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Supplementary Materials for

Can polarity-inverted membranes self-assemble on Titan?

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This PDF file includes:

Section S1. Phonon band structures of the azotosome membrane and the acrylonitrile ice

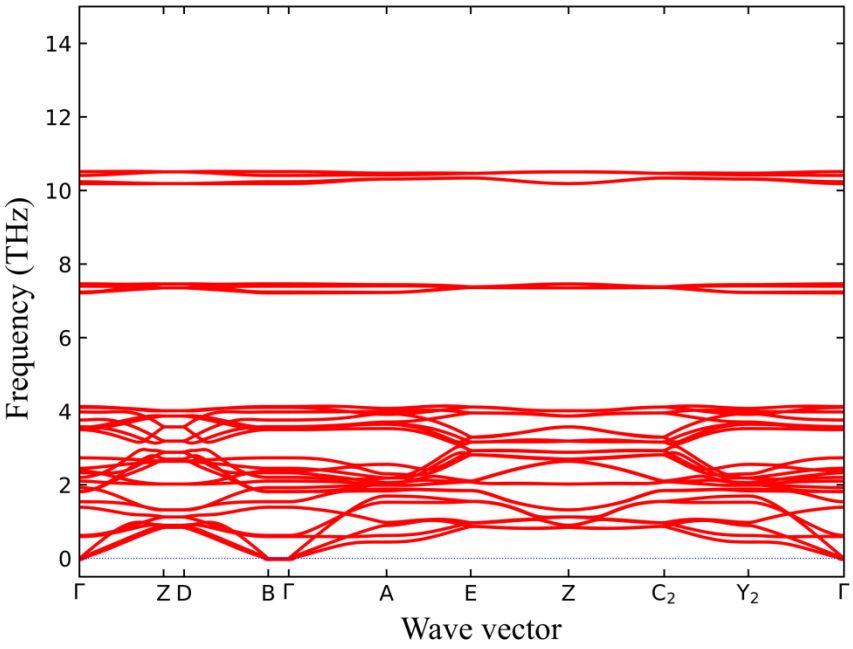

Fig. S1. Phonon band structure of the optimized azotosome membrane.

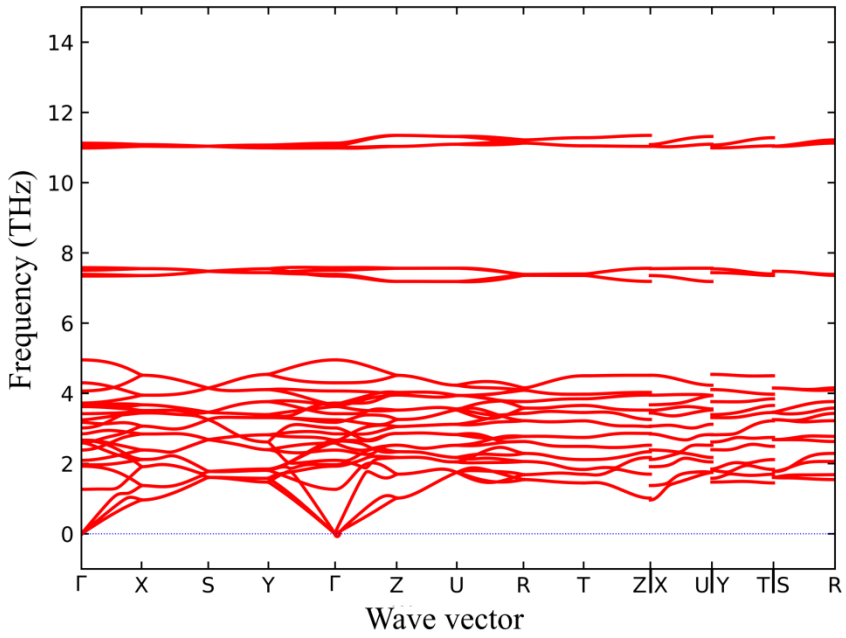

Fig. S2. Calculated phonon band structure of the *Pna*2$_1$ phase of acrylonitrile.

