

## Importance of Cu and Ag Regium– $\pi$ bonds in supramolecular chemistry and biology: A combined crystallographic and *ab initio* study.

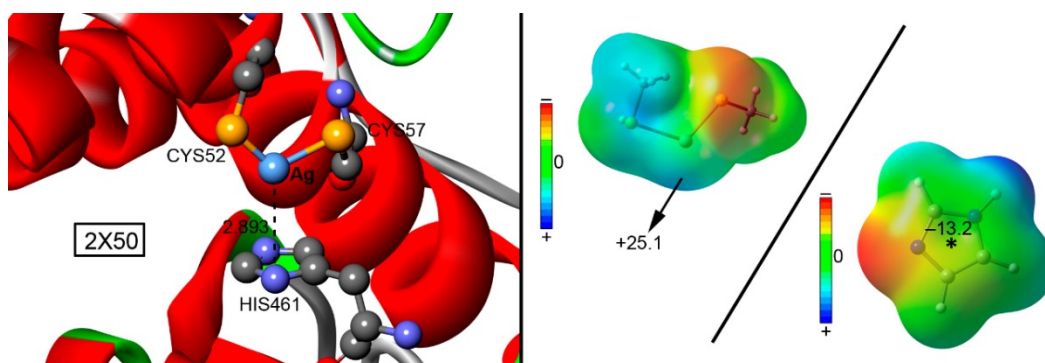
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### Description of additional biological Rg– $\pi$ complexes

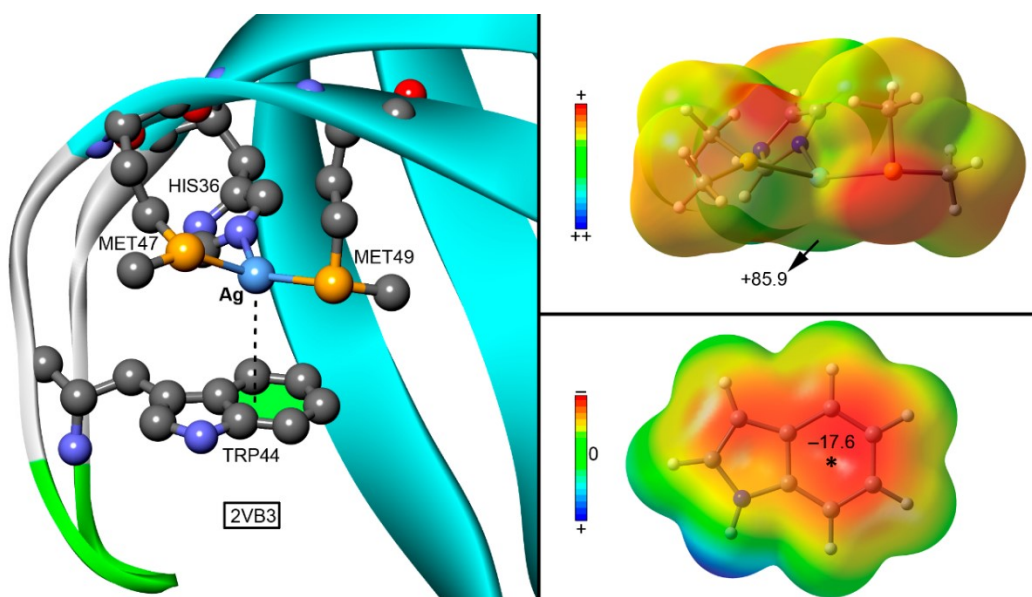
Structure 2X50 corresponds to a protein-inhibitor complex between *Leishmania* Trypanothione Reductase (TR) and silver. Leishmaniasis is suffered by around 12 million people worldwide and owing to the absence of effective vaccines against this disease, the group of Baiocco and collaborators<sup>1</sup> evaluated the inhibitory effect of Ag nanoparticles on the TR Activity. Specifically, they determined and analyzed the X-ray structure of a complex between Ag and TR to understand the molecular basis of protein inhibition. Interestingly, in a parallel way to the commonly used Sb(III) drugs, an Ag ion coordinates to the two known catalytic cysteine residues (CYS52 and CYS57) while also establishing a Rg– $\pi$  bond with the  $\pi$ -system of HIS461 ( $d_{\text{Ag}\cdots\text{C}} = 2.893\text{\AA}$ ), a fact that passed unnoticed to the original authors, which described the Ag $\cdots$ HIS461 interaction as a mere coordination bond. The computed interaction energy strength resulted in  $-11.4$  kcal/mol, which is a moderately strong value. This example highlights the role of Rg– $\pi$  interactions in the inhibition mechanism of TR and their use in the field of rational drug design.



**Figure S1.** (Left) Partial view of the X-ray structure 2X50 exhibiting a Rg– $\pi$  bond. Distance in  $\text{\AA}$ . (Right) MEP surfaces of both Rg– $\pi$  donor and acceptor moieties. Energies at selected points in the surface are given in kcal/mol (0.001 a.u.).

<sup>1</sup> P. Baiocco, A. Ilari, P. Ceci, P. Orsini, M. Gramiccia, T. Di Muccio and G. Colotti, Inhibitory Effect of Silver Nanoparticles on Trypanothione Reductase Activity and *Leishmania infantum* Proliferation. *ACS. Med. Chem. Lett.* 2011, **2**, 230–233.

Structure 2VB3 encompasses the work from Xue and coworkers,<sup>2</sup> where they analysed a novel metal recognition site present in CusF protein. The Cus operon encodes a bacterial copper homeostasis system with several methionine-motif proteins, including the periplasmic protein CusF, which is thought to serve as copper chaperone or regulator. CusF binds metal ions *in vitro*, and a methionine-rich metal site has been proposed based on an apo-CusF structure and NMR chemical shift data. With the purpose to provide more structural insights into this metal-binding protein, the authors solved the crystal structures of Cu(I)-CusF and Ag(I)-CusF. Both metal-bound forms of CusF are defined by a small barrel with two orthogonally packed  $\beta$ -sheets. In both Cu(I)-CusF and Ag(I)-CusF structures, the metal ion is coordinated to HIS36, MET47 and MET49 residues in a trigonal planar fashion. Interestingly, the aromatic system of TRP44 is in contact with the metal ion (see Figure S2 for the Ag(I)-CusF complex) and undergoes a Rg- $\pi$  bond with the S-Ag-S coordination complex. The computed Rg- $\pi$  interaction energy resulted in  $-15.5$  kcal/mol, hence remarking the potential of Rg- $\pi$  bonds to be involved in metal-specific gene regulatory and cation-trafficking protein families.



