The solvates of sulfamerazine: Structural, thermochemical, and desolvation studies

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Electronic Supplementary Information

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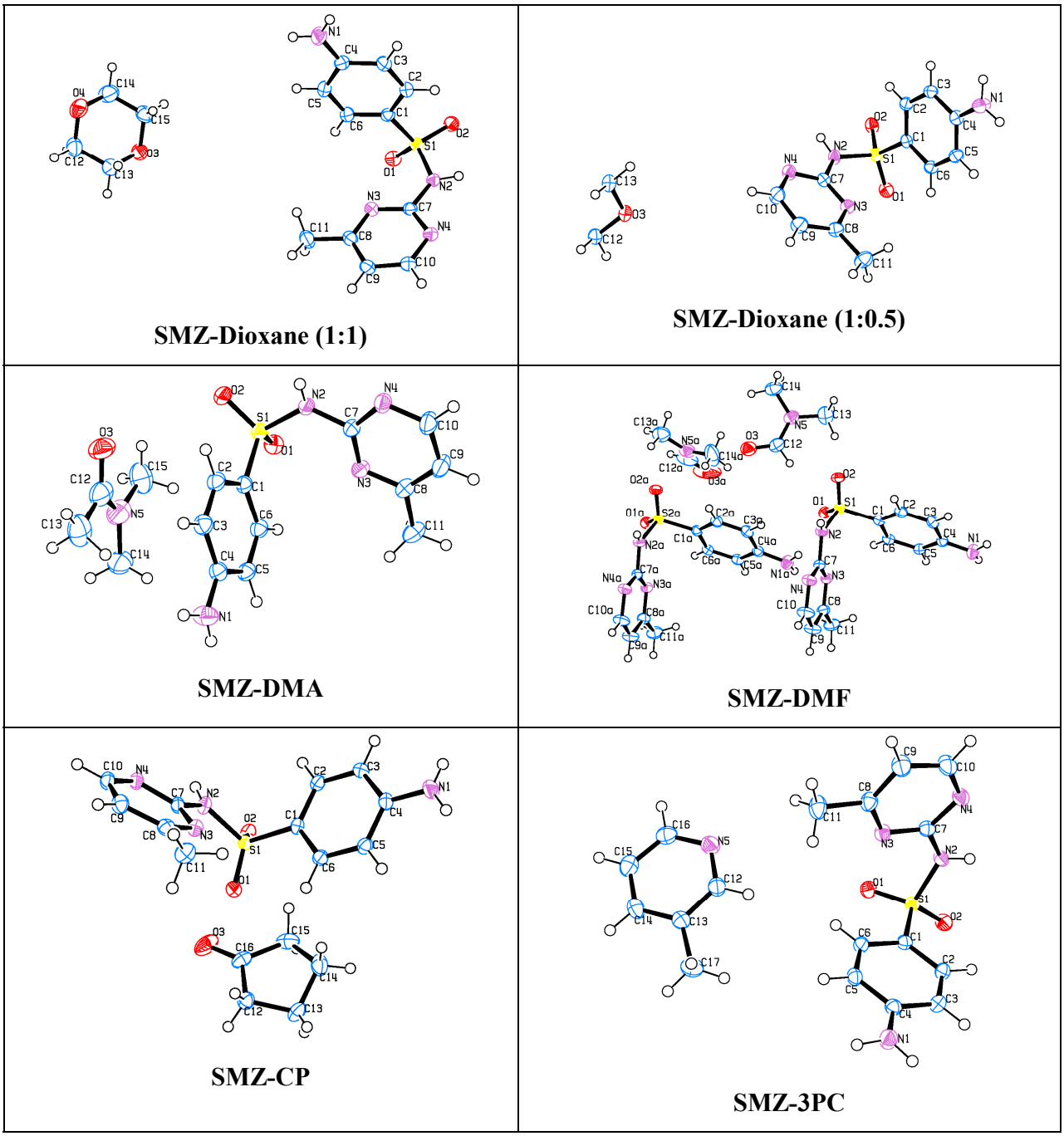

Fig. S1 ORTEP diagrams of crystal structures of the SMZ solvates. Thermal ellipsoids are drawn at 50 % probability.

