Electronic Supplementary Material (ESI) for CrystEngComm.

Insights into the microscopic behaviour of nanoconfined water: Host structure and thermal effects

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Electronic Supporting Information

Table. 1S Properties characterizing LTA-type zeolite and ZIFs: Density, Pore Limiting Diameter (PLD), Large Cavity Diameter (LCD), and Accesible volume (AV).

	Density / kg·m^{-3}	**PLD / Å**	**LCD / Å**	**AV / cm^3·g^{-1}**
Zeolite	1432.8	3.6	10.6	0.22[a] (0.24)[b]
ZIF-20	1016.0	2.8	15.4	0.34(0.27)[c]
Zn(IM)$_2$	634.9	7.2	19.3	0.86

[a]This pore volume corresponds to the framework structure. The presence of cations in LTA-5A slightly reduces this value (see ref. [1]).
[b]Experimental value taken from ref. [2].
[c]Experimental value taken from ref. [3].

Table 2S. Average minimum distances from oxygen atoms of water to the cations and to the metal centres in LTA-5A and the Zn and imidazole-based ZIF with LTA topology, respectively, for selected values of fugacity.

Fugacity [Pa]	**LTA-5A**		**ZIF**
	$d_{min}[O_w\text{-}Na^+]$	$d_{min}[O_w\text{-}Ca^{2+}]$	$d_{min}[O_w\text{-}Zn]$
1	2.00	1.88	2.34
10^2	1.98	1.89	2.31
10^4	1.97	1.88	2.27
10^6	1.96	1.88	2.26

Fig. S1. LTA topology (a) and atomic structures of the zeolite (b) and Zn and imidazole-based ZIF (c).

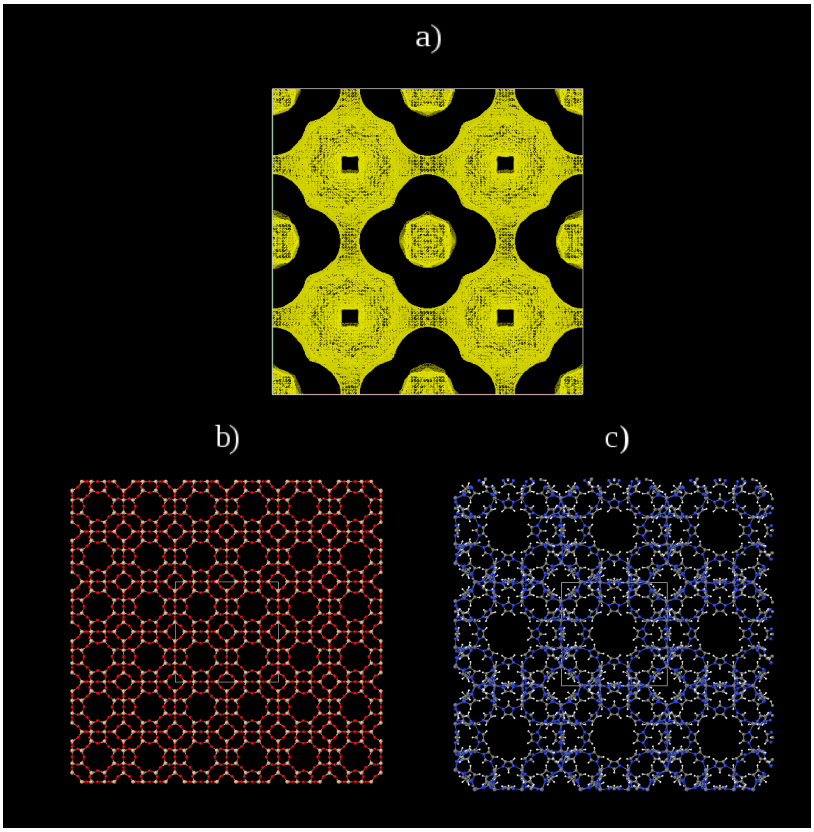


Fig. S2. Pore Size Distribution of LTA-type zeolite and ZIFs for helium as probe molecule.