**Figure S2.** (Left) Partial view of the X-ray structure 2VB3 exhibiting a Rg- $\pi$  bond. Distance in Å. (Right) MEP surfaces of both Rg- $\pi$  donor and acceptor moieties. Energies at selected points in the surface are given in kcal/mol (0.001 a.u.).

<sup>2</sup> Y. Xue, A. V. Davis, G. Balakrishnan, J. P. Stasser, B. M. Staehlin, P. Focia, T. G. Spiro, J. E. Penner-Hahn and T. V. O'Halloran, Cu(I) recognition via cation- $\pi$  and methionine interactions in CusF. *Nature Chem. Biol.* 2008, **4**, 107–109.

## List of PDB structures

Cu(I)-212 hits:

3K0I, 3KSS, 3NT0, 3OMI, 3OMN, 3OMA, 3OM3, 3OW7, 3CVB, 3CVD, 3DSO, 4MAI, 4N3T, 4OUA, 4OZ7, 4DP8, 4DP1, 4DP4, 4DP6, 4DPA, 4DPC, 4F2E, 4F2F, 4L05, 2XMW, 2XMT, 2XMU, 2XMV, 3QJT, 3QJU, 3QJV, 3QJQ, 3QJR, 3QJS, 3QQX, 3HB3, 3I9Z, 3I04, 3I01, 3HW7, 2ZWD, 3FT0, 3FSA, 3FYE, 3FYI, 3ZDW, 3N7D, 4BZ4, 3T0U, 3T5W, 2Z8Y, 2ZKW, 2ZKX, 2ZMZ, 2ZOW, 4BDV, 4TM7, 4RKM, 2YOX, 2YOY, 2XY5, 3EH3, 3EH4, 3EH5, 3EIM, 3F7L, 3F7K, 5AA7, 6TWE, 2QDW, 2QIF, 2QPE, 2QPD, 2RNB, 2RSQ, 2RAC, 2RLI, 1F56, 1FD8, 1FEE, 2PPF, 2PPE, 2PPD, 2PPC, 2PP9, 2PP8, 2PP7, 2PPA, 5ARN, 5C92, 6CPD, 6EK9, 6L9S, 6M98, 6FF2, 5YJS, 5NQM, 5NQO, 5NQN, 5MSZ, 5I0W, 4BTE, 5WEH, 5VDF, 5VDE, 5FEJ, 5FJE, 5K BK, 5KBM, 5KBL, 2XV0, 2XV2, 2XV3, 4M1P, 6Q58, 6Q6B, 6R01, 4P5S, 1K0V, 1DZ0, 6QVH, 6QYB, 6S07, 1HAW, 1A3Z, 1A8Z, 1AQS, 1AQR, 1B3I, 1N18, 6RW7, 1BA9, 1BXA, 6MF0, 6MF2, 6N5U, 2N0M, 2KM0, 2LEL, 2IDS, 2IDU, 2JCW, 2K4W, 2K70, 2K6Z, 2GQM, 2GT6, 2HH7, 2HRN, 2HRF, 2HX9, 2HX8, 2HXA, 1PU0, 1PTZ, 1R1C, 1TL4, 1U96, 6XTO, 6XTQ, 6XTP, 6XTS, 6XTR, 1RJU, 2BZC, 2CAL, 2CAK, 2CCW, 2FJS, 2FK2, 2FT7, 2FT8, 2GA7, 2GBA, 2GBT, 2GBV, 2GGP, 2GIO, 1OF0, 1Q05, 1KQK, 1L3N, 1JXG, 1JZG, 1KVJ, 1MJG, 1N19, 1ZPU, 2B08, 2AQT, 2AQS, 2AQR, 2AQQ, 2AQP, 2AQN, 2B3I, 2AHL, 1WS7, 1X9L, 1S6U, 1SF3, 1SFH, 1SNR, 1UUX, 1UUY, 1YSO, 2BHF, 1YJV, 1YJT, 1YLB, 2E86, 2EIC

Ag(I)-53 hits:

3KSO, 3NSD, 3OPO, 2X17, 2X50, 3UGE, 3H94, 2VB3, 3RU5, 5A4G, 5AFA, 2QCP, 2RVP, 6JR4, 6KA0, 5Z3W, 5AY2, 6LBW, 6LDI, 6M2P, 6IO4, 6IO6, 6G48, 5XUV, 5KU5, 5NXL, 5F0W, 5F0U, 4X89, 4WLV, 5IX7, 6NIZ, 5XJZ, 5FFE, 5FFD, 1A00, 1AQQ, 2MZC, 2KE8, 2M54, 6XTM, 6XTL, 6XTN, 7C17, 7BSF, 7BSG, 7BSE, 7BSH, 7CGC, 7CGD, 2G7N, 1Q06, 2AW0

## List of CSD structures

**Table S1.** List of CSD codes obtained from the CSD search including the CSD code, the size of the aromatic ring and the Rg atom involved.