Section S2. Convergence tests

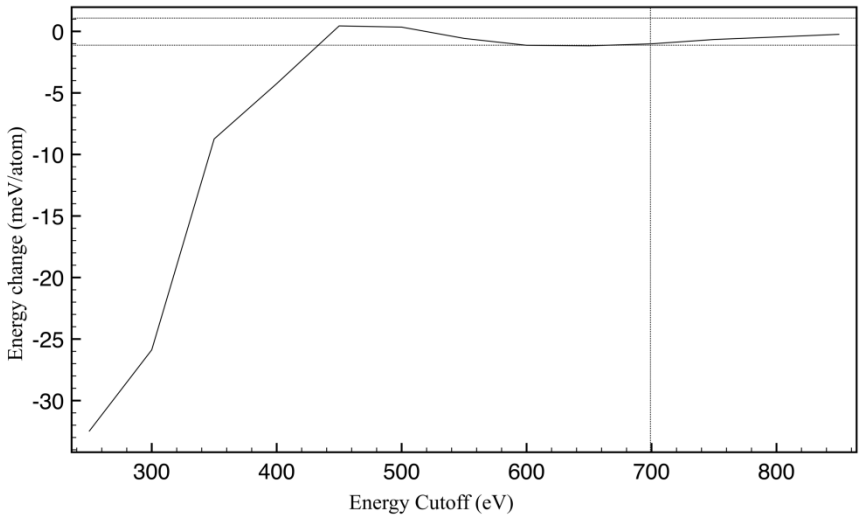

Fig. S3. Convergence of the energy with respect to plane-wave energy cutoff in calculations on the membrane structure. A 9x9x1 *k*-mesh was used for the convergence tests. Used energy cutoff indicated by vertical line.

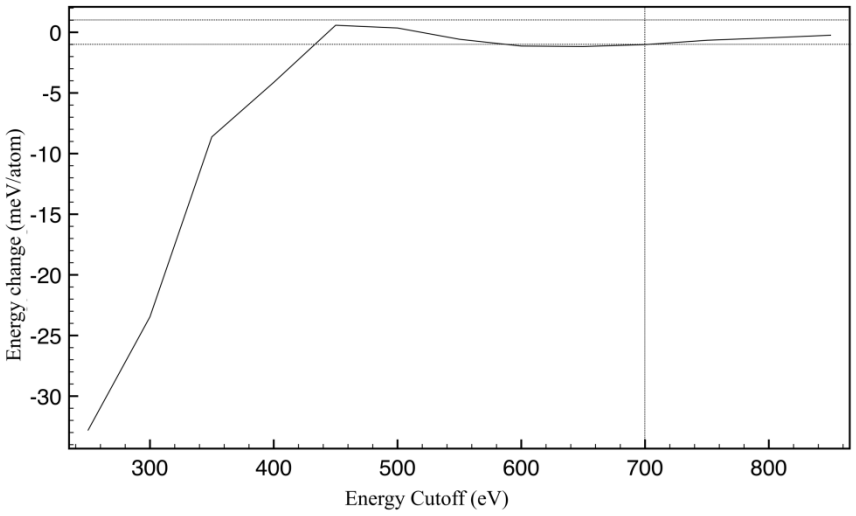

Fig. S4. Convergence of the energy change with respect to plane-wave energy cutoff used in calculations on the *Pna*2_1 phase of the acrylonitrile ice. A 12x12x12 *k*-mesh was used for the convergence tests**.** Used energy cutoff indicated by vertical line.

Table S1. Total energies in eV/atom of the *Pna*2_1 phase of acrylonitrile and the membrane structure as a function of *k*-point density. The energy is unaffected by the number of *k* points in both cases (total change < 0.1 meV/atom).

Pna2₁* phase of the ice, MP *k*-mesh, *k x k x k		**Membrane, Γ-centered *k*-mesh, *k x k x 1***	
k	**Total energy (eV/atom)**	***k***	**Total energy (eV/atom)**
2	-6.5007836	3	-6.4771427
4	-6.5007836	5	-6.4771437
6	-6.5007846	7	-6.4771434
8	-6.5007844	9	-6.4771422
10	-6.5007844	11	-6.4771437
12	-6.5007842	13	-6.4771433
14	-6.5007843	15	-6.4771431

Section S3. Optimized structures

The geometry-optimized membrane structure is shown in Figure S5. Whereas it is possible that other relative orientations of the CH_2-groups might correspond to other kinetically stable azotosome isomers (two-dimensional structures), such structures are unlikely to be significantly lower in energy compared to the considered *Pc* phase. This is evident from the different phases of acrylonitrile ice that are shown in Figure S6. The latter structures demonstrate that in a three-dimensional structure, the energies of rotational isomers are on the order of 1 kJ/mol apart, which is too small to affect our conclusions.

