Supplementary information for *Water-Mediated Conformer-Selective Desorption of n-Propyl Cyanide from Mixed Ices*

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Table S1. Vibrational modes probed for the *gauche:anti* ice-phase ratio analysis

Species	**Freq (cm^{-1})**	**Mode**	**Integration Region**
gauche	1342	CH_2 wag	1348-1334
anti	1352	CH_2 wag	1364-1348
gauche	1260	CH_2 twist	1270-1247
anti	1277	CH_2 twist	1287-1270
gauche	771	CH_2 rock	783-752
anti	740	CH_2 rock	752-723
Mixed	2248	CN stretch	2280-2225

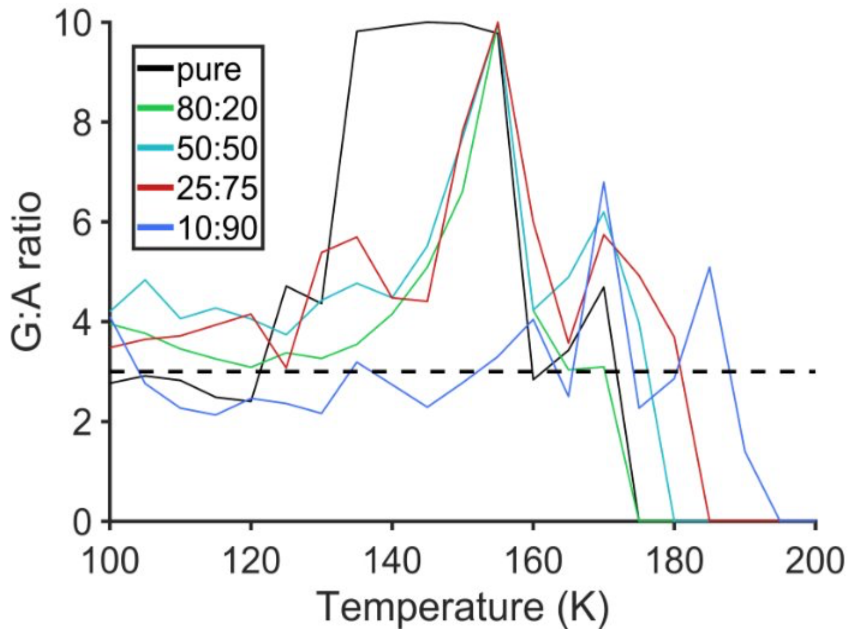

Fig. S2. G:A peak area ratio of mixed *n*-PrCN:Water ices over the expected crystallization and desorption temperature region. The maximum of each data set is normalized to a G:A ratio of 10, which is treated as a pure *gauche* ice.

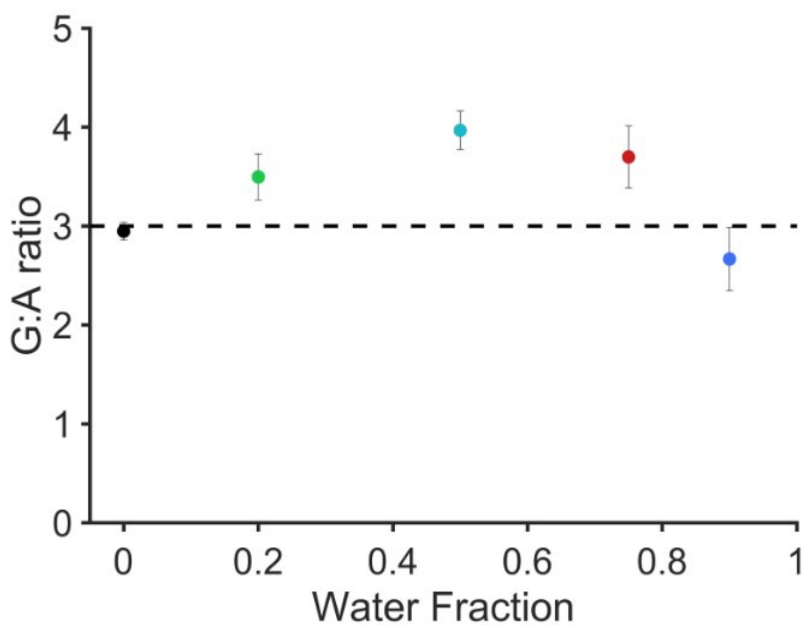

Fig. S3. G:A peak area ratios of mixed *n*-PrCN:Water at different water fractions. This data is an average of the G:A ratio from 5 K to 100 K. Dashed line indicates the expected 3:1 gas phase conformer ratio.