Cu(I) – 6 member ring
CUPORY
ENCCBP10
GALTUI
GOLSOR
NEKDAK

TECCIN	
UQAROU	
WATWET	
Ag(I) – 6 member ring	
ABOREQ	LUXPUR
ACUQUK	LUZHUU
ACUREV	MADYUM
ACURUL	MAFDIH
ADUJOB	MARGIW
AHIDIE	MARGOC
AHIDOK	MARHET
AHIDUQ	MASKID
AJAZAM	MASMEB
AJAZEQ	MASQED
AJEKAD	MAYCAR
AJORAS	MAYCEV
AKIYOI	MEHYEF
AKUJOH	MEKGEP
APAGOP	MEKGIT
ATOMAX	MEKGOZ
AWEGOZ	MEKGUF
AWEHUG	MEVDAV
AWENEW	MICVOM
AWENIA	MOFCAN
AWENOG	MOFDEQ
AWUPIR	MOFDUG
AXAWIF	MOFLIC
AXEGIV	MOFLUO
AXENAS	MOKQIO
AYOGUQ	MOQFOP
AYOHAX	MOTNAL
BADGET	MOZVAZ
BAFDIW	MUKVAR
BAFTIO	MUTMOD
BAFTOU	MUZJUN
BAMLUZ	MUZYOV
BAQGIM	NABYUL
BEHPIO	NAGLOY
BEHPOU	NAGLUE
BEKBOL	NAGMAL
BEKDUR	NANZEI
BEKDUR01	NAPAGP
BIMWAY	NATNEB
BOCFEH	NEBHOT
BOYGIG	NEGDEJ

BULSEI	NEGQOI
BUNFOG	NEKDAK
BUTGAZ	NEKYUY
BUTGAZ01	NEKYUY01
CABMAU	NEKZAF
CABMUO	NEKZEJ
CAGLOC	NEPHEV
CALJEF	NEWNOU
CASQAO	NEXRAK
CEJCOM	NEYJUX
CEJCUS	NEYLOT
CENHOU	NEYMUA
CENHUA	NEYPOX
CETNIY	NEYPUD
CEXKIA	NEYQEO
CEYXOV	NIBMOB
CICVES	NIBMOB01
CIKGEJ	NIBMOB02
CIWWUB	NIBMUH
COCDIJ	NIBNAO
COJKAQ	NISFUQ
COJKEU	NOJNUY01
CUCSOI	NOMBID
CUPORY	NOPHOS
CUTNEL	NOPJAG
CUWNIS	NORDAZ
CUWPAM	NOWGOX
CUWPEQ	NOXYAC
DABFUJ	NUNSEW
DACKAV	NUSGOX
DATJAL	NUSGUD
DATJOZ	NUVBOW
DATKOA	OBECUT
DAXTAY	OBEKOW
DAXTEC	OBIWIH
DECNEF	ODACAX
DEDROW	ODACAX
DEHDIE	OGAQEU
DEHPAI	OGOLEB
DEKRIV	OHACUW
DEKYUQ	OJAROI
DEKZIF	OJEDAJ
DEMKAK	OKABOS
DEMKEO	OKAGIR
DEYKOJ	OKOQAI
DEYKOJ01	OKUGOQ

DIBSIT	OKUXID
DIFMUC	OQAGIX
DIGLAI	OQINUY02
DIGLEM	OROPUH
DIHVOF	OSASEH
DILCUX	OSOQEU
DOHDAG	OTUNUN
DOHXOP	OTUPAV
DOHXOP	OTUPEZ
DONHEV	OVACOE
DOQZER	OXUQAB
DOZYEY	OYIHEL
DUJZAK	OZASIT
DUJZAK01	PAIPAG
DUPMIL	PAJGAL
DURSIT	PALSED
ECETAK	PAWMEG
ECETEO	PAWYOE
ECOCIJ	PAXQIO
EGADOF	PAXQIO01
EGOHAK	PAXQOU01
EJAZOF	PEFPOH
EJEPAM	PEJSOM
EJICOR	PEMROQ
EJIMUG	PEWQIR
EJIROF	PEWYUL
EKOTAZ	PEXGOP
EKOVAB	PEYVOG
EKOYIN	PICTOM
EMIPUN	PIHVAG
ENCCBP10	PITCIF
ENEZAZ	PIVLUE
EPADAC	PIVQIV
EPADEG	PIYJUD
EQEHUE	PIZCIN
EQEQEX	PIZKUF
ERIKEW	PIZKUF
EROBUK	POCPOM
ESASEW	POKBAT
ESASIA	POKBEX
ESETOL	POKBIB
ETIGEU	PORZOM
EWASOK	PORZUS
EYAQAW	POSHOW
EYAYIO	POTYEE
EZASEE	PUCYES

EZUKIT	PUHNEM
EZUKIT01	PUHNEM01
EZUKOZ	PUQDIQ
EZUKOZ01	PURXOR
FASRUO	PURYAD
FAZYIQ	PURZIM
FAZZEN	PURZOS
FEFFII	PUXNUR
FELFAE	QAHYOP
FELFOS	QAJWUT
FELGAF	QAJZOT
FENXAY	QANZIR
FIBSAK	QANZOX
FIGRUJ	QARNOP
FILTEA	QASBIW
FIRROQ	QAVCUN
FIRRUW	QEBVAW
FIWJAZ	QIPXUK
FIZBOG	QIPYIZ
FIZCIB	QIPYOF
FIZCOH	QIXHAH
FOKGAP	QODHUO
FUDFIU	QODHUO03
FUFVOT	QODHUO05
FUFVUZ	QODHUO06
FUFWAG	QODHUO07
FUFWEK	QODHUO09
FUFWIO	QODHUO10
FUFWOU	QODHUO11
FUGPAZ	QODHUO12
FUJLOM	QODHUO13
FULYUI	QOFCAR
FURRUG	QOFCEV
FURRUG01	QOFCIZ
FUXCIM	QOFCOD
GAKNEM	QOFCOF
GALFEF	QOFCUJ
GALTUI	QOFDAS
GAPDEI	QOFDEW
GAQWUT	QOFDIA
GARNUJ	QOFDIA02
GAWYUA	QOFDIA03
GEFDEB	QOFDIA04
GEFJIL	QOFDIA05
GEGBEB	QOFDIA06
GGBOL	QOFDIA07

