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The effective volumes of waters of crystallization: general organic solids

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Supplementary Information

The Effective Volumes of Waters of Crystallization: General Organic Solids

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3 Figures ~2 000 words

Supplementary Tables S1 and S2, Figure S1

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Table S1: Asymmetric-unit volumes, V_m/Å^3, as a function of temperature, T/K, for the anhydrates (CSD refcodes PUBMUU*mn*) and hydrate (CSD refcodes PUBMII*mn*) of hexanitro-azaisowurtzitane (HNIW, $C_6H_6N_{12}O_{12}$). The data is sorted by temperature, and then by asymmetric-unit volume.

$C_6H_6N_{12}O_{12}$	V_m/Å^3	T/K	Polymorph
Anhydrate			$Pb2_1a$
PUBMUU24	365.981	0 (?)	β
PUBMUU03	366.435	298	β
PUBMUU01	366.495	298	β
			$P2_1/n$
PUBMUU25	348.829	100	(ε)
PUBMUU12	349.312	100	ε
PUBMUU13	350.420	150	ε
PUBMUU14	353.001	200	ε
PUBMUU15	355.010	250	ε
PUBMUU20	352.708	298	ε
PUBMUU02	356.036	298	ε
PUBMUU17	356.742	298	ε
PUBMUU19	356.781	298	ε
PUBMUU21	357.122	298	ε
PUBMUU18	357.217	298	ε
PUBMUU16	357.559	298	ε
PUBMUU05	358.005	298	ε
PUBMUU20a	356.326	383	ε
			$P2_1/n$
PUBMUU07	372.488	100	γ
PUBMUU08	375.695	150	γ
PUBMUU09	375.437	200	γ
PUBMUU10	377.336	250	γ
PUBMUU04	377.825	298	γ
PUBMUU06	379.352	298	γ
PUBMUU	379.721	298	γ
PUBMUU11	379.997	298	γ
			$P2_1/n$
PUBMUU23	319.774	298	ζ
Hydrate 0.25H_2O			Pbca
PUBMII02	363.889	86	α
PUBMII	371.190	298	α
PUBMII01	373.159	298	α

Table S2: Asymmetric-unit volumes, V_m/Å^3, of hydrate and anhydrate pairs with the temperatures of their determination, number of waters of crystallization per hydrate, $n(H_2O)$, and effective volume per water of crystallization corrected to 298 K, $V_m(H_2O)$, using a generic volumetric coefficient of thermal expansion of 147 × 10^{-6} K^{-1}. The CSD Refcodes appear in the final two columns. The data is sorted by the values of $V_m(H_2O)$, smallest to largest, with the most egregious outlier values listed in red italics. A value for t-butanol have been added to those from the source list.[1]

