ELECTRONIC SUPPORTING INFORMATION: The Role of Urea on the Solubility of Cellulose in Aqueous Quaternary Ammonium Hydroxide

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1 Two Phase Thermodynamic Method

The two-phase thermodynamic method (2PT)[1, 2] can be used to estimate entropy for MD simulations. This has been implemented successfully to estimate standard molar entropies and heat capacities of common liquid-phase solvents.[3] The following gives further details on how this method was implemented for this study. The velocity of each atom has translational, rotational, and vibrational modes:

$$v_i^{tot} = v_i^{trn} + v_i^{rot} + v_i^{vib} \tag{1}$$

Classical mechanics can be used to easily obtain v_i^{trn} and v_i^{rot}. The remainder, v_i^{vib}, can be found by subtracting the translational and rotational components from the total velocity. Each atom has a velocity autocorrelation function for each mode k:

$$c_i^k(t) = \lim_{t\to\infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} v_i^k(t'+t) v_i^k(t) dt' \tag{2}$$

with correlation time t. The mass-weighted autocorrelation function is obtained for each mode. The DoS is found by applying a Fourier transform $\mathcal{F}$ and weighting:

$$f_{tot}^k(\nu) = \frac{2}{k_B T} \mathcal{F}\left[\sum_{i=1}^{N} m_i c_i^k(t)\right] \tag{3}$$

with Boltzmann's constant k_B, temperature T, number of total atoms N, and mass of atom i m_i. The fluidicity factor g_k for each mode is found:

$$\delta_k^{-4.5} g_k^{7.5} - 3\delta_k^{-3} g_k^5 - \frac{1}{2}\delta_k^{-1.5} g_k^{2.5} + g_k - 1 = 0 \tag{4}$$

$$\delta_k = \frac{2 f_{tot}^k(0)}{9N} \left(\frac{\pi k_B T}{m}\right)^{1/2} \left(\frac{N}{V}\right)^{1/3} \left(\frac{6}{\pi}\right)^{2/3} \tag{5}$$

with m total mass and V partial volume of component. The gas and solid components of the DoS are as follows:

$$f_g^k(\nu) = \frac{f_{tot}^k(0)}{\left(1 + \frac{f_{tot}^k(0)\pi\nu}{6 g_k N}\right)^{1/2}} \tag{6}$$

$$f_s^k(\nu) = f_{tot}^k(\nu) - f_g^k(\nu) \tag{7}$$

The gas component has translational mode weighting factor:

$$\hat{S}_g^{trans} = \frac{1}{3k_B}\left[\frac{5}{2} + \ln\left[\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\frac{V c_1}{N g_{trans}}\right] + c_2\right] \tag{8}$$

$$c_1 = \frac{1 + y + y^2 - y^3}{(1-y)^3} \tag{9}$$

$$c_2 = \frac{y(3y-4)}{(1-y)^2} \tag{10}$$

$$y = g_{trans}^{2.5}\delta_{trans}^{2.5} \tag{11}$$

with c_1 and c_2 compressibility factors from the Carnahan-Starling equation of state. The rotational mode weighting factor (rotational entropy of a polyatomic ideal gas) is:

$$\hat{S}_g^{rot} = \frac{1}{3k_B}\left[\ln\frac{\pi^{1/2}e^{3/2}}{\sigma}\left(\frac{T^3}{\Theta_A\Theta_B\Theta_C}\right)^{1/2}\right] \tag{12}$$

$$\Theta_j = \frac{h^2}{8\pi^2 I_j k_B} \tag{13}$$

$$I_j = \sum_{i=1}^{N} m_i d_i^2 \tag{14}$$

$$COM_j = \frac{1}{M}\sum_{i=1}^{N} m_i j_i \tag{15}$$

with σ rotational symmetry, Θ_j rotational temperature in the j direction, I_j principle moment of inertia in the j direction, d_i distance of atom i from the center of mass (COM), and j_i the j coordinate of atom i. There is no fluidicity factor for the gas-phase vibrational component. The solid component has harmonic oscillator weighting factor for all modes:

$$\hat{S}_s^k(\nu) = \frac{\beta h\nu}{e^{\beta h\nu} - 1} - \ln(1 - e^{-\beta h\nu}) \tag{16}$$

$$\beta = (k_B T)^{-1} \tag{17}$$

Integration is used to obtain the entropy for each mode in either of the phases:

$$\hat{S}_x^k = k_B \int_0^\infty \hat{S}_x^k(\nu) f_x^k(\nu) d\nu \tag{18}$$

with x the gas or solid component. The crystalline bundle and oligomer units were considered rigid rods with translation and rotation, and because the cellulose strands were tethered, these translational and rotational contributions were added to the entropy.