GEGYAU	QOFDOG
GEKYUS	QOJDOJ
GEMDUY	QOLTES
GIQMIF	QOXBUA
GIQMOL	QQQBUV01
GIYVAM	QUXJEZ
GIYVOA	RAKGEQ
GIYZOG	RAKGIU
GOBGOT	RANYEL
GOBNER	RANYIP
GOBQEU01	RANYOV
GOLNIF	RAYZAT
GOLSOR	RAYZEX
GONWAH	RECJIS
GOQMAC	REHHUI
GUBRIF	REJHAQ
GUBYEI	RENNII
GUCYIO	RERQEM
GUCYOU	REXSAO
GUCYUA	RICZAH
GUCZIP	RIDHAQ
GUFYAJ	RIMPAH
GUGCES	RIMVUH
GUPZAU	RIPTIU
GUPZAU01	RISVOF
GUXTOJ	RITHAF
HAKKEL	RIVTOG
HAPFOV	RIYNEU
HAWDUG	ROBNAZ
HAWZAI	ROBNIH
HAYXUC	ROFGAW
HEBDEZ	ROGLAA
HEDRIS	ROJSEQ
HEFFII	ROLNUC
HEQTOO	ROMQQA
HESVEG	RORJAJ
HETQEC	RUKZUT
HILJAO	RULBAC
HILJIW	RULBEG
HILJUI	RULFOU
HIMXEI	SACQOF
HIWHEB	SACQUL
HOQFEY	SADWOL
HORWAN	SADWUR
HORWER	SAJKEU
HUGYOZ	SARNAB



HUHBER	SARNEF
HUMFUQ	SARNOP
HUTTEV	SARPEH
ICEFEB	SARPIL
ICUBOA	SEGFIV
IHUPIK	SEGFUH
IJISIE	SEHBIS
IJISOK	SEHBOY
IJISUQ	SEHCAL
IJUNAE	SEHCEP
IKEWAX	SEHCIT
ILIBUB	SEHCOZ
IQOVEQ	SEMNUU
IQOVIU	SEWSEU
IQOVOA	SEWVUN
IRIPEF	SIJJAZ
IXIVOA	SIXGOV
IZACER	SIXPIZ
IZIJUY	SIYZUV
JABBOE	SOBQEI
JABRUA	SOBQOS
JACVIS	SOMQAM
JADVEQ	SOMQIU
JAQUG	SOWWIL
JAPXEG	SOYFAP
JAQPEX	SOYFET
JAQPOH	SOYFUJ
JAQPOH01	SUFTUK
JEFDEG	SUFVAS
JEHWID	SUHJEL
JEHWUP	SUHVEX
JEHxEA	SUXZER
JIQYUE	TABPES
JOBXAZ	TACYIH
JOFPAY	TAGBOT
JOJNAY	TAGCAG
JOJNEC01	TALQOP
JUJSUE	TECSOK
KAJGAF	TEHMAX
KAJGEJ	TEHMID
KAJGEJ	TEJBOB
KAJGOT	TEJYEM
KAJGUZ	TEPWES
KAPFOY	TEQQEM
KAPFUE	TEWPIW
KAXTOU	TEZGEM

KAYSEK	TIBCAI
KEQWUY	TIFZOY
KETRAD	TIJFOH
KEWBAS	TIJNIK
KICVEY	TINDIE
KICVUO	TINTEQ
KICWEZ	TIRMOZ
KICWUP	TITKIS
KIDNES	TITKOY
KIDNIW	TITKUE
KIDNOC	TITLAL
KIDYIG	TIZCOW
KIDYOM	TOHJUX
KIDYUS	TOHXAR
KIDZED	TOKKEL
KIDZIH	TOLCIH
KIJNUO	TOLCON
KILQAX	TOLCUT
KIMZOY	TONJAI
KIRLUV	TUDNIR
KOHTOR	TUDVOE
KOHWEK	TUHVUO
KOLWOY	TUSKEZ
KUGKUT	TUXRAF
KUGLAA	TUZCUM
KUGLEE	UBEWAB
KUQPOC	UBOGIB
KUXXEH	UBONEE
KUYNOI	UCAKAM
KUZPIG	UDEREB
LAFNIQ	UDERIF
LAGCAZ	UFAGEO
LALMOB	UFOPEK
LALMUH	UGADAI
LALZUW	UHEZAJ
LALZUW	UHEZEN
LAMCIN	UHEZIR
LARMAV	ULACUF
LAYJAY	ULADAM
LEDXAU	ULADIU
LEDXEY	ULAGIX
LEDYEZ	UMIFUT
LEDYID	UMODEG
LEFKOZ	UNOSAT
LELZOR	UPUVEH
LESMUU	UQEVAO

LIKGES	UTAVUH
LINPII	VANLUR
LINQIJ	VANLUR01
LIVKEI	VANMEC
LOKGUO	VATBIB
LOLTUC	VATBUN
LONQUC	VAXTOE
LOPRUF	VAXTUK
LOZQOG	VAXVAS
LUDROR	VEFHIY
LUDSEI	VEFHOE
LULNIR	VEGMIF
LULNOX	VELJOO
LUMNOX	VIGDEW
LURDIM	VIGDOG
VIKBIB	XADYUZ
VILNEK	XADZAG
VINZAV01	XADZEK
VINZID	XANXEP
VIPTOF	XANXOZ
VIYDUE	XAYNIU
VODCUN	XEBGIU
VOPDEL	XECZUB01
VUDKAI	XEDBEO
VUFROF	XEKFIE
VUMBOV	XELYAP
VUQQUV	XENTER
VUSQUW	XIGKAA
VUVGUQ	XIHCEX
WAFWAD	XIWKOE
WAVBUR	XIWKUK
WAVCAY	XIWLAR
WAVCEC	XIWRIG
WAWLAK	XIWSED
WAWLEO	XIXREE
WAWLIS	XOBDIC
WEBHIX	XOBDUI
WEBMIC	XOHVOG
WEGBUI	XOKGAH
WEGVEM	XOLTAT
WESZIE	XOPJUI
WEZSIG	XOPREB
WIHWER	XOPREB
WIJQAI	XORNID
WITLAO	XOVBAN
WIVVOO	XUFLAM