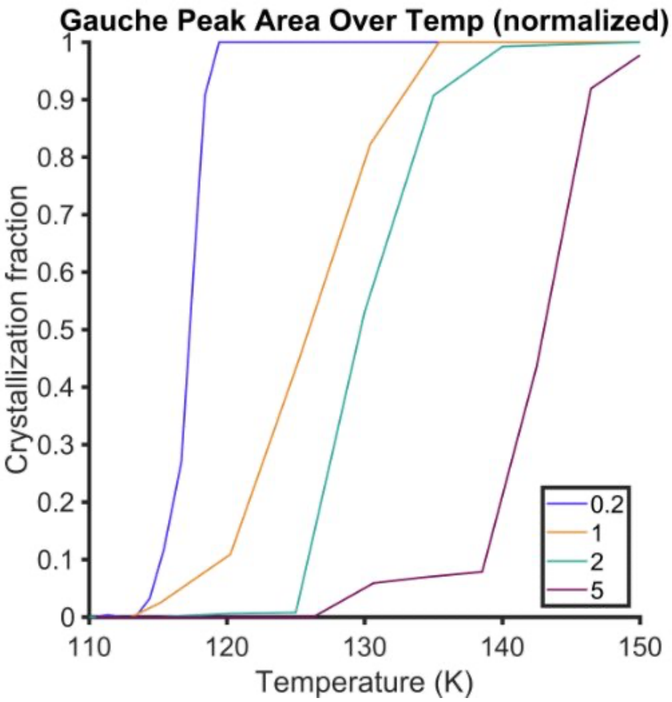

Fig. S4. Crystallization fraction of a pure n-PrCN ice normalized to the *gauche* peak at different ramping rates, 0.2 K/min, 1 K/min, 2 K/min, and 5 K/min over temperature.

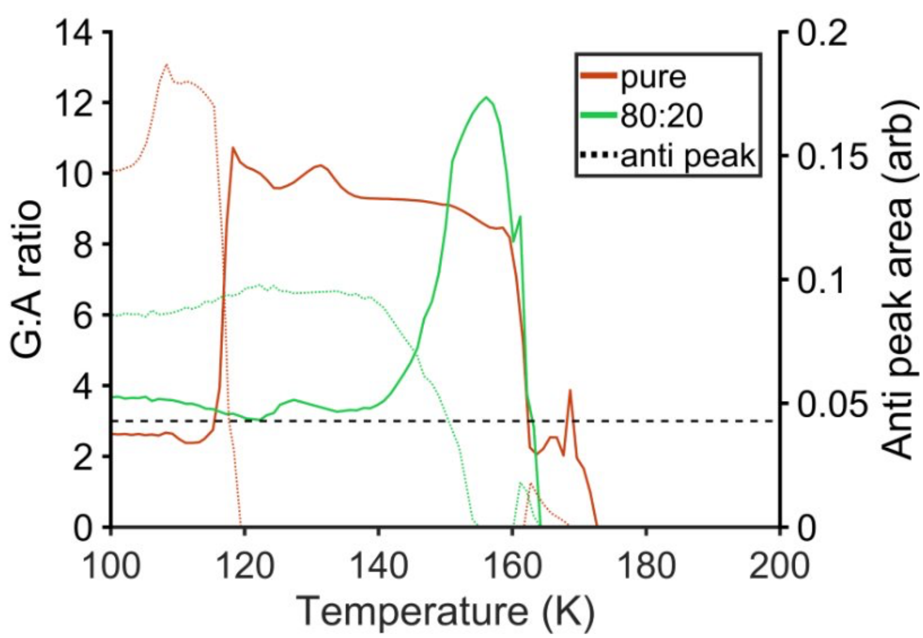

Fig. S5. *gauche:anti* ratio of a pure and 80:20 PrCN:Water mixed ice as the ice is ramped at 0.2 K/min. The dotted lines represent the *anti* peak area over temperature. The dashed line corresponds to a 300 K sample Boltzmann ratio of G:A = 3:1