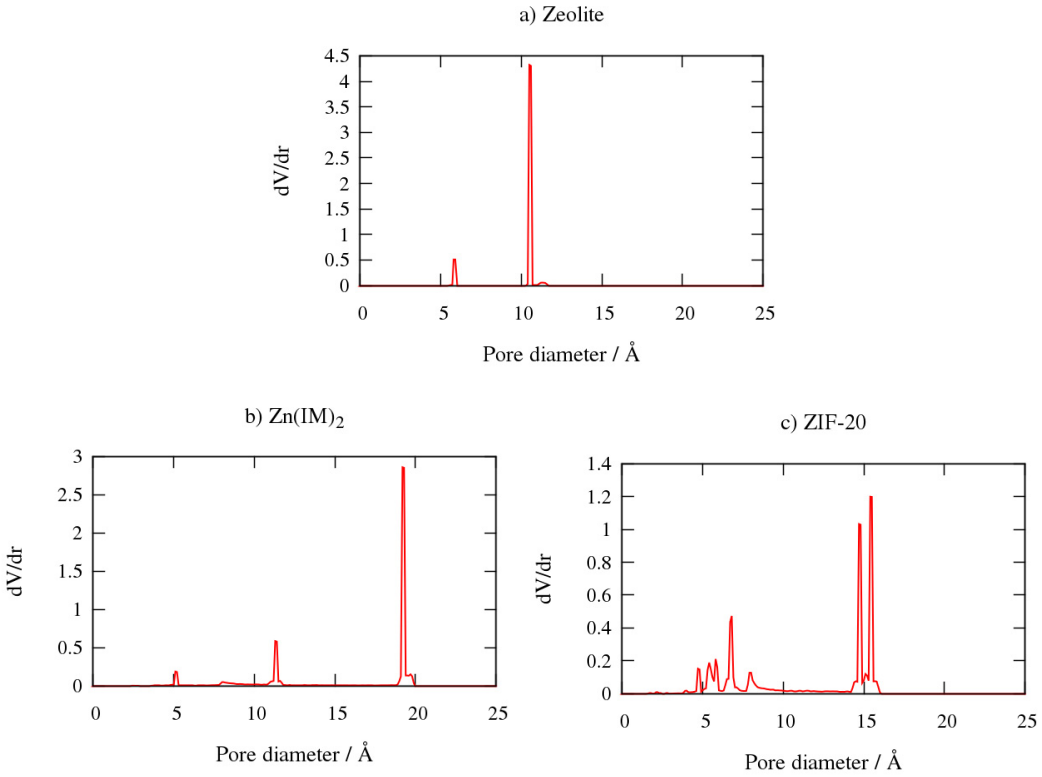
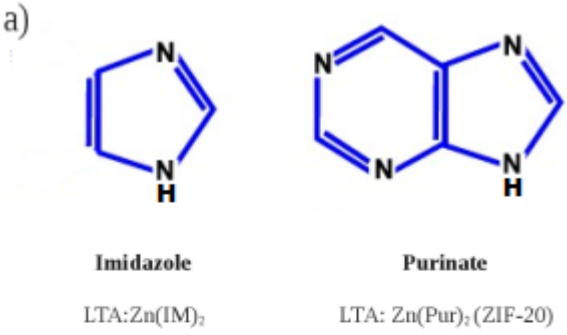


Fig. S3. Zn-based ZIFs with LTA topology: hypothetical $Zn(IM)_2$ and experimentally obtained ZIF-20 [3]. a) Organic linkers and b) picture of the ZIF under study, the LTA-type $Zn(IM)_2$.

a)



Imidazole **Purinate**

LTA:$Zn(IM)_2$ LTA: $Zn(Pur)_2$ (ZIF-20)

b)

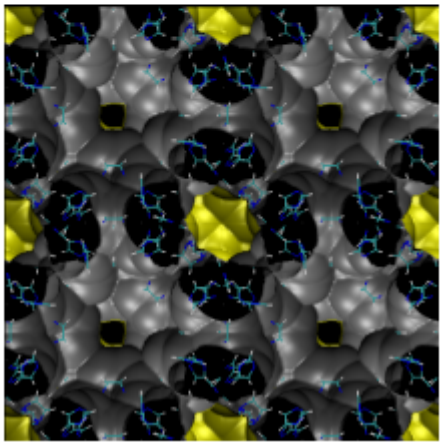


Fig. S4 Oxygen-oxygen (a) and oxygen-hydrogen (b) radial distribution functions and angle distribution for those molecules fulfilling the distance criteria (c) for water in the bulk and in the highly hydrated structures at 298.15 K.