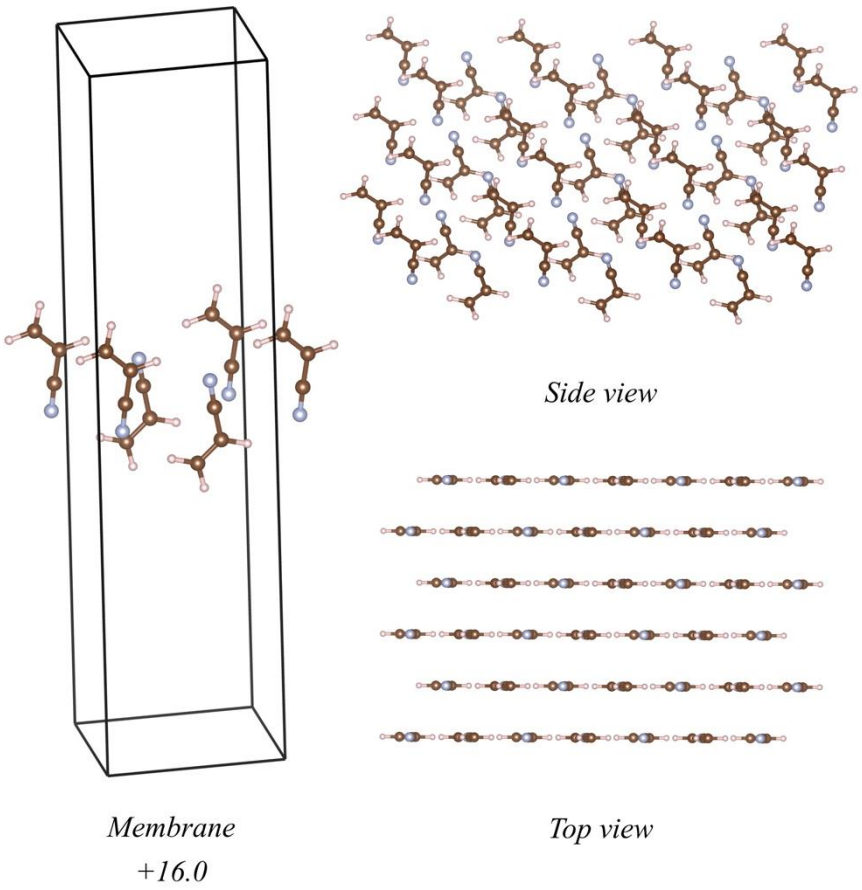

Fig. S5. Structure of the acrylonitrile-based membrane following optimization in vacuum at the PBE-D3 level of theory. The optimization of the membrane structure was done using an energy cutoff 700 eV and a 9x9x1 *k*-point mesh. The energy of the membrane relative to the $Pna2_1$ phase of the acrylonitrile ice is given in the figure in kJ/mol acrylonitrile.