WIWXAD	XUFLEQ
WOHHUX	XUKWAC
WOHJAF	XUSDOF
WOHJIN	XUVZAP
WOHJOT	YALKIH
WOHJUZ	YASMAH
WONKEQ	YASMEL
WONQEW	YECTOQ
WUFMIT	YEGNAA
WULBAI	YETPOD
WUWYAO	YETRAR
WUZBOI	YETTAT
XABLAP	YETTEX
XADYEJ	YEWGAL
XADYIN	YIBVUC
XADYOT	YIJLAF
YIJLAF	YINTUM
YINVAU	
YINVEY	
YINYAX	
YINYEB	
YIQLES	
YIQLOB	
YIQLUH	
YIRYIK	
YISKOB	
YIYHET	
YOGTUM	
YOGVOI	
YOTWIP	
YOYGEZ	
YOZCIB	
YOZSIQ	
YUJKAQ	
YUNKUO	
ZEDFOG	
ZEPDAC	
ZEPWUO	
ZEYMAR	
ZIBPAB	
ZIYXOU	
ZIZXAJ	

ZOLKUJ
ZOTNIH
ZUJPUR
ZUJQAY
ZUJQEC
ZULTOR
ZUWVEU
ZUWVEU
YEGNAA
YETPOD
YETRAR
YETTAT
YETTEX
YEWGAL
YIBVUC

<b>Ag(I) – 5 member ring</b>
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BARJAI
CAGCAQ
DOKJOD
DUKMOM
ECENIK
ECEPEI
EPUSUE
EQUXOE
EROTEK
INEKET
KAWMIH
OMEVUY
RUQMOH
TITKIS
TITKOY

## Cartesian coordinates of the PDB models

### 2XY5

C	1.3303402	2.1446262	-5.6037130
C	1.8273398	1.5286266	-4.4637137
C	0.1213408	2.8186259	-5.5667131
C	-0.6056588	2.8786258	-4.4017138
C	-0.1166590	2.2666262	-3.2717144
C	-1.0146586	2.4136261	-2.0847150
C	1.1013402	1.5836266	-3.2807144
O	1.6023400	0.9926269	-2.2277150
N	-1.2256584	-2.8973709	2.8802822
C	-2.3046578	-2.1173714	3.1662820
N	-2.8366575	-1.5293717	2.1172826
C	-2.0266580	-1.9423714	1.0742832
C	-2.0466580	-1.6703716	-0.3007160
N	-2.9476574	-0.8913720	-0.9027157
N	-1.1006585	-2.2533713	-1.0537156
C	-0.1986590	-3.0483708	-0.4637160
N	-0.0826590	-3.3833706	0.8102834
C	-1.0336586	-2.7813710	1.5292830
C	3.7133388	-2.2503713	2.6312823
C	3.3863390	-1.7113716	1.3882830
C	2.9933392	-1.9053715	3.7652817
C	1.9533398	-1.0043720	3.6642818
C	1.6263400	-0.4673723	2.4402824
C	0.4833406	0.4936272	2.4982824
C	2.3393396	-0.8013721	1.2862830
O	2.0713398	-0.2823724	0.1162837
Cu	0.7103405	0.7866270	-0.4357160
N	-0.8636586	2.0046264	-0.5417159
C	-1.8546580	2.5096260	0.4152836
C	-1.4316583	2.0166263	1.7762828
N	-0.2056590	1.2366268	1.5952829
H	2.7743795	0.9884967	-4.4530408
H	-0.2581709	3.3057571	-6.4680891
H	-1.5606485	3.4085255	-4.3761381
H	-2.6809483	-2.0173346	4.1854955
H	0.5486665	-3.4750637	-1.1430961
H	3.9308966	-1.9676062	0.4789883
H	3.2584250	-2.3327610	4.7351292
H	1.3878678	-0.7153906	4.5544740
H	0.1066012	0.5652292	3.5378673
H	-1.8939545	3.6111483	0.3809368

H	-2.8639945	2.1387895	0.1624672
H	-1.2475945	2.8530917	2.4720335
H	-2.2036430	1.3693058	2.2273156
H	-0.6252685	-3.4053552	3.5162948
H	4.5418857	-2.9600612	2.7068522
H	1.8993423	2.0962291	-6.5361291
H	-2.8632315	-0.7358225	-1.8967544
H	-3.6882391	-0.4614892	-0.3708220
H	-1.9264041	2.9976267	-2.2701506

### 3OW7

C	4.4396030	0.2728490	2.6881947
S	2.6466030	0.2348490	2.6451947
C	2.2376030	1.4198490	3.9041947
C	-0.6843970	2.2468490	-4.8468053
C	-1.0453970	1.0228490	-4.0208053
O	-1.4423970	-0.0181510	-4.5508053
N	-0.9223970	1.1728490	-2.7028053
C	-1.2553970	0.1258490	-1.7488053
C	-2.4283970	0.7008490	-0.9808053
O	-3.5673970	0.5748490	-1.4068053
C	-0.0883970	-0.1301510	-0.8118053
C	-0.1343970	-1.4671510	-0.1398053
C	-0.7783970	-1.6271510	1.0671947
C	0.4656030	-2.5651510	-0.7148053
C	-0.8183970	-2.8581510	1.6871947
C	0.4326030	-3.7941510	-0.0968053
C	-0.2133970	-3.9411510	1.1021947
N	-2.1503970	1.3518490	0.1421947
C	-3.1963970	1.9908490	0.9391947
Cu	3.4296030	-2.2471510	1.5501947
H	4.8525734	-0.1881131	3.5975198
H	4.8198069	-0.2742696	1.8002523
H	2.6964803	2.3807188	3.6267887
H	2.5687820	1.1101880	4.9058899
H	1.1448705	1.5323570	3.9059497
H	-0.3949491	3.1250440	-4.2515886
H	0.0918990	0.6714594	-0.0861553
H	0.8160685	-0.1149645	-1.4445764
H	0.9507893	-2.4617102	-1.6910887
H	-1.2780474	-0.7709387	1.5272984
H	0.8855616	-4.6604627	-0.5876302
H	-1.3475677	-2.9718478	2.6366235
H	-0.2633091	-4.9221020	1.5821497