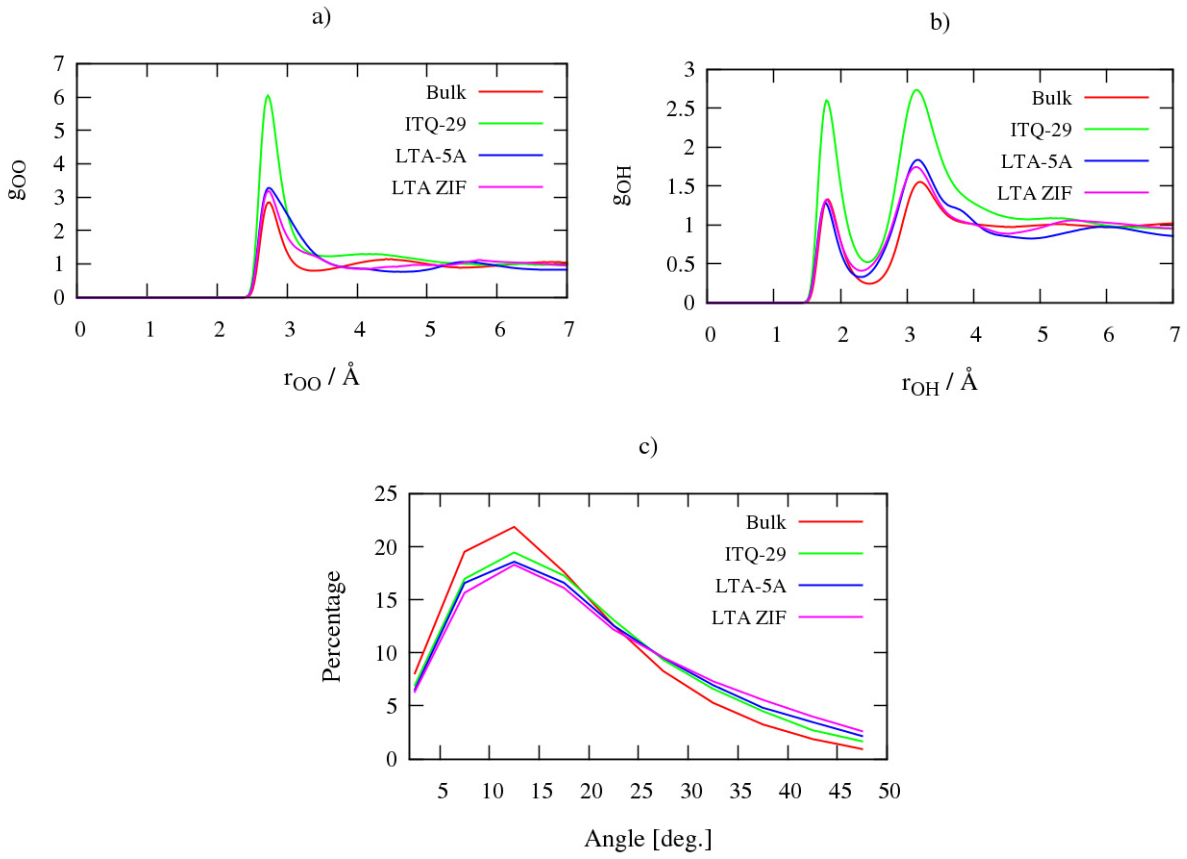


Fig. S5. Water-water and water-surface potential energy for water in ITQ-29 (a), LTA-5A (b), LTA ZIF (c) at 298.15 K (black), 373 K (red), 500 K (green) and 573 K (blue).