V_m(hydrate)	T_{hydr}/K	n(H_2O)	V_m(an)	T_{anhydr}/K	$V_m(H_2O)$	Hydrate	Anhydrate
461.353	*298*	*0.23*	*460.896*	*105*	*-54.87*	*LEZKAC*	*FIQFER*
638.913	*233*	*1*	*664.662*	*233*	*-26.00*	*PEGVEC*	*PEGVAY*
823.370	*173*	*0.5*	*842.710*	*298*	*-8.42*	*RAVBUL*	*NAFMEM*
554.318	*298*	*0.32*	*556.444*	*298*	*-6.64*	*BUJJIZ*	*DADMOK*
655.425	*298*	*2*	*663.342*	*250*	*-6.30*	*MAXVIQ*	*VIQJEK*
475.978	*298*	*1*	*480.125*	*298*	*-4.15*	*SURRIG*	*SURREC*
465.466	*298*	*1*	*469.446*	*298*	*-3.98*	*QOBJEW*	*QOBJAS*
528.420	*298*	*1*	*530.227*	*298*	*-1.81*	*VAXDUT*	*DEMYEZ01*
266.995	298	3	249.316	150	4.08	MEPYRZ	MPYRAZ02
438.804	298	0.5	436.579	298	4.45	HEPNAR	HEPMUK
477.198	298	1	472.046	298	5.15	AMEQAK	AMEPOX
597.687	298	2	585.637	298	6.03	HEVKOI	ZECRUU
254.983	298	1	243.920	173	6.58	SUNGUD	SUNGOX
233.112	298	1	226.450	298	6.66	BOPQAY	COFDUW10
658.867	298	1	652.043	298	6.82	GAJMIN	GAJMOT
402.002	298	0.5	398.390	298	7.22	PANYLB	ANPYAB
282.256	110	1	282.785	298	7.27	IJESIZ	IJESAR
235.547	298	0.67	229.780	298	8.61	BOCNIQ	TICYOT
258.228	298	2	240.786	298	8.72	FONHEW	BTCOAC
274.149	298	1	259.698	173	9.68	PHOLCL	CUZDIK
300.918	298	1	290.447	298	10.47	THMPIM10	IMOXSF
266.877	298	1	252.334	220	11.65	QIHSIJ	CAWKEQ
512.151	298	0.25	509.148	298	12.01	YILKUZ	SEBROG
260.964	298	0.5	254.320	298	13.29	VEBREZ	GEYRAD
576.815	298	4	522.751	298	13.52	JATDUD	JATFAL
485.680	298	1	472.016	298	13.66	EVODOI	EVODUO
385.307	298	2	357.161	298	14.07	CYSTIN10	CYSTBR01
380.782	298	0.5	363.017	100	14.40	JEDTOB	TPEPHO03
563.769	298	1	549.009	298	14.76	DEPDEH	DEPDAD
359.269	298	1.5	336.464	298	15.20	FIXPEH	BODSES
281.055	298	1	265.849	298	15.21	VAMCAO	VAMBUH
690.726	298	1	675.383	298	15.34	BUDTUP	BUDTOJ
250.914	298	1	235.391	298	15.52	HECMUX	VUNYUY10

349.691	150	2	318.937	150	15.71	RALDEN01	XEHKOK
119.361	298	0.5	111.332	298	16.06	AHOXLH	MOYHAJ
300.285	298	1	284.188	298	16.10	PHBARM	PHBARB06
160.975	298	1	144.344	298	16.63	NURAMH	NIMFOE
231.072	113	0.5	222.030	86	16.81	TRMHXD	DMHXDM
422.832	205	2	389.264	205	17.01	WAFPAV	WAFNUN
268.111	298	0.5	259.546	298	17.13	BAJGUO	NASQAZ
420.262	298	1	400.886	263	17.31	THIAMC12	UNEXOA
177.728	298	0.5	166.767	205	17.36	ZZZSBA01	HUYBUY
659.486	298	1	642.002	298	17.48	HAJWAR	HAJWIZ
173.797	298	1.5	142.966	82	17.53	POTPET	GLYGLY04
594.912	298	0.16	592.072	298	17.75	DOBLOV	CUVHAC01
222.377	298	0.5	213.432	298	17.89	QUINCX	QUINCB10
424.741	150	2	389.159	150	18.18	BAFDUI	BAFFAQ
685.917	298	1	667.578	298	18.34	MEYRAJ	MEYQUC
640.270	298	1	621.922	298	18.35	QAMCEN	QAMCAJ
212.032	95	4	142.724	298	18.91	TFMSTH	TFMSUL02
499.114	298	1	480.134	298	18.98	CIZWEN	DAMVIX
371.190	298	0.25	366.435	298	19.02	PUBMII	PUBMUU03
262.519	298	1	243.208	298	19.31	ARGHCL10	LARGIN02
466.700	298	2	421.175	193	19.51	FELCIJ	FELCOP
653.262	298	1	633.545	298	19.72	HOXGEG	HOXGIK
277.310	150	1	257.770	150	19.97	BAFFIY	BAFFOE
202.000	123	2	167.140	298	20.03	PYZDCX01	IYAWAG
308.449	298	1	288.257	298	20.19	BAFPAZ	CALDEY
337.336	298	1	317.104	298	20.23	CIMGUA	CIMETD01
265.613	298	1.5	235.159	298	20.30	RIKBIW	RIKBOC
483.137	298	2	440.930	298	21.10	TUTECD01	THUTEC01
433.661	298	2	391.293	298	21.18	MITCDH01	MITOMC
253.115	298	2	210.225	298	21.45	DILFAF01	FIFGOQ
306.850	233	1	285.541	236	21.64	JEPJOD	BOBZAC02
379.479	298	1	357.370	298	22.11	BIMYEB	BIMYAX
165.710	298	2	117.865	100	22.21	ZAHJIB	CYURAC12
343.548	298	1	321.084	298	22.46	TEJMIE	LETBER
323.492	263	1	302.678	298	22.48	CETMPA01	CLEOZP01
617.697	253	4	528.587	263	22.62	NURJEP01	NURHOX
606.444	298	1	571.590	153	22.67	CUWKAG	CUWJUZ
248.656	298	0.5	233.777	200	23.02	YOYPIL	EGORIB
177.867	298	2	131.781	298	23.04	BARBAD01	BARBAC01
366.670	298	1	337.287	173	23.19	HILMEU	XOMMER
281.684	123	4	195.851	298	23.27	NUYRAA	YAMSAG
190.903	298	1	164.625	178	23.37	MSULIM	POMDAW01
395.986	298	1	370.666	263	23.41	FIMVOM	FESRIE
623.469	298	1	599.979	298	23.49	UJOQUF	KAMPIY

