]-[NB(1.)]-[Zn]-[NB(2.b)])	0.49	3	199.57
([CK(1.)]-[NB(1.)]-[Zn]-[NB(3.a))])	0.49	3	188.04
([CK(1.)]-[NB(1.)]-[Zn]-[NB(3.b))])	0.49	3	188.04
([CK(1.)]-[NB(1.)]-[Zn]-[NB(4.)])	0.49	3	204.13
([CK(2.a)]-[NB(2.a)]-[Zn]-[NB(1.))])	0.49	3	226.42
([CK(2.a)]-[NB(2.a)]-[Zn]-[NB(3.a))])	0.49	3	220.59
([CK(2.a)]-[NB(2.a)]-[Zn]-[NB(3.b))])	0.49	3	139.41
([CK(2.a)]-[NB(2.a)]-[Zn]-[NB(4.)])	0.49	3	244.05
([CK(2.b)]-[NB(2.b)]-[Zn]-[NB(1.))])	0.49	3	133.58
([CK(2.b)]-[NB(2.b)]-[Zn]-[NB(3.a))])	0.49	3	139.41
([CK(2.b)]-[NB(2.b)]-[Zn]-[NB(3.b))])	0.49	3	220.59
([CK(2.b)]-[NB(2.b)]-[Zn]-[NB(4.)])	0.49	3	115.95
([CK(3.a)]-[NB(3.a)]-[Zn]-[NB(1.)])	0.49	3	257.19
([CK(3.a)]-[NB(3.a)]-[Zn]-[NB(2.a))])	0.49	3	113.55
([CK(3.a)]-[NB(3.a)]-[Zn]-[NB(2.b))])	0.49	3	246.45
([CK(3.a)]-[NB(3.a)]-[Zn]-[NB(4.)])	0.49	3	261.44
([CK(3.b)]-[NB(3.b)]-[Zn]-[NB(1.)])	0.49	3	257.19
([CK(3.b)]-[NB(3.b)]-[Zn]-[NB(2.a))])	0.49	3	246.45
([CK(3.b)]-[NB(3.b)]-[Zn]-[NB(2.b))])	0.49	3	113.55
([CK(3.b)]-[NB(3.b)]-[Zn]-[NB(4.)])	0.49	3	261.44
([CK(4.)]-[NB(4.)]-[Zn]-[NB(1.)])	0.49	3	185.6
([CK(4.)]-[NB(4.)]-[Zn]-[NB(2.a))])	0.49	3	161.86
([CK(4.)]-[NB(4.)]-[Zn]-[NB(2.b))])	0.49	3	198.14
([CK(4.)]-[NB(4.)]-[Zn]-[NB(3.a))])	0.49	3	189.84
([CK(4.)]-[NB(4.)]-[Zn]-[NB(3.b))])	0.49	3	189.84

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