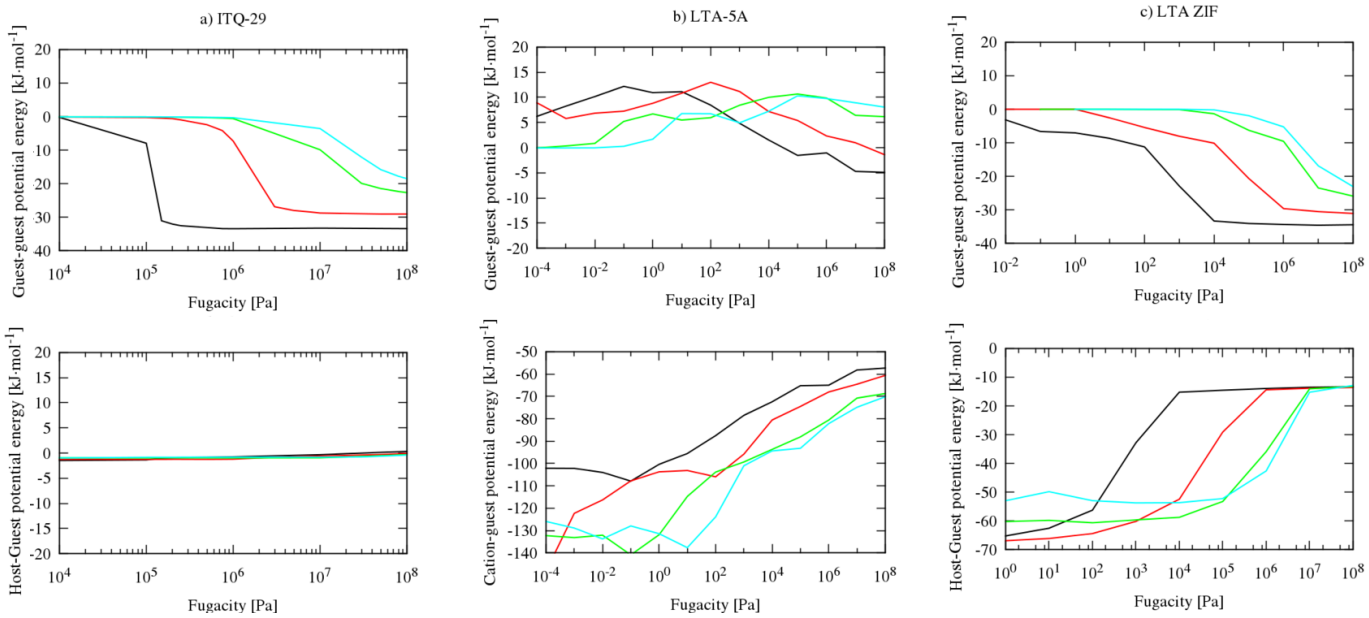
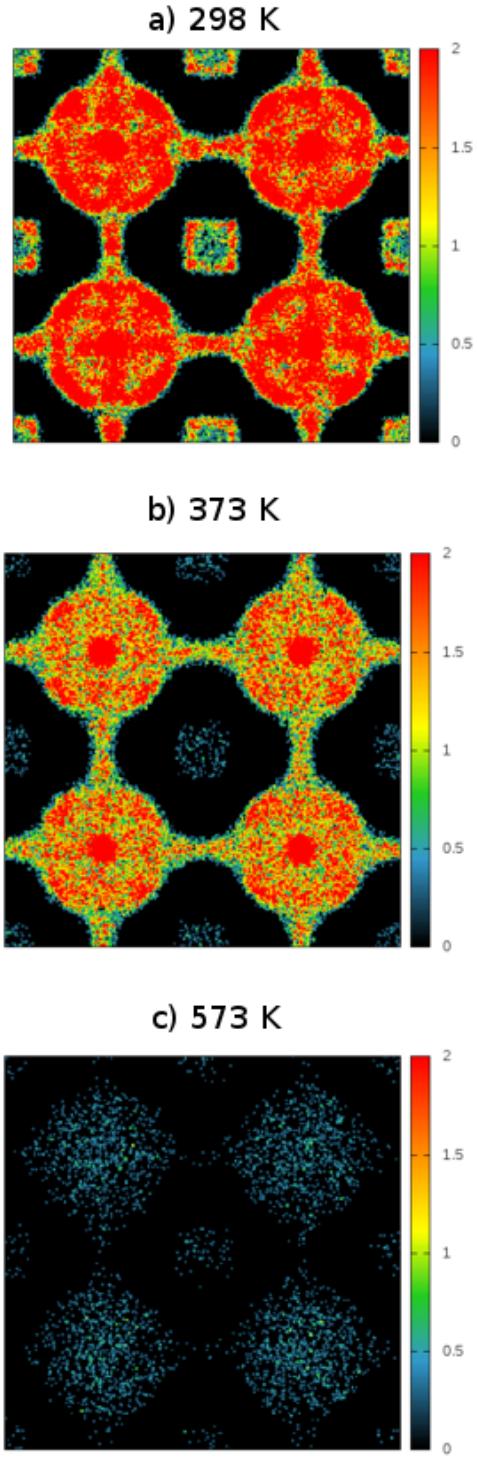


Fig. S6. Density contours of water in ITQ-29 for 10^7 Pa and different temperatures. The relation between colour and probability density occupation (from blue to red) is shown in the bar colour ramp situated on the right side of the figure.