430.384	298	1	406.874	298	23.51	TESTOM	TESTON10
215.337	298	1	191.480	298	23.86	GLUCMH11	GLUCSA10
502.463	298	1	478.415	298	24.05	QIJZUE	RORQEU01
138.036	123	0.5	126.313	123	24.05	RABBUN	NAGVUM
630.626	153	5	523.778	298	24.06	BEQWID	LEWBOE
403.082	298	1	378.994	298	24.09	ZZZTZQ01	ZZZTSE01
184.578	123	3	114.235	130	24.09	GIXDIA	QATVUC
229.521	298	1	205.425	298	24.10	WIKDAV	MUMBEL
138.545	298	1	110.869	100	24.45	LSERMH10	LSERIN20
213.339	298	1	188.815	298	24.52	SULAMH10	SULAMD04
433.921	298	1	409.255	298	24.67	COVMEF	BARWUM01
490.930	298	1.5	453.914	298	24.68	QIDCIP	WIQMUE
327.372	298	1	302.502	298	24.87	NOGKID	NOGKEZ
328.769	298	1	303.895	298	24.87	PAKOJM	PAYKOJ
416.433	298	1	391.471	298	24.96	SOHLAC	KOUMIN
267.457	298	4	164.458	173	24.99	HOMPRO10	QAMVAB
128.544	298	2	78.433	298	25.06	OXACDH28	OXALAC04
222.282	298	0.25	215.995	298	25.15	IBUXIN	UJEMEB
267.227	298	2	216.917	298	25.16	HOSHEC	NANRAV
169.880	298	1	144.700	298	25.18	VEXRUL	VEXREV
356.072	298	1.5	318.253	298	25.21	FAYVUW	FAYVOQ
451.656	110	6	303.548	115	25.40	PUHPOX	BOBHOP
138.947	123	2	89.329	130	25.49	GIXDAS	ETDIAM01
188.397	223	3	111.514	153	25.53	PYRTHA10	PYRDNA01
164.298	298	1	138.742	298	25.56	TARTDL01	ZZZDUI01
300.262	298	2	249.117	298	25.57	PYMDSD	PYMSUL10
178.544	298	1	152.903	298	25.64	KICCOO	WEMWEQ
751.879	298	3	674.729	298	25.72	CAMTOA01	GUCJAP
245.987	298	1	219.891	298	26.10	BANAPQ10	BANAQP10
255.171	298	1	228.927	298	26.24	KOJGUL	GOWZEX
404.124	298	1	377.771	298	26.35	LAKTUM	GULTIQ
339.125	298	2	286.272	298	26.43	FEDBUL	FEDBOF
222.968	173	1	200.345	298	26.72	THEOPH01	BAPLOT01
240.051	173	2	190.916	298	26.77	MAHDOP	LACJEE
433.323	298	1	406.533	298	26.79	GOWCAW	GOWBOJ
943.713	100	7	780.041	298	27.31	DAFNOO	RIZGEM
162.061	298	1	134.719	298	27.34	IJEQET	LASPRT
556.954	123	8	342.306	100	27.38	REGREA	HOXOCD02
318.952	123	7	132.389	220	27.61	LEBKEI	McGregor, 2006[2]
387.837	298	1	360.089	298	27.75	LACTOS03	EYOCUQ01
189.609	298	1	161.815	298	27.79	LEZJEF	LEZJAB01
387.266	298	1	352.736	170	27.89	VALMOL	BERYAZ
320.919	298	1	292.974	298	27.95	IKUROV	IKURUB
298.771	298	4	186.042	298	28.18	BEWYAE	IYAXAH