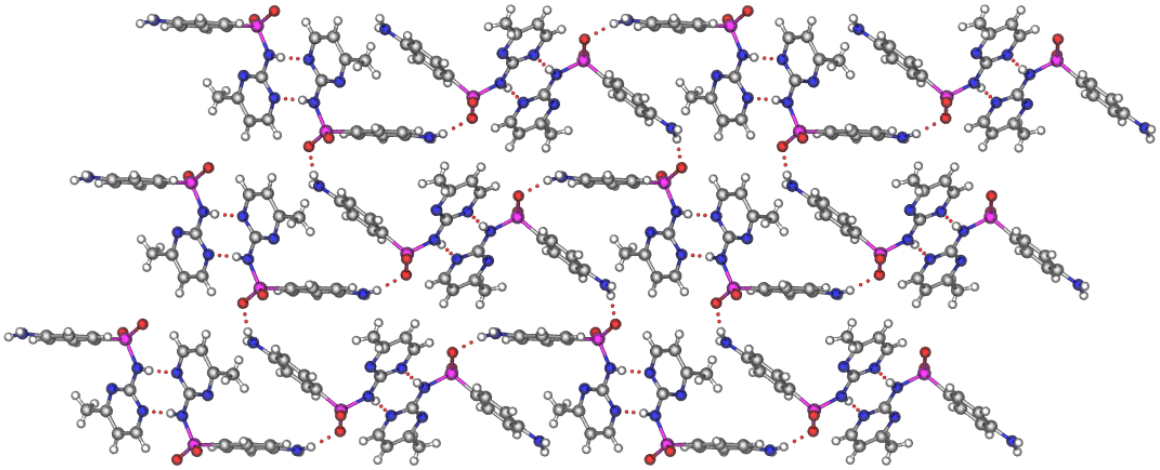

Fig. S2 A distorted hexagonal network in the crystal structure of SMZ Form I.

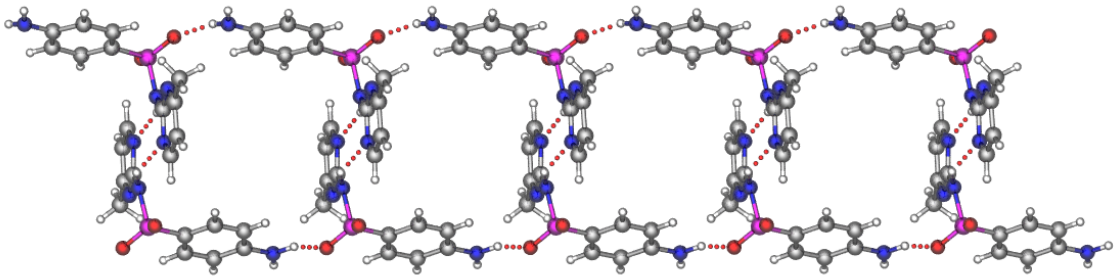

Fig. S3 A ladder network in the crystal structure of SMZ Form II.

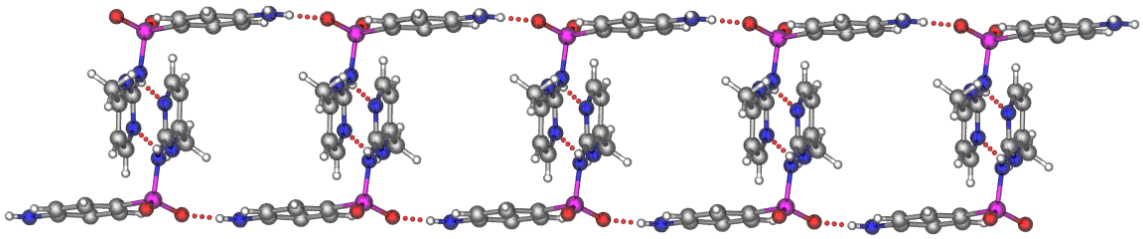

Fig. S4 A ladder network in the crystal structure of SMZ Form III.