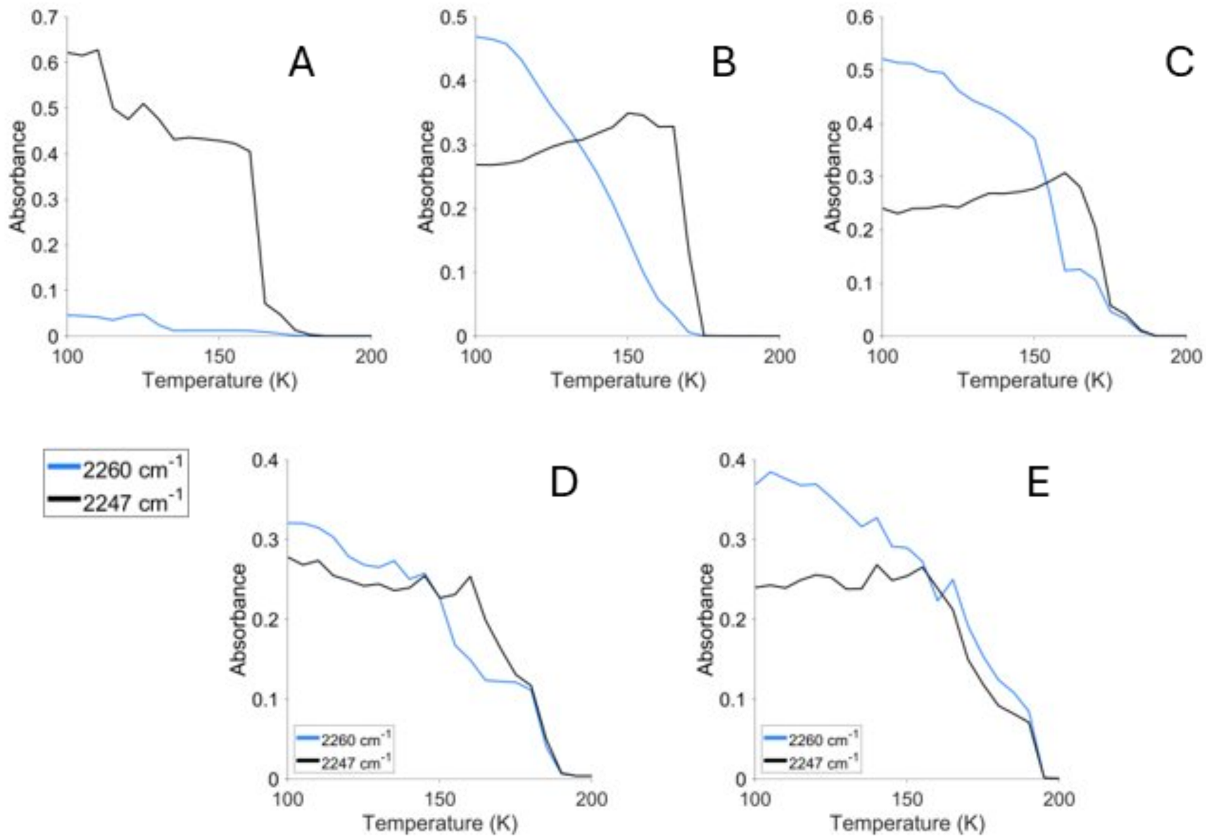

Fig. S6. RAIRS FTIR absorbance of the water-perturbed CN stretch frequency (2260 cm-1) and the pure CN stretch frequency (2247 cm-1) over the temperature region corresponding to crystallization and desorption. (A: pure, B: 80:20, C: 50:50, D: 25:75, E: 10:90)