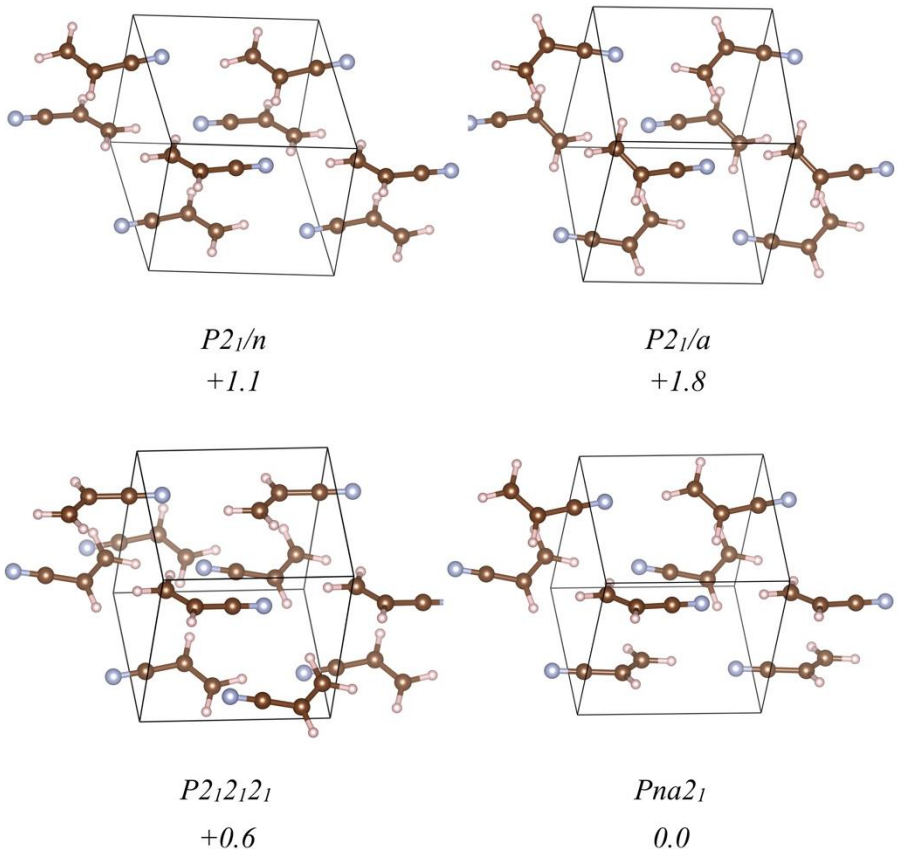

Fig. S6. Crystal structures of different crystalline phases of acrylonitrile and their relative energies in kJ/mol. The structures were optimized at the PBE-D3 level of theory, using an energy cutoff 700 eV and a *k*-mesh of 12x12x12.

The optimized crystal structure of methane and the azotosome membrane solvated by methane are shown in Figures S7 and S8, respectively. The configuration of the methane molecules surrounding the azotosome membrane were arbitrary chosen over a 2 x 2 x 1 supercell prior to optimization. The considered single structure does not strictly correspond to the ground state configuration in solution. Because of the choice of orientation of methane, the energy of the solvated membrane may be slightly overestimated. However, error-cancellation of this modeling effect is likely. This is because we have used crystalline (ordered) methane as our pure methane reference state when calculating the azotosome solvation energy, not liquid (disordered) methane. Liquid methane is the ground state of methane on Titan's surface. Regardless of if the net effect of our solvation modeling is a slight over- or underestimation of the azotosome stability, the high symmetry and nonpolar nature of methane, ensures that this error is small, and inconsequential for our conclusions. To illustrate the insensitivity of the energy calculation with respect to methane orientation, we can, for example, compare the energy per methane molecule in the *P4m2* crystal of methane, with that in the face-centered cubic structure. The difference is less than 3 meV/methane (<0.3 kJ/mol).

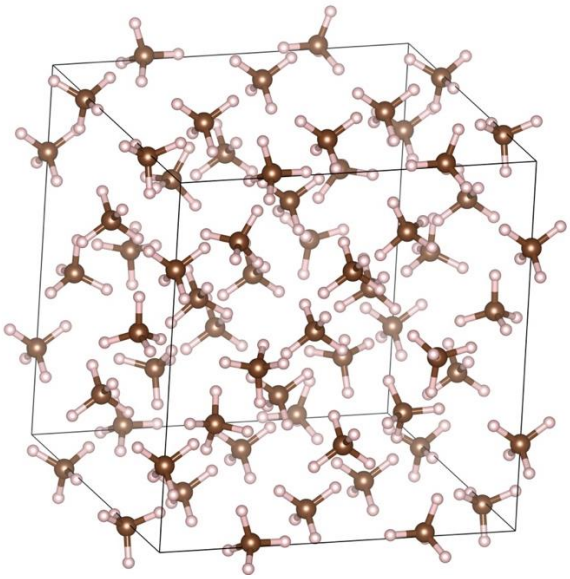

Fig. S7. The optimized *P*4*m*2 crystal structure of methane.