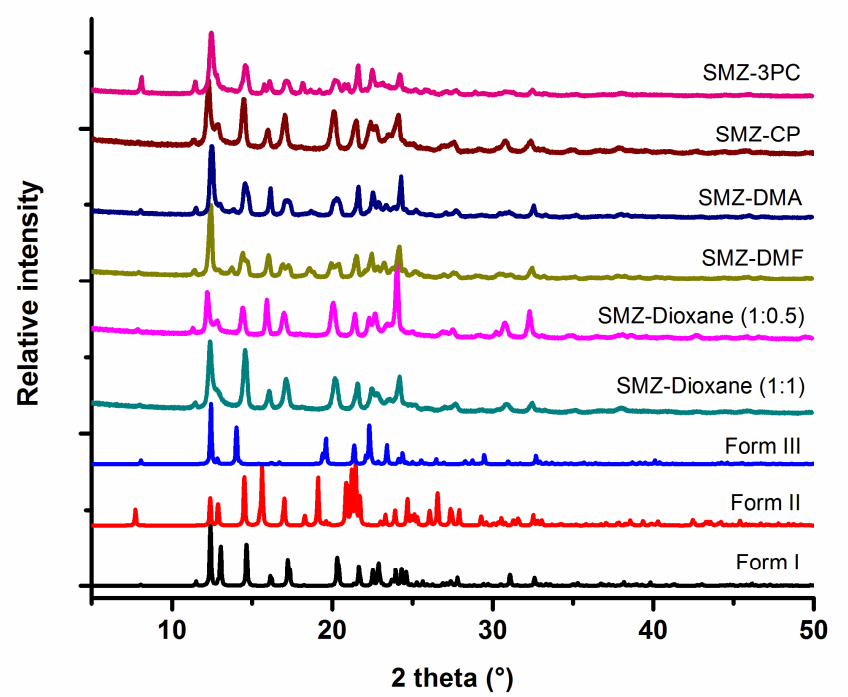

Fig. S5 Comparison of the PXRD patterns of the samples obtained in the desolvation experiments on the solvates of SMZ at ambient conditions.