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LTA-5A.cif

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C2      0.94664   0.26506   0.47042  -0.15400
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H2      0.92531   0.29423   0.55953   0.12100
C1      0.99482   0.80651   0.49934   0.08100
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C2	0.02028	0.52977	0.72161	-0.15400
H1	0.98146	0.49955	0.85127	0.10700
H2	0.03123	0.55974	0.68751	0.12100
H2	0.02764	0.44076	0.68596	0.12100
C1	0.49974	0.80644	0.99453	0.08100
N1	0.45117	0.77462	0.00215	-0.56100
N1	0.54858	0.77589	0.00510	-0.56100
C2	0.47044	0.72083	0.01848	-0.15400
C2	0.52977	0.72161	0.02027	-0.15400
H1	0.49955	0.85127	0.98147	0.10700
H2	0.55974	0.68751	0.03123	0.12100
H2	0.44076	0.68596	0.02763	0.12100
C1	0.50057	0.19762	0.00425	0.08100
N1	0.45160	0.22141	0.98268	-0.56100
N1	0.54902	0.22357	0.98402	-0.56100
C2	0.47019	0.26492	0.94673	-0.15400
C2	0.52953	0.26623	0.94754	-0.15400
H1	0.50095	0.16187	0.03429	0.10700
H2	0.55907	0.29439	0.92484	0.12100

H2	0.44007	0.29175	0.92320	0.12100
C1	0.00425	0.50057	0.19762	0.08100
N1	0.98268	0.45160	0.22141	-0.56100
N1	0.98402	0.54902	0.22357	-0.56100
C2	0.94672	0.47019	0.26492	-0.15400
C2	0.94754	0.52953	0.26623	-0.15400
H1	0.03429	0.50095	0.16187	0.10700
H2	0.92484	0.55907	0.29439	0.12100
H2	0.92320	0.44007	0.29175	0.12100
C1	0.09880	0.09908	0.35905	0.08100
N1	0.15569	0.08689	0.36573	-0.56100
N1	0.08700	0.15602	0.36595	-0.56100
C2	0.18132	0.13917	0.37755	-0.15400
C2	0.13949	0.18128	0.37768	-0.15400
H1	0.06640	0.06691	0.34928	0.10700
H2	0.14339	0.22719	0.38526	0.12100
H2	0.22729	0.14276	0.38499	0.12100
C1	0.90065	0.90037	0.36020	0.08100
N1	0.84370	0.91249	0.36641	-0.56100
N1	0.91238	0.84336	0.36661	-0.56100
C2	0.81794	0.86008	0.37737	-0.15400
C2	0.85977	0.81798	0.37749	-0.15400
H1	0.93315	0.93265	0.35114	0.10700
H2	0.85580	0.77198	0.38452	0.12100
H2	0.77190	0.85642	0.38428	0.12100
C1	0.09866	0.90130	0.63885	0.08100
N1	0.15600	0.91284	0.63606	-0.56100
N1	0.08700	0.84403	0.63511	-0.56100
C2	0.18209	0.85978	0.63022	-0.15400
C2	0.14007	0.81787	0.62964	-0.15400
H1	0.06582	0.93416	0.64354	0.10700
H2	0.14420	0.77151	0.62574	0.12100
H2	0.22848	0.85556	0.62691	0.12100
C1	0.90160	0.09896	0.63878	0.08100
N1	0.84441	0.08687	0.63520	-0.56100
N1	0.91271	0.15638	0.63587	-0.56100
C2	0.81784	0.13974	0.62972	-0.15400
C2	0.85945	0.18207	0.63013	-0.15400
H1	0.93471	0.06637	0.64343	0.10700
H2	0.85488	0.22843	0.62676	0.12100
H2	0.77145	0.14353	0.62593	0.12100
C1	0.35905	0.09880	0.09908	0.08100
N1	0.36573	0.15569	0.08689	-0.56100
N1	0.36595	0.08700	0.15602	-0.56100
C2	0.37755	0.18132	0.13917	-0.15400
C2	0.37768	0.13949	0.18128	-0.15400
H1	0.34928	0.06640	0.06691	0.10700
H2	0.38526	0.14339	0.22719	0.12100
H2	0.38499	0.22729	0.14276	0.12100
C1	0.09908	0.35905	0.09880	0.08100
N1	0.08689	0.36573	0.15569	-0.56100
N1	0.15602	0.36595	0.08700	-0.56100
C2	0.13917	0.37755	0.18132	-0.15400
C2	0.18128	0.37768	0.13949	-0.15400
H1	0.06691	0.34928	0.06640	0.10700
H2	0.22719	0.38526	0.14339	0.12100
H2	0.14276	0.38499	0.22729	0.12100
C1	0.63878	0.90159	0.09896	0.08100
N1	0.63520	0.84441	0.08687	-0.56100
N1	0.63587	0.91271	0.15638	-0.56100
C2	0.62972	0.81784	0.13974	-0.15400
C2	0.63013	0.85945	0.18207	-0.15400
H1	0.64343	0.93471	0.06637	0.10700
H2	0.62676	0.85488	0.22843	0.12100
H2	0.62593	0.77145	0.14353	0.12100