H	-1.5771168	-0.7547002	-2.3182778
H	-4.1589836	1.5785077	0.6121619
H	-3.2159360	3.0818253	0.7873582
H	-1.5497501	2.5023387	-5.4738344
H	-3.0455357	1.7780879	2.0076318
H	0.1384918	1.9812021	-5.5257086
H	4.8237712	1.3013411	2.5990104
H	-0.6831857	2.0837112	-2.3336536
H	-1.2000745	1.5276042	0.4197604

#### 4RKM

C	3.3487566	-2.8019505	-3.3622483
S	2.8417566	-1.2269505	-2.6482483
C	5.1927566	-3.8159505	0.1967517
S	3.6807566	-3.2939505	1.0457517
Cu	2.7197566	-1.9769505	-0.4902483
S	1.5207566	0.9630495	0.0457517
O	1.8347566	1.7950495	-1.1772483
O	2.2447566	1.7450495	1.1237517
C	0.0737566	-2.7689505	0.4527517
C	-0.5362434	0.9070495	3.5937517
C	-1.3802434	3.9350495	-0.1042483
C	-1.6352434	0.0510495	-3.0682483
C	0.0407566	-2.0119505	1.5817517
C	0.2227566	-2.5239505	2.8737517
C	0.0497566	-1.4889505	3.7377517
C	-0.2662434	-0.3329505	2.9997517
C	0.1607566	-1.5289505	5.2367517
C	0.5907566	-3.9499505	3.1927517
C	-0.8142434	2.1220495	2.9347517
C	-0.9592434	3.4140495	3.5157517
C	-1.1982434	4.2870495	2.4697517
C	-1.1712434	3.4970495	1.2237517
C	-0.8852434	3.7310495	4.9887517
C	-1.4042434	5.7410495	2.4567517
C	-1.5172434	3.1200495	-1.2582483
C	-1.8272434	3.5880495	-2.5522483
C	-1.9072434	2.4820495	-3.4042483
C	-1.6632434	1.3350495	-2.6112483
C	-2.0322434	5.0360495	-2.9212483
C	-2.1642434	2.4070495	-4.8622483
C	-1.1792434	-1.0019505	-2.2932483
C	-1.0122434	-2.3289505	-2.8882483
C	-0.5252434	-3.1259505	-1.9112483



C	-0.3902434	-2.2519505	-0.7412483
C	-1.3522434	-2.6879505	-4.3152483
C	-0.1542434	-4.6029505	-1.9132483
N	-0.3032434	-0.6989505	1.6747517
N	-0.9342434	2.2810495	1.6407517
N	-1.4252434	1.7470495	-1.3452483
N	-0.7822434	-0.9929505	-1.0142483
Fe	-0.8362434	0.4790495	0.1807517
H	4.2685501	-3.2144471	-2.9147776
H	2.5601907	-3.5713512	-3.3058391
H	5.8637310	-4.3261265	0.8999370
H	4.8725659	-4.5218102	-0.5807292
H	0.3395382	-3.8215327	0.5150142
H	-0.4633880	0.9507015	4.6807370
H	-1.5202776	5.0067859	-0.2513239
H	-1.8779608	-0.1437342	-4.1108223
H	0.9373407	-0.8369897	5.6003817
H	-0.7855264	-1.2369597	5.7200490
H	0.4184891	-2.5332155	5.5981188
H	0.6786341	-4.1110115	4.2750575
H	1.5519956	-4.2335370	2.7342971
H	0.0973077	3.4559769	5.4055807
H	-1.6496896	3.1768585	5.5575282
H	-1.0400018	4.8022653	5.1772533
H	-2.3880663	6.0080259	2.0353476
H	-0.6449581	6.2481535	1.8383735
H	-1.1220083	5.6295463	-2.7384115
H	-2.8444118	5.4884430	-2.3295439
H	-2.2929266	5.1447067	-3.9826998
H	-3.0285339	1.7618630	-5.0906676
H	-1.2955729	1.9891973	-5.3970497
H	-1.2026042	-3.7609035	-4.4951509
H	-2.3992334	-2.4468319	-4.5558894
H	-0.7086158	-2.1360517	-5.0185779
H	-0.7565918	-5.1671709	-1.1845706
H	0.9079296	-4.7362447	-1.6509555
H	-1.3523987	6.1848952	3.4619978
H	-2.3712134	3.3948945	-5.2974780
H	3.5611035	-2.6403565	-4.4319879
H	5.6884454	-2.9620237	-0.2821248
H	-0.3128877	-5.0483187	-2.9045549
H	-0.1685358	-4.6538420	2.8148810
H	4.2227439	-2.3854573	1.8907160