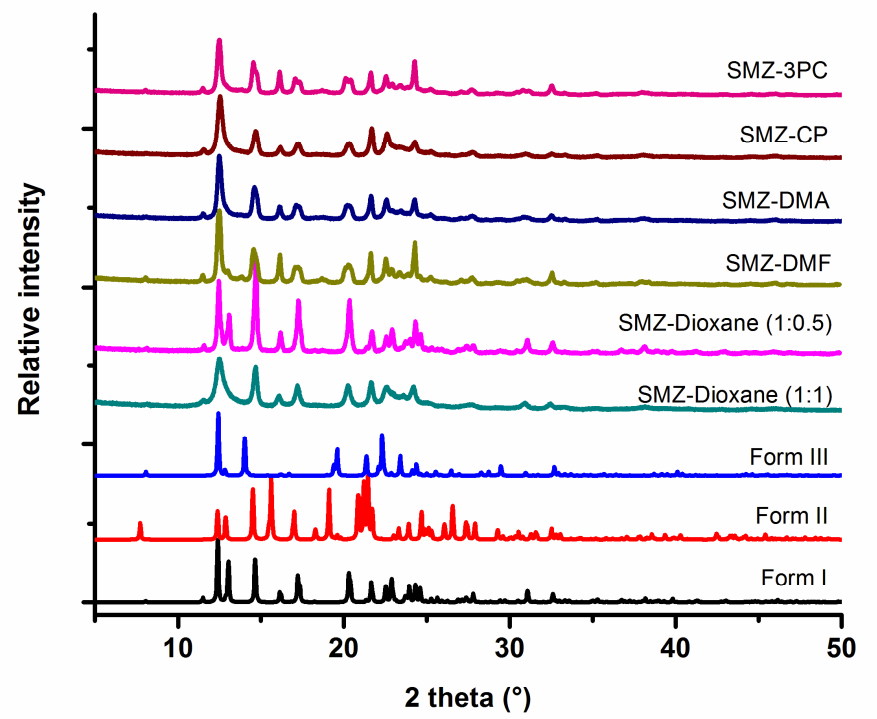

Fig. S6 Comparison of the PXRD patterns of the samples obtained in the desolvation experiments on the solvates of SMZ at 90 °C in a vacuum oven. Notice that all the solvates converted to Form I.

Table S1. List of CSD Refcodes of sulfonamide drug solvates and their packing motifs.

Solvates of sulfonamide drugs – 41				
Refcode	**Solvent**	**Molar ratio (sulfonamide:solvent)**	**Hydrogen bond network involving sulfonamide molecules[a]**	**Remark**
ADEDIX	Pyridine	1:1	1D ladder	
ADEFOF	DMA	1:2	2D layer	
BABYIN	Acetonitrile	1:1	2D bilayer	
BABYOT	*N*-formyl piperidine	1:1	1D chain	
BIXMIF	Ethylacetate	1:1	2D layer	
BIZXEO	Pyridine	1:3	0D (not a dimer)	
BONROM	Ethylacetate	1:0.5	1D ladder	
CASMAL	Aniline	1:1	2D layer	
DAHNIJ	Acetonitrile	1:1	1D chain	
DATTUN	Acetonitrile	1:1	1D chain	
DIKCUW	Caprylic acid	1:1	0D dimer	
DIKDUX	1,4-dioxane	1:0.25	0D dimer	
FAYGOC	Ethyl methyl ketone	1:0.5	1D chain	
GIMRUQ	Acetone	1:1	2D layer	
GIMSAX	DMF	1:1	3D channel	
HEZNEF	1-Butanol	1:1	1D chain	
HEZNIJ	1-Pentanol	1:1	1D chain	
HEZNOP	1,4-Dioxane	1:1	1D chain	
HOMZIS	Methanol	1:0.5	0D (not a dimer)	
IRILOK	Methanol	1:1	2D layer	cocrystal
IRILUQ	Ethanol	1:1	2D layer	cocrystal
JENGIS	Methanol	2:3	1D column mediated by malate ions	Salt of *S*-Malic acid
KEFGAD	Acetone	1:1	Complex 3D structure	
LIWMIN	1,4-Dioxane	1:1	0D (not a dimer)	
LOWKOX	Methanol	1:1	0D (not a dimer)	
MAJQOE	Methanol	1:1	1D chain	
MAJQUK	Ethanol	1:1	1D chain	

MALVOL	Dimethylsulfoxide	1:1	1D chain	
MAPPUP	Acetonitrile	1:1	1D chain	
NIKROP	Dimethylsulfoxide	1:2	1D chain	
NUQGOV	Chloroform	1:1	3D coordinates not available	
ODATIX	DMF	1:1	2D layer	
ODEFEJ	Dimethylsulfoxide	1:1	0D dimer	
PEHYEH	Tetrahydrofuan	1:2	1D chain	
PIWWAU	Acetone	1:1	1D chain	
RASSUZ	Methanol	1:1	2D layer	cocrystal
VIDMUR	DMA	1:2	0D dimer	
VIDNEC	Dimethylsulfoxide	1:1	1D chain	
WOMYAZ	Acetone	1:1	1D chain	
YABMIX	Methanol	1:1	0D dimer	
YESKIR	N-methyl-2-pyrrolidone	1:2	1D chain	

[a] Only the strong hydrogen bonds between the molecules of sulfonamide drugs are considered.

Table S2. List of CSD Refcodes of sulfonamide drug hydrates and their packing motifs.