C1	0.90037	0.36020	0.90065	0.08100
N1	0.91249	0.36641	0.84370	-0.56100
N1	0.84336	0.36661	0.91238	-0.56100
C2	0.86008	0.37737	0.81794	-0.15400
C2	0.81798	0.37749	0.85977	-0.15400
H1	0.93265	0.35114	0.93315	0.10700
H2	0.77198	0.38452	0.85579	0.12100
H2	0.85642	0.38428	0.77190	0.12100
C1	0.36020	0.90065	0.90037	0.08100
N1	0.36641	0.84370	0.91249	-0.56100
N1	0.36661	0.91238	0.84336	-0.56100
C2	0.37737	0.81794	0.86008	-0.15400
C2	0.37749	0.85977	0.81798	-0.15400
H1	0.35114	0.93315	0.93264	0.10700
H2	0.38452	0.85579	0.77198	0.12100
H2	0.38428	0.77190	0.85642	0.12100
C1	0.90130	0.63885	0.09866	0.08100
N1	0.91284	0.63606	0.15600	-0.56100
N1	0.84403	0.63511	0.08700	-0.56100
C2	0.85978	0.63022	0.18209	-0.15400
C2	0.81787	0.62964	0.14007	-0.15400
H1	0.93416	0.64354	0.06582	0.10700
H2	0.77152	0.62574	0.14420	0.12100
H2	0.85556	0.62691	0.22848	0.12100
C1	0.63885	0.09866	0.90129	0.08100
N1	0.63606	0.15600	0.91284	-0.56100
N1	0.63511	0.08700	0.84403	-0.56100
C2	0.63022	0.18209	0.85978	-0.15400
C2	0.62964	0.14007	0.81787	-0.15400
H1	0.64354	0.06582	0.93416	0.10700
H2	0.62574	0.14420	0.77151	0.12100
H2	0.62691	0.22848	0.85556	0.12100
C1	0.09896	0.63878	0.90160	0.08100
N1	0.08687	0.63520	0.84441	-0.56100
N1	0.15638	0.63587	0.91271	-0.56100
C2	0.13974	0.62972	0.81784	-0.15400
C2	0.18207	0.63013	0.85945	-0.15400
H1	0.06637	0.64343	0.93471	0.10700
H2	0.22843	0.62676	0.85488	0.12100
H2	0.14353	0.62593	0.77145	0.12100
C1	0.87816	0.87798	0.62698	0.08100
N1	0.85330	0.92223	0.65618	-0.56100
N1	0.92247	0.85359	0.65647	-0.56100
C2	0.88368	0.92603	0.70710	-0.15400
C2	0.92582	0.88422	0.70728	-0.15400
H1	0.86417	0.86370	0.58477	0.10700
H2	0.95775	0.87418	0.73984	0.12100
H2	0.87325	0.95802	0.73948	0.12100
C1	0.12090	0.12108	0.62810	0.08100
N1	0.14591	0.07698	0.65740	-0.56100
N1	0.07672	0.14560	0.65769	-0.56100
C2	0.11578	0.07344	0.70850	-0.15400
C2	0.07364	0.11523	0.70867	-0.15400
H1	0.13468	0.13514	0.58575	0.10700
H2	0.04186	0.12543	0.74133	0.12100
H2	0.12637	0.04161	0.74098	0.12100
C1	0.12137	0.87873	0.37314	0.08100
N1	0.14703	0.92220	0.34348	-0.56100
N1	0.07725	0.85418	0.34348	-0.56100
C2	0.11741	0.92531	0.29206	-0.15400
C2	0.07491	0.88388	0.29206	-0.15400
H1	0.13463	0.86512	0.41581	0.10700
H2	0.04335	0.87351	0.25924	0.12100
H2	0.12859	0.95659	0.25925	0.12100
C1	0.87892	0.12153	0.37310	0.08100