2 Statistical Measurement of Thermodynamic Properties

2.1 Statistical Measurements of a Given Composition and a Given State

The averages of the thermodynamic quantities and their uncertainties reported in the manuscript were calculated in the following manner. For a single simulation of a given composition j (e.g. TBAH with 60 wt% water and no urea) and a given state k (e.g. crystalline or dissociated) the thermodynamic quantity of interest, denoted generically as X, at a given moment in time i can be represented as $X_i^{j,k}$. These data were recorded once every 100 fs throughout the 10 ns production run equating with a total of 100 000 data points, denoted by N. The average value of that quantity is calculated as:

$$\langle X \rangle^{j,k} = \frac{1}{N} \sum_{i=1}^{N} X_i^{j,k}. \tag{19}$$

The instantaneous enthalpy $H_i^{j,k}$ is calculated as the sum of the instantaneous internal energy $H_i^{j,k}$ and the product of the instantaneous pressure $p_i^{j,k}$ and the instantaneous volume $V_i^{j,k}$

$$H_i^{j,k} = U_i^{j,k} + p_i^{j,k} V_i^{j,k}. \tag{20}$$

Due to the deterministic nature of the computations each of the above quantities were considered as exact measurements of the instantaneous state of the system. The standard deviation of the thermodynamic quantity of interest at a given composition and given state is calculated as

$$\sigma^{j,k}(X^{j,k}) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (X_i^{j,k} - \langle X \rangle^{j,k})^2}, \tag{21}$$

and the standard uncertainty of that thermodynamic quantity as

$$u_c^{j,k}(X^{j,k}) = \frac{\sigma^{j,k}(X^{j,k})}{\sqrt{N}}, \tag{22}$$

and the *relative* standard uncertainty as

$$u_{c,r}^{j,k}(X^{j,k}) = \frac{u_c^{j,k}(X^{j,k})}{|X^{j,k}|}. \tag{23}$$

The standard uncertainty is a measure of the standard deviation of the mean. Unless otherwise noted, this is the measure represented as the error bars throughout the figures of the main manuscript.

For a single simulation of a given composition j and a given state k the average Gibbs free energy is calculated as the combination of the average enthalpy, average temperature, and average entropy of that respective simulation

$$\langle G \rangle^{j,k} = \langle H \rangle^{j,k} - \langle T \rangle^{j,k} \langle S \rangle^{j,k}. \tag{24}$$

The standard uncertainty (u_c) is obtained through error propagation:

$$u_c^{j,k}(\langle T \rangle^{j,k} \langle S \rangle^{j,k}) = |\langle T \rangle^{j,k} \langle S \rangle^{j,k}| \sqrt{u_{c,r}^{j,k}(T^{j,k})^2 + u_{c,r}^{j,k}(S^{j,k})^2} \tag{25}$$

$$u_c^{j,k}(G^{j,k}) = \sqrt{u_c^{j,k}(H^{j,k})^2 + u_c^{j,k}(\langle T \rangle^{j,k} \langle S \rangle^{j,k})^2}. \tag{26}$$

2.2 Statistical Measurement of Thermodynamic Changes

The average change in the Gibbs free energy, enthalpy, energy, pairwise interaction energy, temperature, and entropy, denoted here generally as $\langle \Delta X \rangle$, at a given composition j is calculated as the difference between the dissociated (diss) and crystalline (crys) states:

$$\langle \Delta X \rangle^j = \langle X \rangle^{j,diss} - \langle X \rangle^{j,crys}, \tag{27}$$

and the standard uncertainty is estimated through the propagation of error

$$u_c^j((\Delta X)^j) = \sqrt{u_c^{j,diss}(\langle X \rangle^{j,diss})^2 + u_c^{j,crys}(\langle X \rangle^{j,crys})^2}. \tag{28}$$

3 Difference in the Change of the Pairwise Interaction Energy

The difference in the change of the pairwise interaction energy upon dissolution ($\Delta\Delta U_{pair}$), given in kcal/mol-AGU, between selected compositions. The interactions are grouped into five different resolutions. Interactions at the higher resolutions combine to form the merged cells at the lower resolutions. Abbreviations represent (CAT) cations, (HOX) hydroxide, (URE) urea, (HOH) water, (CEL) cellulose, (IL) ionic liquid, (MOL) molecular/IL mixture, (AQ) aqueous/molecular/IL mixture, and (TOTAL) all of the components. Colors indicate key changes that are (red) unfavorable, (blue) neutral, and (green) favorable.