Table S2. mm-wave transitions probed during TPD experiment as reported in the Cologne Database for Molecular Spectroscopy[1]

Species	Freq (GHz)	Intensity (18 K)	Rotational Transition	$S\mu^2$
anti	84.050	2.7389×10^{-4}	19 3 17 – 18 3 16	296.43
anti	84.073	2.7396×10^{-4}	19 3 16 – 18 3 15	296.41
gauche	84.122	7.2196×10^{-3}	14 6 9 – 13 6 8	244.841
gauche	84.124	7.2195×10^{-3}	14 6 8 – 13 6 7	244.79

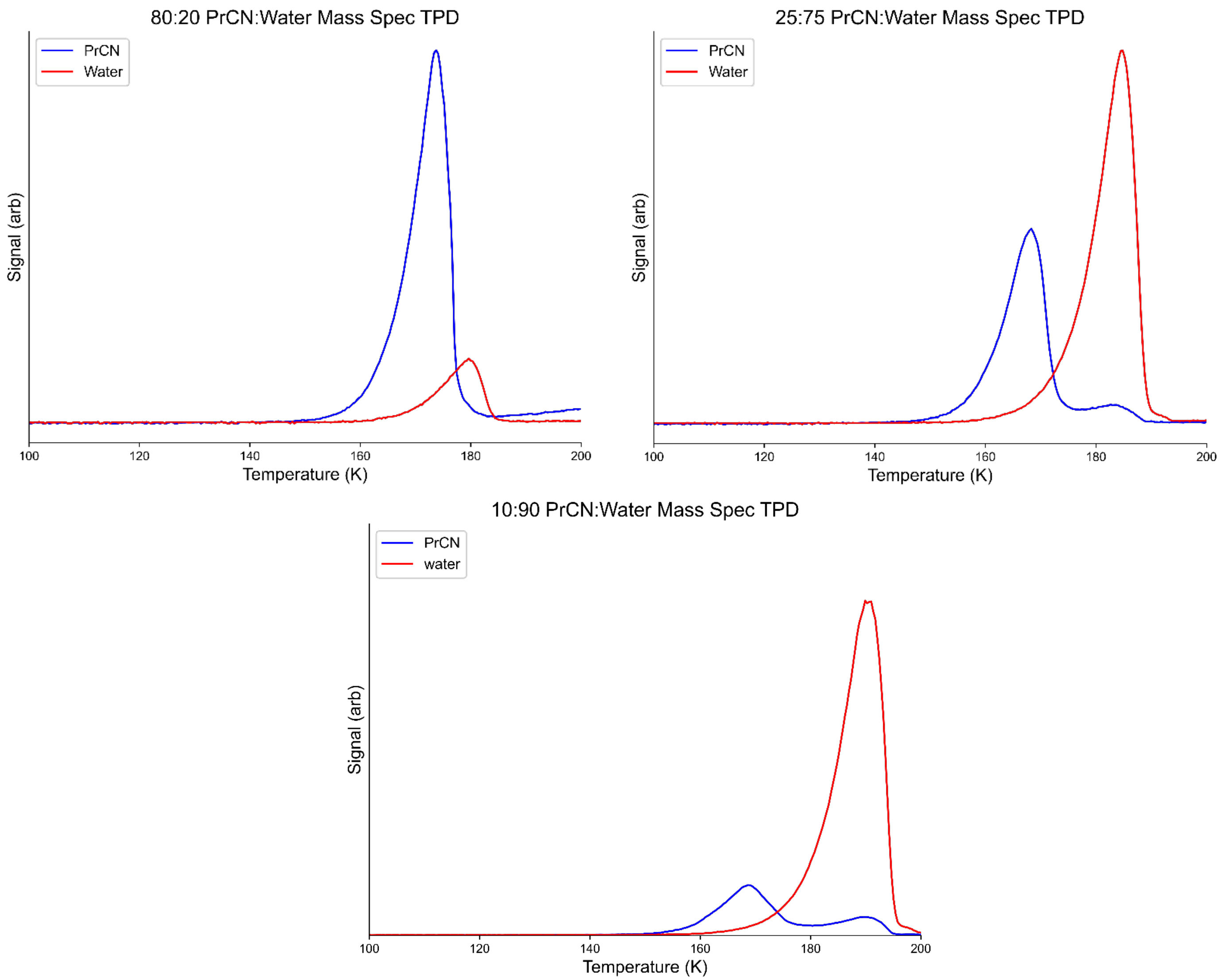

Fig. S7. Mass spectrometry TPD plots of an 80:20, 25:75, and 10:90 *n*-PrCN:Water mixed ice

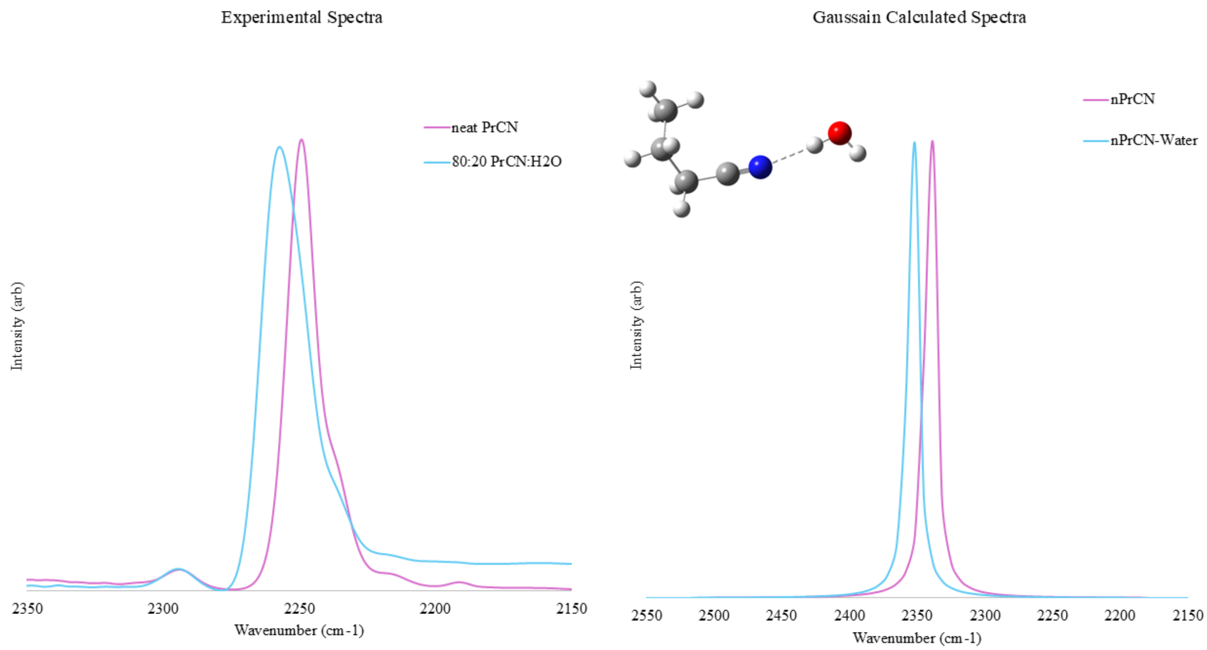

Fig. S8. CN-stretch band of neat and 80:20 *n*-PrCN:H_2O mixed ices. Experimental spectra (left) and Gaussian spectra computed at the B3LYP/aug-cc-pVDZ level of theory (right). Inset is the Gaussian optimized structure of *n*-PrCN- H_2O complex.