## 2QCP

C	3.7652796	-0.2136012	-3.9388492
N	3.2982796	0.7953988	-3.1158492
C	3.1532796	-1.3516012	-3.5088492
C	2.4202796	0.2653988	-2.2548492
N	2.3012796	-1.0416012	-2.4718492
C	-3.9287204	5.1333988	1.5551508
C	-2.8357204	4.1103988	1.9111508
O	-2.7087204	3.6923988	3.0671508
N	-1.9797204	3.7503988	0.9291508
C	-0.8597204	2.8923988	1.2341508
C	0.4272796	3.6803988	1.2331508
O	0.6912796	4.5353988	0.3711508
C	-0.7097204	1.7633988	0.1941508
C	-1.7297204	0.7173988	0.2571508
C	-2.6827204	0.5123988	1.2201508
C	-1.9017204	-0.3246012	-0.6838492
N	-3.4237204	-0.5946012	0.9211508
C	-2.9817204	-1.1126012	-0.2618492
C	-1.2607204	-0.6316012	-1.8958492
C	-3.4327204	-2.1976012	-0.9918492
C	-1.6957204	-1.6976012	-2.5988492
C	-2.8127204	-2.4516012	-2.1798492
N	1.2752796	3.4323988	2.2391508
C	2.6182796	3.9973988	2.2361508
C	1.1082796	2.4433988	3.3541508
C	3.2512796	-2.5616012	1.2131508
S	1.4432796	-2.7036012	1.0241508
C	1.1212796	-1.0826012	1.6301508
C	1.0232796	-5.8316012	-2.3828492
S	-0.2287204	-4.5376012	-2.1048492
C	-0.9967204	-5.1426012	-0.5998492
Ag	0.8972796	-2.3556012	-1.3398492
H	3.2502972	-2.3645477	-3.8921415
H	1.8816065	0.8445494	-1.5062215
H	-3.5926667	6.1233336	1.8983698
H	0.2947045	1.3186814	0.3348049
H	-0.6774159	2.2293387	-0.8070410
H	-2.9065087	1.1117109	2.1043649
H	-0.4695700	0.0161895	-2.2833109
H	-1.2439880	-1.9387763	-3.5646054
H	-4.2906192	-2.7885697	-0.6611306
H	-3.1516736	-3.2789548	-2.8070395
H	-1.0694416	2.4757402	2.2223057

H	0.0664353	2.3933176	3.6937707
H	1.4562775	1.4401906	3.0569382
H	2.7201472	4.6643291	1.3721998
H	0.5230243	-6.7996924	-2.5268514
H	1.5625825	-5.5663616	-3.3022233
H	-0.2845081	-5.1686636	0.2376706
H	-1.8099624	-4.4426503	-0.3623588
H	-1.4209373	-6.1422689	-0.7718000
H	3.4812925	-2.3995156	2.2753932
H	3.7176889	-3.4995727	0.8828989
H	1.7023225	-0.3328610	1.0737698
H	1.3770094	-1.0150131	2.6988576
H	0.0507409	-0.8525295	1.5154746
H	-4.1455977	5.1793799	0.4789152
H	-4.8353978	4.8723618	2.1145552
H	1.7147644	2.7891474	4.2006540
H	2.7940374	4.5754092	3.1566546
H	3.3743666	3.1958237	2.1758466
H	3.6301254	-1.7302338	0.6022493
H	4.4918048	-0.0294104	-4.7258198
H	1.7303730	-5.8924927	-1.5433281
H	3.5564071	1.7739605	-3.1736019
H	-4.2225591	-0.9194451	1.4471581
H	-1.9469579	4.2704834	0.0602557

### 2VB3

C	0.7523193	4.0579550	-3.5597337
N	1.5213178	3.2159564	-2.7907351
C	-0.5296787	3.6609557	-3.3857341
C	0.7423194	2.3409578	-2.1847361
N	-0.5106787	2.5969575	-2.5187355
C	3.7783141	-1.8360352	4.9672519
C	3.0943153	-2.1920346	3.6512540
O	2.7003159	-3.3440326	3.4322544
N	2.9543154	-1.1880362	2.7882555
C	2.4353164	-1.3780358	1.4322577
C	3.5703146	-1.3540358	0.4272594
O	4.4133130	-0.4500375	0.4592593
C	1.4443182	-0.2860376	1.0472585
C	0.1483201	-0.3600376	1.7362573
C	-0.3756788	-1.4330358	2.3712562
C	-0.8236781	0.6819606	1.8372571
N	-1.6056769	-1.1250364	2.8892553
C	-1.9096763	0.1669615	2.5662558

C	-0.8796781	2.0039584	1.3912579
C	-3.0386745	0.9249602	2.8582553
C	-2.0006762	2.7499572	1.6802574
C	-3.0656744	2.2099582	2.4082561
N	3.5843146	-2.3340342	-0.4887390
C	4.5253129	-2.3310343	-1.5937372
C	2.6833159	-3.5010322	-0.5477389
C	-0.3026789	-0.7120370	-3.2347343
S	-1.6966767	-1.0320364	-2.1127363
C	-1.3906771	-2.7630334	-1.7647369
C	-5.2886705	1.3029596	-2.5037355
S	-4.6986716	1.4469594	-0.8027384
C	-5.2736707	3.0809566	-0.4137391
Ag	-2.0326762	1.3409595	-1.2977377
H	4.8647135	-1.9808639	4.8587256
H	1.9302990	0.6926588	1.2049871
H	1.2868282	-0.3558959	-0.0488520
H	0.0741764	-2.4068926	2.5672475
H	-0.0314857	2.4573144	0.8697212
H	-2.0467892	3.7954134	1.3644414
H	-3.8649255	0.5067647	3.4376177
H	-3.9221267	2.8445486	2.6495387
H	1.9399298	-2.3531233	1.4477761
H	2.4849676	-3.9083084	0.4535562
H	1.7264969	-3.2595224	-1.0420879
H	5.1505795	-1.4321581	-1.5249559
H	2.5318596	3.2626549	-2.7172718
H	-1.4495775	4.0575673	-3.8067206
H	1.0932868	1.5643017	-1.5077762
H	0.6552271	-0.7503283	-2.6946798
H	-0.4428692	0.2834544	-3.6720122
H	-2.1543786	-3.1017661	-1.0519175
H	-1.4825810	-3.3404131	-2.6952997
H	-0.3977583	-2.9100800	-1.3164857
H	-6.3881865	1.3120466	-2.5236625
H	-4.9315687	0.3389901	-2.8919420
H	-6.3730537	3.1047864	-0.4383000
H	-4.9391673	3.3135707	0.6049032
H	-4.8706480	3.8361324	-1.1037908
H	3.4191669	-2.5275688	5.7382544
H	3.5937897	-0.7967569	5.2744781
H	3.1780930	-4.2884613	-1.1290331
H	5.1775972	-3.2176322	-1.5525498
H	3.9896736	-2.3338836	-2.5576338