Table S1: The difference in the change of the pairwise interaction energy upon dissolution ($\Delta\Delta U_{pair}$), given in kcal/mol-AGU, between TBAH with 40 wt% water and TBAH with 60 wt% water.

Ultra		Very-High		High		Medium		Low	
Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$
CAT-CAT	16.3	**IL-IL**	1.9	**MOL-MOL**	1.9	**AQ-AQ**	0.4	**TOTAL**	1.7
CAT-HOX	-34.5								
HOX-HOX	20.1								
CAT-URE	–	**IL-URE**	–						
HOX-URE	–								
URE-URE	–	**URE-URE**	–						
CAT-HOH	1.1	**IL-HOH**	-11.2	**MOL-HOH**	-11.2				
HOX-HOH	-12.3								
URE-HOH	–	**URE-HOH**	–						
HOH-HOH	9.7	**HOH-HOH**	9.7	**HOH-HOH**	9.7				
CAT-CEL	2.2	**IL-CEL**	11.6	**MOL-CEL**	11.6	**AQ-CEL**	2.3		
HOX-CEL	9.4								
URE-CEL	–	**URE-CEL**	–						
HOH-CEL	-9.3	**HOH-CEL**	-9.3	**HOH-CEL**	-9.3				
CEL-CEL	-1.0	**CEL-CEL**	-1.0	**CEL-CEL**	-1.0	**CEL-CEL**	-1.0		

Table S2: The difference in the change of the pairwise interaction energy upon dissolution ($\Delta\Delta U_{pair}$), given in kcal/mol-AGU, between TBAH with 60 wt% water/no urea and TBAH with 60 wt% water/33 wt% urea.

Ultra		Very-High		High		Medium		Low	
Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$
CAT-CAT	10.8	**IL-IL**	1.9	**MOL-MOL**	8.3	**AQ-AQ**	0.4	**TOTAL**	0.3
CAT-HOX	-21.6								
HOX-HOX	12.7								
CAT-URE	1.7	**IL-URE**	5.8						
HOX-URE	4.1								
URE-URE	0.6	**URE-URE**	0.6						
CAT-HOH	-2.7	**IL-HOH**	-16.5	**MOL-HOH**	-16.9				
HOX-HOH	-13.8								
URE-HOH	-0.4	**URE-HOH**	-0.4						
HOH-HOH	8.9	**HOH-HOH**	8.9	**HOH-HOH**	8.9				
CAT-CEL	2.6	**IL-CEL**	9.5	**MOL-CEL**	2.3	**AQ-CEL**	0.2		
HOX-CEL	6.9								
URE-CEL	-7.2	**URE-CEL**	-7.2						
HOH-CEL	-2.1	**HOH-CEL**	-2.1	**HOH-CEL**	-2.1				
CEL-CEL	-0.2	**CEL-CEL**	-0.2	**CEL-CEL**	-0.2	**CEL-CEL**	-0.2		

Table S3: The difference in the change of the pairwise interaction energy upon dissolution ($\Delta\Delta U_{pair}$), given in kcal/mol-AGU, between TBAH with 40 wt% water/33 wt%urea and TBAH with 40 wt% water/40 wt%urea.

Ultra		Very-High		High		Medium		Low	
Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$	Interaction	$\Delta\Delta U_{pair}$
CAT-CAT	4.9	**IL-IL**	-4.7	**MOL-MOL**	-3.0	**AQ-AQ**	1.4	**TOTAL**	1.3
CAT-HOX	-11.4								
HOX-HOX	1.8								
CAT-URE	0.8	**IL-URE**	0.8						
HOX-URE	0.0								
URE-URE	0.9	**URE-URE**	0.9						
CAT-HOH	0.4	**IL-HOH**	9.0	**MOL-HOH**	6.7				
HOX-HOH	8.6								
URE-HOH	-2.2	**URE-HOH**	-2.2						
HOH-HOH	-2.3	**HOH-HOH**	-2.3	**HOH-HOH**	-2.3				
CAT-CEL	1.0	**IL-CEL**	0.8	**MOL-CEL**	0.1	**AQ-CEL**	-0.1		
HOX-CEL	-0.2								
URE-CEL	-0.7	**URE-CEL**	-0.7						
HOH-CEL	-0.2	**HOH-CEL**	-0.2	**HOH-CEL**	-0.2				
CEL-CEL	-0.1	**CEL-CEL**	-0.1	**CEL-CEL**	-0.1	**CEL-CEL**	-0.1		

4 Changes in Hydrogen Bonding upon Dissolution

Table S4: Breakdown in hydrogen bonds for (top) 40 wt% water and 0wt% urea, (middle) 40 wt% water and 33wt% urea, and (bottom) 40 wt% water and 55wt% urea. Columns in gray represent numbers for the dissolved state and columns in white represent numbers for the crystalline state.