Table S3. Cartesian coordinates for *g*-PrCN with ωb97xd/6-311+G(d,p) level of theory with very tight optimization and quadratically convergent SCF

Element	X (Å)	Y (Å)	Z (Å)
C	-1.6136620	-0.8549580	0.1643350
C	-1.1220000	0.4777400	-0.3900550
H	-2.5473440	-1.1535530	-0.3168720
H	-0.8802720	-1.6479320	-0.0044850
H	-1.7966150	-0.7895510	1.2410760
C	0.1795440	0.9614820	0.2684970
H	-0.9670950	0.4025090	-1.4700880
H	-1.8772300	1.2527880	-0.2313970
H	0.4686520	1.9415920	-0.1198770
H	0.0425310	1.0689580	1.3490460
C	1.2949940	0.0429270	0.0464990
N	2.1605890	-0.6911380	-0.1404370

*No imaginary frequencies were found

Table S4. Cartesian coordinates for water with ωb97xd/6-311+G(d,p) level of theory with very tight optimization and quadratically convergent SCF

Element	X (Å)	Y (Å)	Z (Å)
O	0.0000000	0.0000000	0.1163160
H	0.0000000	0.7607400	-0.4652640
H	0.0000000	-0.7607400	-0.4652640

*No imaginary frequencies were found

Table S5. Cartesian coordinates for *g*-PrCN-water with ωb97xd/6-311+G(d,p) level of theory with very tight optimization and quadratically convergent SCF

Element	X (Å)	Y (Å)	Z (Å)
C	-1.9226530	1.4334630	-0.2501750
C	-2.1551080	0.1190190	0.4868780
H	-2.4889150	2.2420480	0.2162260
H	-0.8663760	1.7150710	-0.2373410
H	-2.2395490	1.3606570	-1.2947680
C	-1.4069050	-1.0671750	-0.1433390
H	-1.8531300	0.2140780	1.5335710
H	-3.2195790	-0.1312430	0.4854450
H	-1.6358720	-1.9969440	0.3838950
H	-1.7102390	-1.2008580	-1.1862960
C	0.0419520	-0.8849530	-0.1205790
N	1.1783410	-0.7188100	-0.0901320
O	3.8634760	0.6368190	0.1069580
H	4.5059270	-0.0631560	-0.0062160
H	3.0078210	0.1953510	0.0440370

*No imaginary frequencies were found

Table S6. Cartesian coordinates for *g*-PrCN-*g*-PrCN dimer with ωb97xd/6-311+G(d,p) level of theory with very tight optimization and quadratically convergent SCF

Element	X (Å)	Y (Å)	Z (Å)
C	-2.6040780	1.0884830	0.9453850
C	-3.1931180	0.0500610	-0.0038730
H	-3.3943420	1.5836900	1.5142270
H	-1.9181320	0.6234520	1.6593300
H	-2.0470060	1.8489320	0.3926090
C	-2.1293780	-0.6463540	-0.8677730
H	-3.7527740	-0.7038100	0.5578580
H	-3.9015150	0.5278170	-0.6865200
H	-2.5929920	-1.3529480	-1.5612940
H	-1.5760730	0.0926950	-1.4547730
C	-1.1532930	-1.3783310	-0.0650030
N	-0.3917680	-1.9447410	0.5859320
C	2.8994450	-1.1221930	-0.4997130
C	2.6035030	-0.3098280	0.7548820
H	3.0865580	-2.1662760	-0.2423020
H	2.0501610	-1.1025040	-1.1875640
H	3.7778260	-0.7371970	-1.0277090
C	2.3590130	1.1800150	0.4659580
H	1.7318390	-0.7278500	1.2626540
H	3.4455860	-0.3676930	1.4507500
H	2.1667180	1.7279150	1.3923510
H	3.2407690	1.6309790	-0.0006860
C	1.2264230	1.4093230	-0.4288530
N	0.3392360	1.5869910	-1.1395030

*No imaginary frequencies were found

Table S7. Electronic energies calculated for binding energy calculation

Element	Electronic Energy (Hartree)	Electronic energy +ZPE (Hartree)
g-PrCN	-211.367253	-211.263767
Water	-76.432257	-76.410574
g-PrCN-water	-287.808184	-287.680815
g-PrCN-*g*-PrCN	-422.745409	-422.537337

References

1. References cited in the SI have been listed in the article's reference list