

Investigating the competitive factors of metal-anion coordination, coordination by water, and hydrogen bonding in complexes of cyanuric acid with the alkaline earth metals

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Supplementary material

Table S1: CSD REFCODES for CYH and its solvates and cocrystals

AGEREJ
AGERIN
AGEROT
AGEROT01
AMIGUA
BADCUR
BULLEB
BUVLEM
CYURAC03
CYURAC04
CYURAC05
CYURAC10
CYURAC12
CYURAC13
CYURAC14
CYURAC15
HADKUT
HADKUT01
HIQZOY
HOPJOM
ILECAG
IQUKUD
IQULAK
IZIHEE
JAGPEQ
JAGPIU
JAGPOA
JAGPOA01
JAGPUG
JAGQAN
JAGQAN01
JAGQER
JAGQIV
JAGQIV01
JAGQOB
JAGQOB01

JOLSAE
KEMWUU
KIRGIF
KIRGOL
LEPKOH
MOPYAR
MOXNAR
NONYOH
OYAPOW
OYAPUC
OYEJOU
PANVUV
PAVDID
PAVDOJ
PAVDUP
QACSUI
QACSUI01
QACSUI02
QACSUI03
QAGDEK
TEBREZ
TEBRID
UCUSIY
UFOGOP
VEDFAM
VEXQOE
VEXQUK
XAKSOU
XAKSUA
XANVER
XASWUN
XENFAB
XENFAB01
XEPZID
XURGID
XURGOJ
YIWBOV
YIZWUA
YIZXAH
YIZXEL
YIZXIP
YIZXOV
ZAHJIB
ZAHJIB01
ZAHJIB02
ZAHJIB03
ZAHJIB04

Table S2: CSD REFCODES for organic salts of CY⁻

BUHMAU
CIHHUX
DIRNUP
IDIDUX
KADMAG
KADMEK
KADMIO
KADMOU
KADMUA
KADNAH
KADNEL
KAYSOT
KEDYUO
LAFLOV
MOHCUI
MOPYEV
MOPYEV01
POHFAW
QAGDAG
QAGQAT
QELXEL
TUBMOV
WEGTAE
WEYCEM
XASWUN
XORMOH

Table S3: CSD REFCODES for cyanurate complexes of transition and post-transition metals

AYOBIC
AYOBOI
AZIYEQ
BIPYEG
CENKUC
DACMIH
DOKFOZ
DOVTEN
DUCJOA
DUCJOA01
DUCJOA10
EDEREK
EMEWEB
FETGAM
FETGAM01
FETGIU
FETGIU01
HASQIF

HIGMIU
HILKIX
HOLFIX
HOPZAQ
HOPZEU
ICOREX
ICYUCU
ICYUCU01
IDOGUH
IQEYUB
IYUGAM
JEDGOS
JOKKAX
JOXZOO
JOXZOO01
JUGMEG
KARDEM
KARDIQ
KEQGIW
KEQGIW01
KOKVAI
KUXFAK
KUXFAK01
KUXFAK02
MAXMAD
MIPCEX
MIRGEB
MIRGIF
MIRGOL
NECTEU
NECTIY
NECTIY01
NECTIY02
NECTIY03
NECTIY04
NECTIY05
NECTIY06
NECTIY07
NECTIY08
NECTIY09
NECTOE
NECTUK
NIDDOV
RADNIX
RADNOD
SIBBEK
SUQCEN
SUQCIR
TAQWIR
TESZOJ

TOSQAV
TUDQAN
TUDQER
TUDQIV
UKIFAV
VEZJAP
WEYMUJ
WICCIV
XILLEK
XIXQOO
XIXQUU
ZETDOR

Table S4: CSD REFCODES for cyanurate complexes of alkali metals

CUQTIU
CUQTIU01
DODTEY
DODTEY01
FUSMIS
FUSMIS01
GONPIL
GONPOR
GONPOR01
GUMZAS
ILECAG
IQUKOX
IQUKUD
IQULAK
JOKKAX
KOJJAX
KOJJEB
KOJJIF
KOJJOL
KUTFAI
KUTFEM
LEPKIB
LEPKIB01
LEPKOH
LIZQOD
LIZQUJ
LOVBOQ
NOMSIU
NOMSOA
OYANUA
RONLUE
RONLUE01
UCUSIY
VOKKIP
VOKKIP01

VOKKIP02
WIVSAY
XIBPII
XIBPII01
XIBPII02

Table S5: CSD REFCODES for cyanurate complexes of alkaline earth metals.

FUSMEO
FUSMEO01
VUQVUB
VUQVIP
YIWBOV
YIWBOV01
ZACZEM
QEHKOG
QEHKOG01
VUQTOT
VUQTOT01
VUQTOT02
OYEJUA
VUQTIN
GONNEF
GONNUV
VUQVOV
GONPEH
YOZREM
YOZREM01
YOZREM02
UPECAU
UPECAU01
UPECAU02
XENFEF
GONPAD
SIXKAO
SOVMAU
HIJSEB
HIJTAY
YOKYUV