Pair	Per AGU	u_c	Per AGU	u_c	Per IL	u_c	Per IL	u_c	Per HOH	u_c	Per HOH	u_c	Per URE	u_c	Per URE	u_c
CEL-CEL	1.279	±0.004	0.313	±0.003	0.3789	±0.0012	0.0928	±0.0007	0.03947	±0.00013	0.009670732	±0.00008	–	–	–	–
CEL-HOX	0.1608	±0.0010	1.393	±0.003	0.0476	±0.0003	0.4128	±0.0009	0.004962787	±0.00003	0.042994194	±0.00009	–	–	–	–
CEL-HOH	0.5936	±0.0018	1.952	±0.004	0.1759	±0.0005	0.5784	±0.0011	0.018320929	±0.00006	0.06024	±0.00011	–	–	–	–
CEL-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
HOX-HOH	18.095	±0.006	16.750	±0.006	5.3616	±0.0017	4.9631	±0.0018	0.55845	±0.00018	0.51694	±0.00018	–	–	–	–
HOX-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
HOH-HOH	28.23	±0.02	27.99	±0.02	8.363	±0.006	8.293	±0.006	0.8711	±0.0007	0.8638	±0.0007	–	–	–	–
HOH-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
URE-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
TOTAL	48.35	±0.02	48.40	±0.02	14.327	±0.007	14.340	±0.007	1.4923	±0.0007	1.4936	±0.0007	–	–	–	–

Pair	Per AGU	u_c	Per AGU	u_c	Per IL	u_c	Per IL	u_c	Per HOH	u_c	Per HOH	u_c	Per URE	u_c	Per URE	u_c
CEL-CEL	1.248	±0.004	0.205	±0.002	0.4438	±0.0014	0.0728	±0.0007	0.04623	±0.00015	0.00758	±0.00007	0.3083	±0.0010	0.0506	±0.0005
CEL-HOX	0.1518	±0.0004	0.930	±0.003	0.05397	±0.00015	0.3306	±0.0010	0.00562	±0.00002	0.03444	±0.00010	0.03749	±0.00010	0.2296	±0.0007
CEL-HOH	0.595	±0.002	1.980	±0.004	0.2117	±0.0006	0.7039	±0.0013	0.02205	±0.00006	0.07332	±0.00014	0.1471	±0.0004	0.4890	±0.0009
CEL-URE	0.1851	±0.0010	0.798	±0.002	0.0658	±0.0003	0.2837	±0.0007	0.00686	±0.00004	0.02955	±0.00007	0.0457	±0.0002	0.1971	±0.0005
HOX-HOH	12.461	±0.006	11.820	±0.006	4.4306	±0.0022	4.2027	±0.0022	0.4615	±0.0002	0.4378	±0.0002	3.0779	±0.0015	2.9195	±0.0015
HOX-URE	2.852	±0.006	2.752	±0.004	1.0142	±0.0021	0.9787	±0.0015	0.1056	±0.0002	0.10194	±0.00016	0.7045	±0.0015	0.6799	±0.0011
HOH-HOH	21.943	±0.020	21.419	±0.019	7.8018	±0.0069	7.6158	±0.0069	0.8127	±0.0007	0.7933	±0.0007	5.4198	±0.0048	5.2906	±0.0048
HOH-URE	8.731	±0.009	8.768	±0.007	3.1042	±0.0032	3.1175	±0.0026	0.3234	±0.0003	0.3247	±0.0003	2.1564	±0.0023	2.1657	±0.0018
URE-URE	2.525	±0.007	2.107	±0.008	0.8977	±0.0023	0.7493	±0.0028	0.0935	±0.0002	0.0780	±0.0003	0.6236	±0.0016	0.5205	±0.0020
TOTAL	50.69	±0.05	50.78	±0.02	18.024	±0.009	18.055	±0.009	1.8775	±0.0009	1.8807	±0.0009	12.521	±0.006	12.542	±0.006