261.105	105	2	212.141	298	28.19	SEFSOL	VAYJIO
246.944	298	1	218.736	298	28.21	RUWKEZ	RUWKAV
301.241	298	1	272.968	298	28.27	DUHKEW	BURLOP
519.628	298	1	491.177	298	28.45	SATSEL	DURDAV
449.947	298	3	364.543	298	28.47	SUGBIF	YADSOL
420.430	298	0.25	413.302	298	28.51	ZOYMUV	ZOYMOP
318.514	298	1.5	275.652	298	28.57	THIRDN10	BELZEX
706.274	298	4	591.965	298	28.58	SUMMOC	SUMMIW
337.404	298	1	308.788	298	28.62	ZOZVUF	WISGEK
427.411	298	2	369.187	298	29.11	CIZQAD01	MENMIB01
138.149	193	1	108.812	173	29.47	DIPMUK	NILYAI
415.591	173	2	357.679	173	29.49	SUPKET	SUPKIX
234.637	298	1	205.109	298	29.53	RUVPUT	RUVPON
238.085	298	0.5	223.236	298	29.70	RAVZOD	RAVZIX
189.445	298	1	165.587	543	29.82	YEJNEG	QAMXUY
425.088	298	1	395.229	298	29.86	VUXGAW	DORMOM
148.110	298	1	117.846	298	30.26	JIYWET	JOWWIB
245.713	143	1	217.034	173	30.29	POSTAS	POSTEW01
122.693	210	1	91.067	83	30.33	BULMAW10	TFACET
469.652	198	2.5	400.218	298	30.54	AQOMEY	UNOGIN
259.588	298	1	229.026	298	30.56	ZZZAMS04	OPENAN
256.298	153	1	226.293	153	30.64	QIMKOM	QIMKIG
632.803	298	2	570.917	298	30.94	ETUTEC	ZZZEII01
313.850	298	1	274.159	90	31.31	RAWBIA	RAWBEW01
270.767	298	1	239.415	298	31.35	HAXBUD	LABJON
322.807	298	1	291.106	298	31.70	NOJWAK	NOJVUD
367.405	298	4	237.412	213	31.76	EACLTH10	HIVROT
229.703	298	1	197.869	298	31.83	PUVMAU	SAQJEZ
306.633	298	0.33	296.123	298	31.85	ANSFON01	DAPSUO05
531.019	298	1	499.130	298	31.89	TOHGIG	OMIXUD
721.941	123	2	659.133	124	32.26	HAKDUT	HAKDON
191.794	298	1	159.302	298	32.49	SAJRUQ	SAJQUP
342.780	298	2	277.440	298	32.67	AZTHPN	CIPWUT
422.043	298	1	389.372	298	32.67	GAFVIS	VUXBAR
187.516	298	1	153.335	298	34.18	CADVUY	YUYMOU
268.428	298	1	227.446	130	35.36	SOWSIG	QATWUD
378.339	298	1	337.026	193	36.11	IVUQIZ	IVUQOF
476.836	298	1	440.523	298	36.31	AMEVET	AMEVAP
221.002	100	0.67	202.775	298	36.81	HIPKAS	GLUCIT03
508.288	298	1	471.403	298	36.89	CAZWAB	CAZWEF
261.205	150	3	155.470	298	37.14	XOMWOL	HXACAN12
461.522	298	1	424.128	298	37.39	QIQLUX	QIQLIL
218.083	298	0.5	199.367	298	37.43	RATBOD	RATBIX
578.184	298	1	540.728	298	37.46	GESKUK	GESKOE