Hydrates of sulfonamide drugs – 27			
Refcode	**Molar ratio (sulfonamide:water)**	**Hydrogen bond network involving sulfonamide molecules[a]**	**Remark**
ACIGEY	1:1	0D	No sulfonamide-sulfonamide hydrogen bonds. The sulfonamide molecules are connected through water molecules and generate a 3D structure
AHUXOR	1:2	0D	No sulfonamide-sulfonamide hydrogen bonds. 1D hydrogen bond ladder mediated by water molecules
CIDYAP	1:1	0D tetramer	2D layer mediated by water molecules
CITYEJ	1:2	3D coordinates not available	
CUBKEQ	1:1	0D	No sulfonamide-sulfonamide hydrogen bonds. 1D hydrogen bond

			ladder mediated by water molecules
DAGGIC	1:1	3D structure	
DICVOB	1:1	1D chain	2D sheet structure mediated by water molecules
FEDTEO	1:1	3D structure	Salt of citric acid.
GUSHAD	1:0.5	3D coordinates not available	
IRIMEB	1:1	3D structure	Tetroxoprim sulfametrole cocrystal
JEBNUZ	1:1	2D layer	
KOCLUK	1:1	1D chain	
LEPMOJ	1:1	1D chain	Crystal structure contains water and ethanol.
MAJQIY	1:1	1D chain	3D structure mediated by water molecules
MIVNIO01	1:1	0D (not a dimer)	A four component unit with 2 each molecules of sulfonamide and water
QACQUH	1:1	1D chain	
QOGHUQ	1:2	3D structure mediated by water molecules	norfloxacinium saccharinate saccharin cocrystal
RIWLOY	1:1	2D layer	cocrystal
SOBZIM	1:1	3D coordinates not available	
SULAMH10	1:1	1D chain	
WECXEI	1:1	0D	No sulfonamide-sulfonamide hydrogen bonds. 2D hexagonal layer, each hexagon composed of 3 each molecules of sulfonamide and water
WINJAE	1:3	2D layer	Sodium salt
WODBEW	1:1	1D chain	
WODBIA	1:1	2D layer	
ZOWDUK	1:1	0D	No sulfonamide-sulfonamide hydrogen bonds. 3D structure mediated by water molecules
BURXOC	0.22:18.7	1D chain	β-cyclodextrin inclusion complex. Crystal structure also contains ethanol molecule.
BURXUI	0.5:9.2	1D chain	β-cyclodextrin inclusion complex.

[a] Only the strong hydrogen bonds between the molecules of sulfonamide drugs are considered.

Table S3. List of CSD Refcodes of sulfonamide drug crystal structures.