Pair	Per AGU	u_c	Per AGU	u_c	Per IL	u_c	Per IL	u_c	Per HOH	u_c	Per HOH	u_c	Per URE	u_c	Per URE	u_c
CEL-CEL	1.067	±0.008	0.150	±0.002	0.468	±0.004	0.0657	±0.0007	0.0488	±0.0004	0.00684	±0.00007	0.1351	±0.0010	0.0189	±0.0002
CEL-HOX	0.1694	±0.0006	0.644	±0.002	0.0744	±0.0003	0.2826	±0.0010	0.00775	±0.00003	0.02944	±0.00011	0.02145	±0.00007	0.0815	±0.0003
CEL-HOH	0.529	±0.002	1.790	±0.003	0.2322	±0.0007	0.7859	±0.0013	0.02419	±0.00008	0.08186	±0.00013	0.0670	±0.0002	0.2267	±0.0004
CEL-URE	0.2695	±0.0013	1.407	±0.003	0.1183	±0.0006	0.6175	±0.0013	0.01232	±0.00006	0.06432	±0.00014	0.0341	±0.0002	0.1781	±0.0004
HOX-HOH	8.656	±0.005	7.944	±0.006	3.800	±0.002	3.488	±0.002	0.3958	±0.0002	0.3633	±0.0003	1.0963	±0.0007	1.0061	±0.0007
HOX-URE	4.189	±0.005	4.148	±0.007	1.839	±0.002	1.821	±0.003	0.1915	±0.0003	0.1897	±0.0003	0.5305	±0.0007	0.5253	±0.0009
HOH-HOH	15.671	±0.016	15.270	±0.018	6.880	±0.007	6.704	±0.008	0.7166	±0.0007	0.6983	±0.0008	1.985	±0.002	1.934	±0.002
HOH-URE	15.506	±0.014	14.965	±0.011	6.807	±0.006	6.570	±0.005	0.7091	±0.0006	0.6843	±0.0005	1.964	±0.002	1.8953	±0.0014
URE-URE	7.258	±0.011	6.590	±0.012	3.186	±0.005	2.893	±0.005	0.3319	±0.0005	0.3014	±0.0005	0.9192	±0.0014	0.8346	±0.0015
TOTAL	53.31	±0.06	52.9069	±0.0259	23.406	±0.012	23.227	±0.011	2.4380	±0.0012	2.4194	±0.0012	6.752	±0.003	6.7006	±0.0033

Table S5: Breakdown in hydrogen bonds for (top) 60 wt% water and 0wt% urea, (middle) 60 wt% water and 33wt% urea, and (bottom) 60 wt% water and 55wt% urea. Columns in gray represent numbers for the dissolved state and columns in white represent numbers for the crystalline state.

Pair	Per AGU	u_c	Per AGU	u_c	Per IL	u_c	Per IL	u_c	Per HOH	u_c	Per HOH	u_c	Per URE	u_c	Per URE	u_c
CEL-CEL	0.827	±0.005	0.1926	±0.0018	0.367	±0.002	0.0856	±0.0008	0.01701	±0.00010	0.00396	±0.00004	–	–	–	–
CEL-HOX	0.1481	±0.0007	1.022	±0.004	0.0658	±0.0003	0.4544	±0.0018	0.003046	±0.000014	0.02103	±0.00008	–	–	–	–
CEL-HOH	0.938	±0.002	3.031	±0.004	0.4170	±0.0011	1.3470	±0.0019	0.01930	±0.00005	0.06235	±0.00009	–	–	–	–
CEL-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
HOX-HOH	12.444	±0.006	11.509	±0.007	5.531	±0.002	5.115	±0.003	0.25602	±0.00011	0.23679	±0.00014	–	–	–	–
HOX-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
HOH-HOH	55.84	±0.03	54.61	±0.03	24.819	±0.015	24.271	±0.014	1.1489	±0.0007	1.1235	±0.0006	–	–	–	–
HOH-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
URE-URE	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
TOTAL	70.20	±0.03	70.36	±0.03	31.20	±0.02	31.273	±0.015	1.4443	±0.0007	1.4477	±0.0007	–	–	–	–