N1	0.85391	0.07747	0.34374	-0.56100
N1	0.92248	0.14672	0.34315	-0.56100
C2	0.88339	0.07465	0.29222	-0.15400
C2	0.92515	0.11683	0.29186	-0.15400
H1	0.86559	0.13509	0.41575	0.10700
H2	0.95639	0.12761	0.25887	0.12100
H2	0.87264	0.04302	0.25959	0.12100
C1	0.87798	0.62698	0.87816	0.08100
N1	0.92223	0.65618	0.85330	-0.56100
N1	0.85359	0.65647	0.92247	-0.56100
C2	0.92603	0.70710	0.88368	-0.15400
C2	0.88422	0.70728	0.92582	-0.15400
H1	0.86370	0.58477	0.86417	0.10700
H2	0.87418	0.73984	0.95775	0.12100
H2	0.95802	0.73948	0.87325	0.12100
C1	0.62698	0.87816	0.87798	0.08100
N1	0.65618	0.85330	0.92223	-0.56100
N1	0.65647	0.92247	0.85359	-0.56100
C2	0.70710	0.88368	0.92603	-0.15400
C2	0.70728	0.92582	0.88422	-0.15400
H1	0.58477	0.86417	0.86370	0.10700
H2	0.73984	0.95775	0.87418	0.12100
H2	0.73948	0.87325	0.95802	0.12100
C1	0.12153	0.37310	0.87892	0.08100
N1	0.07747	0.34374	0.85391	-0.56100
N1	0.14672	0.34315	0.92248	-0.56100
C2	0.07465	0.29222	0.88339	-0.15400
C2	0.11683	0.29186	0.92515	-0.15400
H1	0.13509	0.41575	0.86559	0.10700
H2	0.12761	0.25887	0.95639	0.12100
H2	0.04302	0.25959	0.87264	0.12100
C1	0.62810	0.12090	0.12108	0.08100
N1	0.65740	0.14591	0.07698	-0.56100
N1	0.65769	0.07672	0.14560	-0.56100
C2	0.70850	0.11578	0.07344	-0.15400
C2	0.70867	0.07364	0.11523	-0.15400
H1	0.58575	0.13468	0.13514	0.10700
H2	0.74133	0.04186	0.12543	0.12100
H2	0.74098	0.12637	0.04161	0.12100
C1	0.12108	0.62810	0.12090	0.08100
N1	0.07698	0.65740	0.14591	-0.56100
N1	0.14560	0.65769	0.07672	-0.56100
C2	0.07344	0.70850	0.11578	-0.15400
C2	0.11523	0.70867	0.07364	-0.15400
H1	0.13514	0.58575	0.13468	0.10700
H2	0.12543	0.74133	0.04186	0.12100
H2	0.04161	0.74098	0.12637	0.12100
C1	0.37314	0.12137	0.87873	0.08100
N1	0.34348	0.14704	0.92220	-0.56100
N1	0.34348	0.07725	0.85418	-0.56100
C2	0.29206	0.11741	0.92531	-0.15400
C2	0.29206	0.07491	0.88388	-0.15400
H1	0.41581	0.13463	0.86512	0.10700
H2	0.25924	0.04335	0.87351	0.12100
H2	0.25925	0.12859	0.95659	0.12100
C1	0.87873	0.37314	0.12137	0.08100
N1	0.92220	0.34348	0.14703	-0.56100
N1	0.85418	0.34348	0.07725	-0.56100
C2	0.92531	0.29206	0.11741	-0.15400
C2	0.88388	0.29206	0.07491	-0.15400
H1	0.86512	0.41581	0.13463	0.10700
H2	0.87350	0.25924	0.04335	0.12100
H2	0.95659	0.25925	0.12859	0.12100
C1	0.37310	0.87892	0.12153	0.08100
N1	0.34374	0.85391	0.07747	-0.56100