253.092	100	1	222.702	298	37.76	EDOKOX	RIZFEL
387.886	298	1	349.488	298	38.40	THIMCH10	GEYXOX
323.077	200	1	289.244	298	38.49	WUTVIQ	RENCUI
343.921	298	1	305.122	298	38.80	CAKFAV	BUBTIB
335.531	298	0.5	316.092	298	38.88	UKORUH	IZAJUO
570.405	298	1	531.488	298	38.92	FIFFUV	ACPRET
234.370	*298*	*0.5*	*214.315*	*298*	*40.11*	*AHEREK*	*JAYPUU*
198.119	*150*	*1*	*160.550*	*298*	*41.88*	*YAKWAJ*	*BISMEV04*
411.060	*298*	*0.5*	*388.957*	*298*	*44.21*	*VIPCUS*	*ZOKSUN*
667.044	*298*	*1*	*622.342*	*298*	*44.70*	*REQWEP*	*REQWAL*
406.115	*298*	*1*	*361.070*	*298*	*45.05*	*NINSIM*	*NINSEI*
210.857	*143*	*0.25*	*199.046*	*143*	*48.32*	*EDUHIU*	*EDUGOZ*
588.339	*298*	*2*	*477.703*	*298*	*55.32*	*DOFTAT*	*DOFSUM*
285.821	*253*	*0.25*	*269.329*	*253*	*66.40*	*NABWET*	*NABWAP*

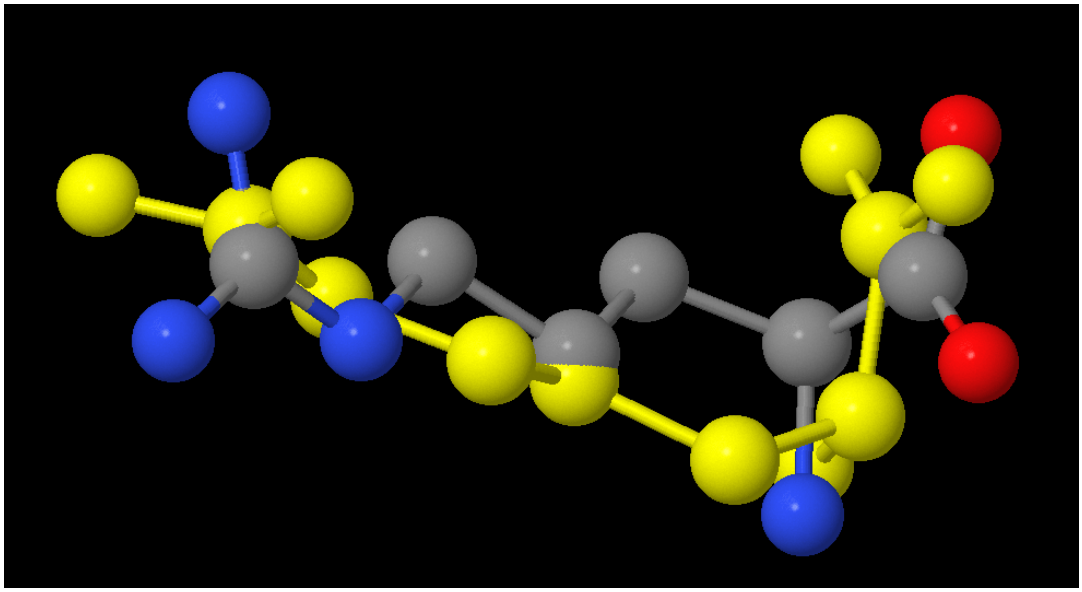

Figure S1: Overlay of molecular units from the amino-acid CSD files L-arginine L-dihydrate,[3] ARGIND.cif, and L-arginine,[4] TAQBIY.cif ($C_6H_{14}N_4O_2$), illustrating the conformational changes between the hydrate and anhydrate in this flexible molecular system. One molecule has been rotated and translated as a rigid body to a minimised RMSD of 1.5Å with reference to the other molecule. This diagram has been prepared in Jmol using the "compare" function.[5]

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