Pair	Per AGU	u_c	Per AGU	u_c	Per IL	u_c	Per IL	u_c	Per HOH	u_c	Per HOH	u_c	Per URE	u_c	Per URE	u_c
CEL-CEL	0.849	±0.006	0.1406	±0.0017	0.491	±0.004	0.0813	±0.0010	0.0227	±0.0002	0.00376	±0.00004	0.1515	±0.0011	0.0251	±0.0003
CEL-HOX	0.0776	±0.0007	0.692	±0.003	0.0448	±0.0004	0.3999	±0.0015	0.00207	±0.00002	0.01850	±0.00007	0.01384	±0.00012	0.1234	±0.0005
CEL-HOH	0.709	±0.002	2.570	±0.004	0.4101	±0.0013	1.486	±0.002	0.01896	±0.00006	0.06875	±0.00011	0.1265	±0.0004	0.4587	±0.0007
CEL-URE	0.4122	±0.0018	1.009	±0.003	0.2384	±0.0010	0.5834	±0.0019	0.01102	±0.00005	0.02698	±0.00009	0.0735	±0.0003	0.1800	±0.0006
HOX-HOH	8.341	±0.006	7.778	±0.005	4.824	±0.004	4.498	±0.003	0.2231	±0.0002	0.20803	±0.00014	1.4884	±0.0011	1.3879	±0.0009
HOX-URE	1.375	±0.005	1.281	±0.004	0.795	±0.003	0.741	±0.002	0.03677	±0.00012	0.03427	±0.00011	0.2453	±0.0008	0.2287	±0.0007
HOH-HOH	37.31	±0.03	36.00	±0.03	21.576	±0.015	20.817	±0.016	0.9979	±0.0007	0.9627	±0.0007	6.6574	±0.0045	6.4229	±0.0048
HOH-URE	15.794	±0.011	15.335	±0.011	9.134	±0.006	8.869	±0.006	0.4224	±0.0003	0.4102	±0.0003	2.8183	±0.0020	2.7364	±0.0020
URE-URE	3.670	±0.010	3.491	±0.009	2.122	±0.006	2.019	±0.005	0.0982	±0.0003	0.0934	±0.0002	0.6549	±0.0018	0.6230	±0.0015
TOTAL	68.54	±0.07	68.29	±0.03	39.636	±0.018	39.494	±0.018	1.8331	±0.0008	1.8265	±0.0008	12.230	±0.006	12.186	±0.006

Pair	Per AGU	u_c	Per AGU	u_c	Per IL	u_c	Per IL	u_c	Per HOH	u_c	Per HOH	u_c	Per URE	u_c	Per URE	u_c
CEL-CEL	1.123	±0.004	0.0978	±0.0014	0.860	±0.003	0.0749	±0.0011	0.03980	±0.00013	0.00347	±0.00005	0.1102	±0.0004	0.00959	±0.00014
CEL-HOX	0.0227	±0.0004	0.458	±0.002	0.0174	±0.0003	0.351	±0.002	0.000805	±0.000013	0.01622	±0.00008	0.00223	±0.00004	0.0449	±0.0002
CEL-HOH	0.590	±0.003	2.039	±0.005	0.452	±0.002	1.562	±0.003	0.02090	±0.00010	0.0723	±0.0002	0.0579	±0.0003	0.2000	±0.0004
CEL-URE	0.569	±0.002	1.932	±0.004	0.436	±0.002	1.480	±0.003	0.02017	±0.00009	0.06849	±0.00015	0.0558	±0.0002	0.1896	±0.0004
HOX-HOH	5.441	±0.005	5.105	±0.005	4.167	±0.004	3.910	±0.004	0.1928	±0.0002	0.1809	±0.0002	0.5337	±0.0005	0.5008	±0.0005
HOX-URE	2.170	±0.005	1.895	±0.005	1.662	±0.004	1.451	±0.004	0.0769	±0.0002	0.0671	±0.0002	0.2128	±0.0005	0.1858	±0.0005
HOH-HOH	23.270	±0.021	22.410	±0.020	17.824	±0.016	17.165	±0.016	0.8247	±0.0007	0.7943	±0.0007	2.283	±0.002	2.198	±0.002
HOH-URE	23.266	±0.014	22.354	±0.014	17.821	±0.011	17.122	±0.011	0.8246	±0.0005	0.7923	±0.0005	2.2822	±0.0014	2.1928	±0.0014
URE-URE	10.373	±0.014	9.893	±0.014	7.945	±0.011	7.578	±0.010	0.3676	±0.0005	0.3506	±0.0005	1.0175	±0.0014	0.9704	±0.0013
TOTAL	66.82	±0.07	66.1839	±0.0299	51.184	±0.023	50.694	±0.023	2.3684	±0.0011	2.3457	±0.0011	6.555	±0.003	6.4922	±0.0029

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