N1	0.34315	0.92248	0.14672	-0.56100
C2	0.29222	0.88339	0.07465	-0.15400
C2	0.29186	0.92515	0.11683	-0.15400
H1	0.41575	0.86559	0.13509	0.10700
H2	0.25887	0.95639	0.12761	0.12100
H2	0.25959	0.87264	0.04302	0.12100
C1	0.99382	0.28336	0.28365	0.08100
N1	0.01241	0.33657	0.26779	-0.56100
N1	0.01273	0.26784	0.33686	-0.56100
C2	0.04495	0.35580	0.31363	-0.15400
C2	0.04515	0.31393	0.35571	-0.15400
H1	0.96687	0.25626	0.25682	0.10700
H2	0.06598	0.31373	0.39750	0.12100
H2	0.06559	0.39769	0.31313	0.12100
C1	0.99644	0.71486	0.28593	0.08100
N1	0.02225	0.66704	0.26412	-0.56100
N1	0.02523	0.73703	0.33184	-0.56100
C2	0.07015	0.65850	0.29824	-0.15400
C2	0.07196	0.70113	0.33949	-0.15400
H1	0.95719	0.73329	0.26860	0.10700
H2	0.10307	0.70839	0.37356	0.12100
H2	0.09943	0.62288	0.29083	0.12100
C1	0.00110	0.71607	0.71579	0.08100
N1	0.97522	0.66786	0.73665	-0.56100
N1	0.97487	0.73667	0.66766	-0.56100
C2	0.93000	0.65740	0.69955	-0.15400
C2	0.92979	0.69931	0.65752	-0.15400
H1	0.03856	0.73591	0.73539	0.10700
H2	0.90088	0.70512	0.62132	0.12100
H2	0.90130	0.62106	0.70560	0.12100
C1	0.99654	0.28563	0.71463	0.08100
N1	0.02499	0.33163	0.73705	-0.56100
N1	0.02273	0.26403	0.66692	-0.56100
C2	0.07190	0.33956	0.70145	-0.15400
C2	0.07052	0.29837	0.65873	-0.15400
H1	0.95725	0.26810	0.73280	0.10700
H2	0.10004	0.29116	0.62327	0.12100
H2	0.10281	0.37375	0.70895	0.12100
C1	0.28365	0.99382	0.28336	0.08100
N1	0.26779	0.01241	0.33657	-0.56100
N1	0.33685	0.01273	0.26784	-0.56100
C2	0.31363	0.04495	0.35580	-0.15400
C2	0.35571	0.04515	0.31393	-0.15400
H1	0.25682	0.96687	0.25626	0.10700
H2	0.39750	0.06598	0.31373	0.12100
H2	0.31313	0.06558	0.39769	0.12100
C1	0.28336	0.28365	0.99382	0.08100
N1	0.33657	0.26779	0.01241	-0.56100
N1	0.26784	0.33686	0.01273	-0.56100
C2	0.35580	0.31363	0.04495	-0.15400
C2	0.31393	0.35571	0.04515	-0.15400
H1	0.25626	0.25682	0.96687	0.10700
H2	0.31373	0.39750	0.06598	0.12100
H2	0.39769	0.31313	0.06558	0.12100
C1	0.71463	0.99654	0.28563	0.08100
N1	0.73705	0.02499	0.33163	-0.56100
N1	0.66692	0.02273	0.26403	-0.56100
C2	0.70145	0.07190	0.33956	-0.15400
C2	0.65873	0.07052	0.29837	-0.15400
H1	0.73280	0.95725	0.26810	0.10700
H2	0.62327	0.10004	0.29116	0.12100
H2	0.70895	0.10281	0.37375	0.12100
C1	0.71486	0.28593	0.99644	0.08100
N1	0.66704	0.26412	0.02225	-0.56100
N1	0.73703	0.33184	0.02523	-0.56100

C2	0.65850	0.29824	0.07015	-0.15400
C2	0.70113	0.33949	0.07196	-0.15400
H1	0.73329	0.26860	0.95719	0.10700
H2	0.70839	0.37356	0.10307	0.12100
H2	0.62288	0.29083	0.09943	0.12100
C1	0.28593	0.99644	0.71486	0.08100
N1	0.26412	0.02225	0.66704	-0.56100
N1	0.33184	0.02523	0.73703	-0.56100
C2	0.29824	0.07015	0.65850	-0.15400
C2	0.33949	0.07196	0.70113	-0.15400
H1	0.26860	0.95719	0.73329	0.10700
H2	0.37356	0.10307	0.70839	0.12100
H2	0.29083	0.09943	0.62288	0.12100
C1	0.71607	0.71579	0.00110	0.08100
N1	0.66786	0.73665	0.97522	-0.56100
N1	0.73667	0.66766	0.97487	-0.56100
C2	0.65740	0.69955	0.93001	-0.15400
C2	0.69931	0.65752	0.92979	-0.15400
H1	0.73591	0.73539	0.03856	0.10700
H2	0.70512	0.62132	0.90088	0.12100
H2	0.62106	0.70560	0.90130	0.12100
C1	0.71579	0.00110	0.71607	0.08100
N1	0.73665	0.97522	0.66786	-0.56100
N1	0.66766	0.97487	0.73667	-0.56100
C2	0.69955	0.93001	0.65740	-0.15400
C2	0.65752	0.92979	0.69931	-0.15400
H1	0.73539	0.03856	0.73591	0.10700
H2	0.62132	0.90088	0.70512	0.12100
H2	0.70560	0.90130	0.62106	0.12100
C1	0.28563	0.71463	0.99654	0.08100
N1	0.33163	0.73705	0.02499	-0.56100
N1	0.26403	0.66692	0.02273	-0.56100
C2	0.33956	0.70145	0.07190	-0.15400
C2	0.29837	0.65873	0.07052	-0.15400
H1	0.26810	0.73280	0.95725	0.10700
H2	0.29116	0.62327	0.10004	0.12100
H2	0.37375	0.70895	0.10281	0.12100

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