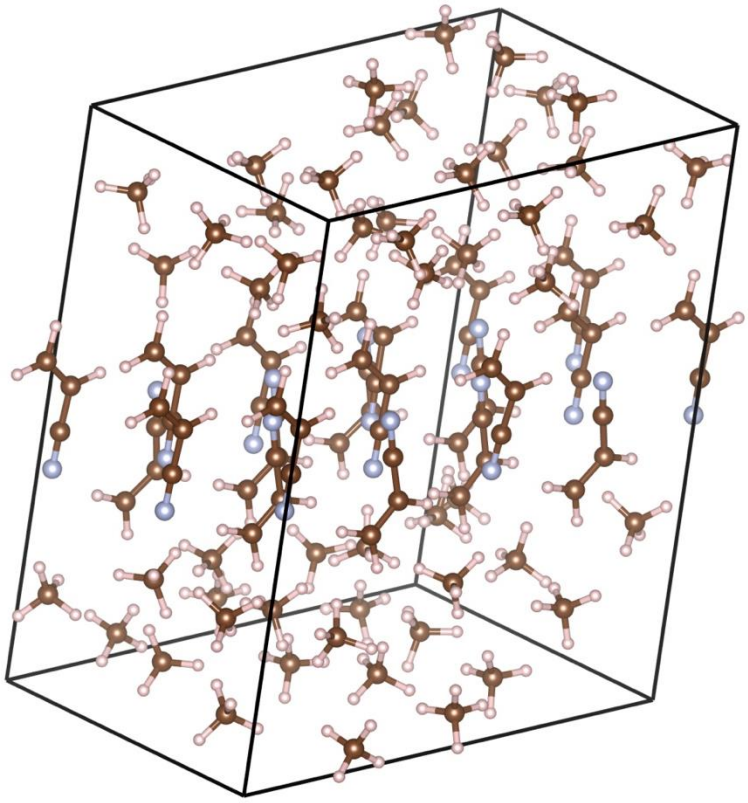

Fig. S8. The optimized structure of the azotosome membrane solvated by methane.

Section S4. The dynamics of the solvated membrane

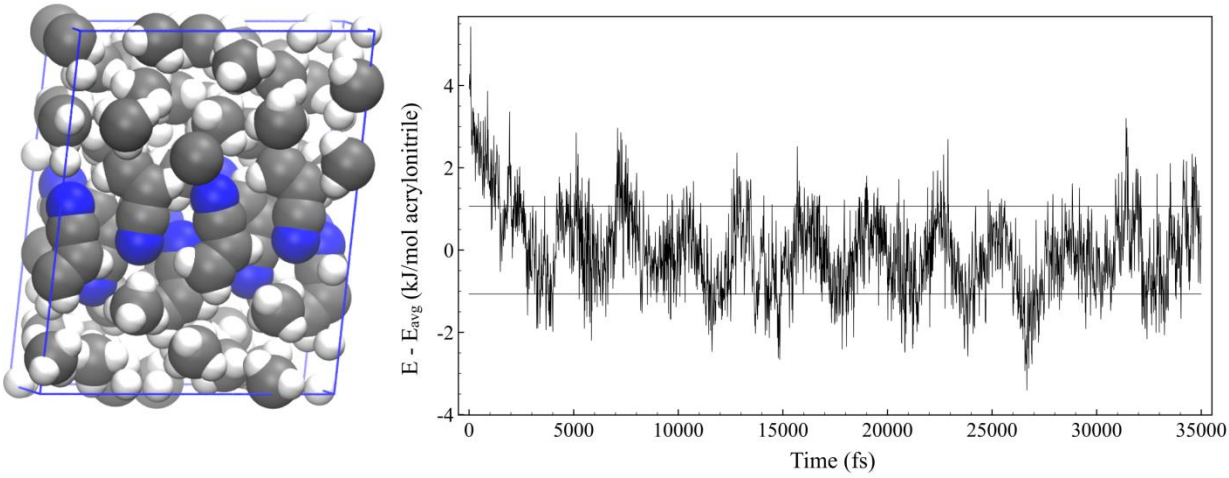

Fig. S9. The dynamic stability of the azotosome. Left: A snapshot of the solvated membrane from the ab initio simulation performed in CP2K. Right: Difference between the potential energy and the average potential energy of the azotosome in a 35 ps ab initio simulation of the 2 x 2 x 1 azotosome cell solvated by methane. Horizontal lines indicate the 1 kJ/mol acrylonitrile standard deviation.