Hydrates of sulfonamide drugs - 27		**Solvates of sulfonamide drugs - 41**		**Polymorphs of sulfonamide drugs - 25**	
ACIGEY	MIVNIO01	ADEDIX	JENGIZ	ATDZSA	SLFNMD10
AHUXOR	QACQUH	ADEFOF	KEFGAD	BEDMIG	SLFNMF
CIDYAP	QOGHUQ	BABYIN	LIWMIN	BEWKUJ04	SLFNMG
CITYEJ	RIWLOY	BABYOT	LOWKOX	BIYSEH	SULDAZ03
CUBKEQ	SOBZIM	BIXMIF	MAJQOE	FOGVIG	SUTHAZ
DAGGIC	SULAMH10	BIZXEO	MAJQUK	FURSEM	TOHBUN
DICVOB	WECXEI	BONROM	MALVOL	HCSBTZ	TORSEM
FEDTEO	WINJAE	CASMAL	MAPPUP	KUMCEB	VUHFIO
GUSHAD	WODBEW	DAHNIJ	NIKROP	QQQAUG	WURMOM
IRIMEB	WODBIA	DATTUN	NUQGOV	QQQBSS	YUCCIJ
JEBNUZ	ZOWDUK	DIKCUW	ODATIX	SAMPYM	ZZZAYP
KOCLUK	BURXOC	DIKDUX	ODEFEJ	SLFNMA	ZZZPUS
LEPMOJ	BURXUI	FAYGOC	PEHYEH	SLFNMB03	
MAJQIY		GIMRUQ	PIWWAU		
		GIMSAX	RASSUZ		
		HEZNEF	VIDMUR		
		HEZNIJ	VIDNEC		
		HEZNOP	WOMYAZ		
		HOMZIS	YABMIX		
		IRILOK	YESKIR		
		IRILUQ			
Sulfonamide drugs (including hydrates, solvates, and polymorphs) - 418					
ACICAQ	GARFEK	MOKXOA	SOJNEK	VUQWIO	
ACIGEY	GEHZAV	MORJIM	SOLSIW	VUWBEV	
ADAGUI	GEYSAE	MORJUY	SOTALC	UKIFIE	
ADEDIX	GIMRUQ	MOWYON	SOVDOW		
ADEFOF	GIMSAX	NADLIN	SOVDUC		
AHEMUV	GODRUM	NAFVIA	SUKHOV		
AHUXOR	GODSAT	NAWQOR	SULAMD06		
AJULUM	GODYED	NAWQUX	SULAMH10		
AMAVIT	GODYIH	NEDSUK	SULDAZ01		
ASUMEG	GUCMEW	NERQEH	SULPIA		
ATDZSA	GUSHAD	NIFKIX	SULTAM		
BABYIN	HADTEL	NIKCEQ	SUTHAZ		
BABYOT	HAGMAD	NIKROP	SUVGUL		
BAGVUA	HANFUY	NITQOX	TAHDUB		
BAPYIB	HAWZEL	NUNGIM	TAMRUV		
BEBZIS	HCSBTZ	NUQGOV	TAMXAG		
BEDMIG	HEZNEF	OBAWIX	TAQVUD		
BEGSEL	HEZNIJ	OBAWOD	TEDXAB		

BEWKUJ04	HEZNOP	ODATIX	TELWAI		
BILSEU	HOLTUY	ODEFEJ	THTHXN		
BIVTAB	HOMZIS	OFEHAJ	TIKQEK		
BIXMIF	HOQZET	OFIHIV	TOHBUN		
BIXMUR	HORNEI	OFIHOB	TORSEM		
BIYSEH	HOSCAU	OFIHUH	TUDTOB		
BIZXEO	HOTPAI	PABJOR	UDEWUV		
BONROM	HUHWAI	PECTAT	UFERED		
BUDYEF	IDIMOY	PEHVEE	UNEZAO		
BUDYUV	IDUSUV	PEHVII	VAKPIH		
BUNDHA10	IFAFAX	PEHWEF	VAZTIA		
CABCOX	IFODOX	PEHYEH	VEFXEJ		
CABCUD	IFODUD	PEMYOV	VEKSEK		
CASMAL	INEDUA	PEXYEX	VENLUV		
CAVGOV	IRILOK	PIDVEE	VIDMUR		
CEKHIJ	IRILUQ	PILPEG	VIDNEC		
CELNAJ	IRIMEB	PIWVIB	VIGVOW		
CIDYAP	IZEBEU	PIWVUN	VITWIE		
CIHFAA	IZEBIY	PIWWAU	VOHZIC		
CIRTIG	JABJAY	POHYER	VOKSET		
CISKUL	JABJEC	PONZIC	VOKXEY		
CITSON	JAGWAP	PUBZOB	VOKXIC		
CITYEJ	JAQVAY	PUBZUH	VONZIH		
CIVBAK	JATLOF	PYMSBZ	VORBAF		
COMFOZ	JATMEW	QACQUH	VUGMIT		
COXYOE	JAWHOF	QASFIZ	VUGMOZ		
COYVER	JAYJUP	QAXSUD	VUHFIO		
COYVIV	JAZVEL	QEFQOH	VUXPEJ		
CUBKEQ	JAZZOZ10	QIHPAY	VUXPUZ		
CUQTEN	JEBNUZ	QIJZOY	WACJIT		
CUZQOD	JENGIS	QIMBET	WASNOT		
DAGGIC	JIRKIE	QIMDIZ	WECXEI		
DAHNIJ	JIRKOK	QIMDOF	WENROX		
DATTUN	JIRLAX	QIMDUL	WEWVUQ		
DATWOK	JIZGII	QIYMEQ	WIKNAF		
DAWRAU	JIZHEG	QODGIA	WINJAE		
DEFZEU	JUWTUQ	QOGHUQ	WINWUL		
DEVLIZ	JUWWAZ	QORSOG	WOBHUR		
DEVSON	KASXIM	QOVQIC	WODBEW		
DEZQUU	KATBEN	QOVQOI	WODBIA		
DIBBUL	KEFGAD	QQQAUD	WODBOG		
DICVOB	KEFROC	QQQAUG	WOMYAZ		
DIKCIK	KEGXAW	QQQBSS	WURBER		
DIKCOQ	KENDOX	RALSED	WURMOM		
DIKCUW	KIFZUV	RASSUZ	WUVSOW		