Section S5. Coordinates and cell parameters

Methane (P1)

a: 4.40160 Å b: 4.03972 Å c: 3.98000 Å
α: 61.75989 β: 56.46137 γ: 57.00145

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Methane (P4m2)

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α: 90.00000 β: 90.00000 γ: 90.00000

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Methane Solvated Membrane

a: 12.39420 Å b: 14.96420 Å c: 18.47110 Å
α: 95.20520 β: 95.54470 γ: 91.02860

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H 10.11663 13.88138 2.44227
H 11.23678 12.13574 0.31174
H 0.27880 11.57086 1.21528
H 11.03349 11.14585 1.78713
H 8.75745 10.38346 3.53582
H 11.68015 10.40249 0.29654
H 10.41689 9.73722 3.72547
H 9.29059 8.98680 2.56071
H 9.02846 8.79088 4.32203
H 11.44803 7.79132 2.11370
H 9.52858 6.43652 3.81827
H 0.54258 7.96057 1.13364
H 11.34956 7.78001 0.32675
H 10.25886 5.19130 2.76261
H 8.97485 6.25460 2.12486
H 12.07274 6.39512 1.19130
H 8.57112 5.00740 3.33849
H 10.38099 3.38955 1.21748
H 11.77464 3.66404 0.13253
H 8.38911 1.55775 17.75088
H 8.24769 2.58157 3.70332
H 9.05654 1.19406 4.49813
H 9.81311 1.98413 3.08131
H 11.10131 2.01566 0.32547
H 8.34023 0.99999 2.86915
H 4.74017 13.31509 16.73677
H 4.82238 13.31227 14.95348
H 5.36315 11.87452 15.86984
H 3.62506 12.28351 15.78875
H 4.96243 11.03266 12.89177
H 6.56107 10.92531 13.70068
H 5.23748 9.82983 14.18156
H 3.40264 10.29008 17.47630
H 6.02854 9.63871 12.57711
H 4.76766 9.22677 17.03350
H 3.22322 9.12132 16.13526

H 3.31474 8.53681 17.82154
H 5.18217 7.10500 15.49623
H 3.25646 5.53090 16.61504
H 6.62341 6.37198 14.74627
H 5.60301 7.49351 13.80191
H 4.55461 4.32212 16.41167
H 3.01717 4.13677 15.51985
H 4.98894 5.86488 14.22238
H 3.05848 3.88875 17.29270
H 4.75983 3.80661 12.49364
H 6.11992 3.61997 13.64888
H 5.79676 2.36084 12.42005
H 2.28700 1.49172 16.24894
H 3.24497 0.17351 16.98096
H 4.01205 1.29127 15.81877
H 4.67139 2.58747 13.80099
H 2.80333 0.09547 15.25332
H 0.93474 -1.13930 16.97199
H 0.30081 -1.34140 15.31849
H 1.06206 12.34549 16.04008
H -0.60196 12.60161 16.64323
H 2.37593 11.77000 13.24268
H 2.57733 10.27892 14.20627
H 0.93846 10.92726 13.90753
H -0.82509 10.10528 16.86564
H 1.86602 10.20061 12.56338
H 0.74779 9.56111 16.20995
H -0.77077 9.05385 15.41843
H -0.33654 8.39443 17.02563
H 1.19954 6.87741 15.15008
H -0.68216 5.96725 16.63847
H 2.80450 7.47388 14.64559
H 1.37519 7.78873 13.61885
H 0.55289 4.70074 16.37067
H -0.95107 4.70535 15.39921
H 2.03709 6.12867 13.75889
H -1.00988 4.28511 17.13692
H 0.82592 3.63076 13.97251
H 2.12401 3.59242 12.73673
H 0.81057 2.39076 12.67339
H 10.51753 2.08291 15.70162
H -1.12485 0.67273 16.50686
H -0.20626 1.60157 15.28334
H 2.02923 2.31317 13.98276
H 10.80958 0.58075 14.77958
H 9.56122 -1.33792 16.12941

H 8.22969 12.78416 14.96264
H 9.33218 11.83584 15.99889
H 7.90900 12.65251 16.71664
H 9.61781 11.15557 11.90970
H 10.90971 10.14873 12.61262
H 10.38608 11.63922 13.45612
H 7.45924 9.96215 16.86985
H 9.30318 10.21894 13.40597
H 8.88225 9.12907 16.18048
H 7.29642 9.01734 15.36077
H 7.55775 8.17779 16.91818
H 8.79975 7.65726 13.67450
H 7.98831 5.55508 16.66703
H 10.58304 7.61859 13.78269
H 9.69239 6.17905 13.19967
H 8.94009 4.05735 16.43675
H 7.24914 4.14210 15.86032
H 9.59735 6.65344 14.92072
H 7.59674 4.09169 17.61597
H 9.07659 3.93872 13.80209
H 10.34333 2.84920 13.16397
H 9.32559 3.77980 12.02740
H 6.54230 1.75391 15.76404
H 6.98286 0.05169 16.09774
H 8.10485 1.10767 15.18724
H 8.61339 2.43450 12.95987
H 6.57576 0.56759 14.43160
N 3.52113 3.84876 9.73304
N 3.83312 0.26347 7.90984
N 0.46501 5.56348 8.19742
N 9.90897 0.12270 7.41579
N 3.47574 11.40222 9.99919
N 0.40697 13.08206 8.41250
N 3.55618 7.69512 7.77219
N 9.70619 3.68169 9.33472
N 9.65562 11.28334 9.12457
N 9.79812 7.69580 6.70500
N 6.59848 13.06409 8.24592
N 6.55233 9.22806 10.02061
N 6.78251 1.66563 10.03983
N 6.70058 5.61217 7.91936
N 0.44724 9.24269 10.48117
N 0.31866 1.65137 10.27761

Non-solvated Membrane

a: 6.38654 Å b: 7.25887 Å c: 29.79710 Å

α: 90.00000 β: 90.00000 γ: 90.00030

N 1.61029 2.33895 15.80528
N 1.61027 5.96839 13.99182
N 4.80421 0.95033 13.97514
N 4.80419 4.57977 15.82196
C 1.60843 2.93534 12.33749
C 1.60914 1.94785 13.24511
C 1.60984 2.19094 14.64557
C 1.60842 6.56478 17.45961
C 1.60912 5.57728 16.55199
C 1.60982 5.82038 15.15153
C 4.79711 1.55035 17.43905
C 4.80191 0.56002 16.53441
C 4.80325 0.80102 15.13454
C 4.79709 5.17978 12.35805
C 4.80189 4.18946 13.26269
C 4.80323 4.43045 14.66256
H 1.60921 0.88928 12.97366
H 1.60830 3.98672 12.62533
H 1.60793 2.69144 11.27522
H 1.60919 4.51872 16.82344
H 1.60832 0.35728 17.17177
H 1.60791 6.32088 18.52188
H 4.80443 6.76135 16.81063
H 4.79449 2.60035 17.14615
H 4.79577 1.30957 18.50191
H 4.80445 3.13191 12.98647
H 4.79447 6.22978 12.65095
H 4.79575 4.93901 11.29519

Acrylonitrile ice (Pn21a)
a: 7.06881 Å b: 6.37355 Å c: 6.90727 Å
α: 90.00000 β: 90.00000 γ: 90.00000

N 4.24772 1.56375 2.64217
N 6.35550 4.75053 6.09580
N 0.71331 1.56375 0.81147
N 2.82109 4.75053 4.26510
C 4.18778 2.10028 6.09719
C 4.35644 1.39695 3.79437
C 6.41544 5.28705 2.64355
C 6.08731 4.35791 1.73283
C 6.24678 4.58373 0.34074
C 0.65337 2.10028 4.26372
C 0.98150 1.17114 5.17444

C 2.88103 5.28705 0.81008
C 2.55290 4.35791 1.72081
C 2.71237 4.58373 3.11290
C 4.51591 1.17114 5.18646
C 0.82203 1.39695 6.56653
H 4.32470 1.90824 0.25412
H 4.93304 0.19943 5.46192
H 3.78026 3.06313 5.79119
H 6.82296 6.24990 2.33756
H 6.27852 5.09502 3.70775
H 5.67018 3.38620 2.00829
H 0.24585 3.06313 4.56971
H 0.79029 1.90824 3.19952
H 1.39863 0.19943 4.89898
H 2.74411 5.09502 6.65315
H 2.13577 3.38620 1.44535
H 3.28855 6.24990 1.11608