DIKDAD	KIKCUD	RAYLOT	XACVEC		
DIKDEH	KIKFEQ	RETLEI	XETKUD		
DIKDIL	KIXJIL	RETLIM	XIGLAB		
DIKDOR	KOCLOE	RETLOS	XIYRUT		
DIKDUX	KOCLUK	REVJAE	XOXYAK		
DIWSAE	KOLHUP	REZNOA	XUDTIZ01		
DIYJOL	KOMVEO	RIQKOS	XUGNAO		
DOLJIX	KONJAY	RIWLOY	XUYTUG		
DONTOP	KOQHAZ	RIYXED	YABGUD		
DONTUV	KOWZIF	RIZKOB	YABMIX		
DUGPAW	KUMCEB	RUGFUU	YAMPUY		
DUNLEE	KUSVEZ	RUWCER	YANNEH		
DUNXAL	LADTOZ	SAMPYM	YAWZIF		
DUXYIE	LAWKUP	SEBJAK	YEKGUQ		
DUXYOK	LEPMOJ	SEBLEQ	YESKIR		
EDEZES	LICZOM	SEBPAQ	YESMEO		
EFOFAH	LISCUL	SECDAF	YEZJET		
ENIROI	LIVPUB	SEDZOQ	YEZJIX		
ETITEG	LIVQAI	SEQJUT	YIBFEU		
EWUHAF01	LIWBOJ	SEQKAA	YIGBEW		
EXOCUP	LIWMIN	SEQKEE	YIGMUX		
FAXVAB	LOCHUH	SETSOA	YIHRUC		
FAXZIO	LOCJAP	SEVHAD	YIZQAA		
FAYGOC	LOWKOX	SFDMOX02	YOCVOC		
FEDTEO	LUJBOH	SIBDAI	YODGUU		
FEYKIE	MAJQIY	SIFFUJ	YOWTIN		
FEYKOK	MAJQOE	SIMJEE	YUCCIJ		
FIDDAY	MAJQUK	SIQRAM	YUKKUK		
FIKHEM	MALVEB	SIVZIG	ZEXWOO		
FIKHIQ	MALVOL	SLFNMA	ZIKKAF		
FIXNUV	MAPPUP	SLFNMB03	ZOWDUK		
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FOMZOX	MEJTAX	SLFNMD01	ZOYPIM		
FORFEY	MENPEB	SLFNMF	ZUWRIS		
FOWSUG	MENPIF	SLFNMG	ZZZAYP		
FOWTAN	MENPUR	SLFQUI	ZZZPUS		
FOZXUO	MILFIW	SLFSMD10	BURXOC		
FURSEM	MINGOF	SLFSXZ	BURXUI		
GAQTUO	MISMUX	SOBJUO	FULHUQ		
GAQVAW	MISNAE	SOBZIM	NAJLOB		
	MIVNIO01		QQQAUG09		
	MOCVEF				