Acrylonitrile ice (P212121)
a: 7.09294 Å b: 6.41706 Å c: 6.84612 Å
α: 89.94250 β: 90.00000 γ: 90.00000

N 4.14327 1.53955 2.65458
N 6.41812 4.88712 6.08599
N 0.59680 1.67242 0.76848
N 2.87165 4.74878 4.18318
C 4.30279 2.25689 6.08668
C 4.44961 1.25341 5.20811
C 4.26988 1.43034 3.81185
C 6.26945 4.16800 2.67368
C 6.12263 5.17068 1.79423
C 6.29647 4.99133 0.39749
C 0.75632 0.96194 4.18250
C 0.90314 1.96543 5.06106
C 0.72341 1.78850 6.45733
C 2.72298 5.46103 0.74938
C 2.57616 4.45835 1.62883
C 2.75000 4.63769 3.02557
H 4.45252 2.07847 0.30643
H 4.72872 0.24277 5.51311
H 4.03149 3.25826 5.75478
H 6.12390 4.34162 3.73983
H 5.84820 6.18270 2.09847
H 6.53650 3.16545 2.34206
H 0.90605 1.13349 3.11663
H 1.18225 2.97606 4.75607

H 0.48502 6.37763 4.51440
H 2.57743 5.29427 6.52935
H 2.30173 3.44633 1.32459
H 2.99003 0.04652 1.08100

Acrylonitrile ice (P21/a)
a: 7.25667Å b: 6.41311Å c 6.84102Å
α: 90.00360 β: 89.96450 γ: 83.08380

N 4.50493 1.55578 2.65671
N 7.09048 4.80844 6.06976
N 0.87583 1.55592 0.73856
N 3.46106 4.80883 4.16632
C 4.89138 2.06137 6.10321
C 4.43678 1.16478 5.21443
C 4.47433 1.39614 3.81442
C 6.70031 4.30354 2.67532
C 7.15314 5.20088 1.78646
C 7.11638 4.96921 0.38645
C 1.26180 2.06209 4.13266
C 0.80865 1.16506 5.02172
C 0.84799 1.39591 6.42180
C 3.07095 4.30413 0.71995
C 3.52486 5.20110 1.60860
C 3.48983 4.96897 3.00861
H 4.85457 1.84985 0.33090
H 4.02751 0.19653 5.50770
H 5.30585 3.01702 5.78538
H 6.73244 4.51616 3.74402
H 7.56028 6.17001 2.07967
H 6.28792 3.34690 2.35776
H 1.67632 3.01778 4.45029
H 1.22785 1.84998 3.06396
H 0.39922 0.19683 4.72865
H 2.65874 3.34740 1.03765
H 3.10600 4.51616 6.49233
H 3.93172 6.17037 1.31525

Acrylonitrile ice (P21/n)
a: 7.04064Å b: 6.57525 Å c: 6.93965 Å
α: 81.54240 β: 90.17400 γ: 91.17420

N 4.15048 2.06033 2.67806
N 6.36072 5.87765 6.08922
N 0.64457 1.74429 0.72067
N 2.83183 5.52163 4.22106

C 4.20787 2.89074 6.07810
C 4.37615 1.85068 5.24760
C 4.24158 1.98007 3.84106
C 6.14701 5.73156 2.60901
C 6.09494 4.66963 1.79059
C 6.26230 4.78790 0.38618
C 0.83280 1.94151 4.18440
C 0.74325 2.99472 5.01010
C 0.67140 2.85042 6.41979
C 2.68516 4.68098 0.82638
C 2.70492 5.59703 3.06115
C 2.53038 5.72198 1.65839
H 4.34921 1.74834 0.29022
H 4.64652 0.85355 5.59959
H 3.94778 3.87728 5.69432
H 6.33422 6.73197 2.21940
H 6.00319 5.61614 3.68318
H 5.89457 3.65894 2.15165
H 0.89780 2.08241 3.10563
H 2.95788 3.69639 1.20569
H 2.51920 5.81876 6.61686
H 2.24472 6.71634 1.30900
H 0.74058 4.02505 4.65151
H 0.83860 0.92271 4.57106