H	-0.3006630	-1.4599557	-4.0411775
H	1.1953738	4.8527133	-4.1546255
H	-4.8972500	2.1152160	-3.1328096
H	-2.1796405	-1.7462969	3.4408890
H	3.4616682	-0.3244949	2.9453088

## 2x50

C	-3.4470404	-5.2340085	1.9072932
S	-2.9060404	-4.3170085	3.3692932
C	0.4909596	-3.8220085	-0.4927067
S	-1.2890404	-3.7500085	-0.1827067
C	-0.6890404	5.1559915	-2.8447067
C	0.1099596	4.2689915	-1.8917068
O	1.1939596	4.6599915	-1.4537067
N	-0.4220404	3.0879915	-1.5727068
C	-0.0240404	2.3669915	-0.3467068
C	1.4679596	2.0629915	-0.0927067
O	2.0419596	2.6039915	0.8582932
C	-0.8600404	1.1039915	-0.1117067
C	-0.3830404	0.2969915	1.0542933
N	-0.6160404	0.6679915	2.3602933
C	0.3599596	-0.8330085	1.1102932
C	-0.0620404	-0.2140085	3.1722933
N	0.5339596	-1.1370085	2.4382933
N	2.0919596	1.1739915	-0.8927067
C	3.4699596	0.8369915	-0.5327068
C	1.6549596	0.4179915	-2.0757068
Ag	-1.1900404	-3.1820085	2.0792932
H	-1.4755302	4.6265396	-3.4029799
H	-1.9195743	1.3860364	0.0243233
H	-0.8349929	0.4445365	-0.9912551
H	0.7511471	-1.4485876	0.3086445
H	-0.0974908	-0.1731201	4.2593608
H	-0.2147327	3.0538691	0.4969225
H	0.7261457	0.8336073	-2.4861896
H	2.4285714	0.4979926	-2.8542911
H	3.7099225	1.2994462	0.4296510
H	-4.0713572	-6.0862327	2.2103810
H	-4.0598394	-4.5290569	1.3292310
H	1.1135283	-3.7167821	0.4079745
H	0.8095202	-3.0434710	-1.2096645
H	-2.5983099	-5.5277866	1.2734527
H	1.5060610	-0.6483113	-1.8344276
H	3.5786986	-0.2576034	-0.4578727

H	4.1705066	1.2088457	-1.2994482
H	0.0123689	5.6253046	-3.5457085
H	-1.1547746	5.9582478	-2.2523705
H	-1.3434744	2.8640783	-1.9281507
H	-1.1004538	1.5141215	2.6332573
H	0.7563860	-4.7890979	-0.9503806
H	-2.2183004	-5.3075507	3.9809924

### 3H94

C	-4.6225555	-0.0086008	3.0470927
S	-2.9485578	0.4993984	2.6560932
C	-2.0765592	-0.6616001	3.6530917
C	0.7144370	-2.5555973	-4.7038966
C	0.7914368	-1.2675991	-3.9818976
O	0.6534371	-0.2226006	-4.6018967
N	0.9684367	-1.3365991	-2.6748993
C	1.1264363	-0.1596006	-1.8659005
C	2.3174348	-0.4996001	-1.0359017
O	3.3944333	0.0253990	-1.2009013
C	-0.0585619	0.0283990	-0.9719018
C	0.0224379	1.2653974	-0.2169028
C	0.8754368	1.3503972	0.8830957
C	-0.5915612	2.4143957	-0.6509022
C	1.0514365	2.5553954	1.6140947
C	-0.4425613	3.6093939	0.0360968
C	0.3684375	3.6753939	1.1700952
N	2.1134350	-1.4255988	-0.1389028
C	3.1954335	-2.0115981	0.6410959
Ag	-2.8455580	2.5123955	2.9370927
H	-0.1243294	-3.1705225	-4.3388586
H	-0.2209154	-0.8402208	-0.3164955
H	-0.9532445	0.0511643	-1.6173475
H	1.4134161	0.4602010	1.2147180
H	-1.2124174	2.3857474	-1.5517187
H	1.7292478	2.5943926	2.4689402
H	-0.9310028	4.5145085	-0.3343808
H	0.5033050	4.6358809	1.6771538
H	1.3285702	0.7023919	-2.5109603
H	4.1411858	-1.6352106	0.2319298
H	-4.8362337	0.1007637	4.1189597
H	-5.3242549	0.5997144	2.4601346
H	-2.3292395	-0.5731816	4.7186852
H	-2.3357307	-1.6636675	3.2824405
H	-0.9988496	-0.4977041	3.5127558

H	1.6329823	-3.1519352	-4.5777554
H	0.5683792	-2.3517141	-5.7695495
H	3.1349164	-1.7167253	1.7014023
H	3.1750601	-3.1090244	0.5750866
H	1.1802381	-2.2353976	-2.2630132
H	1.2003053	-1.8379972	-0.0220068
H	-4.7377084	-1.0597268	2.7450594

### 3OPO

C	-4.0372970	0.2595603	-6.1999167
C	-4.2922963	0.1485605	-4.6889203
O	-4.8262950	-0.8574369	-4.2319214
N	-3.8112976	1.1715580	-3.9699221
C	-3.8492976	1.3215576	-2.5089258
C	-4.1052968	2.8045539	-2.2099266
O	-3.9172972	3.6415519	-3.0919242
C	-2.5063008	0.9305586	-1.8809275
C	-1.7153030	-0.1494387	-2.6109257
S	0.0026929	-0.2544384	-2.0349269
C	0.5886913	-1.6584350	-2.9779248
N	-4.5342958	3.1495530	-0.9929296
C	-4.8112950	4.5565495	-0.6969304
C	2.0596877	2.0805557	6.0570526
C	2.4556866	0.7425591	5.4480542
O	3.1736848	-0.0534389	6.0640526
N	1.9846877	0.4925596	4.2330572
C	2.3636868	-0.7314371	3.5470589
C	3.7946832	-0.6234375	3.0280601
O	4.6386812	-1.4564353	3.3580596
C	1.3906893	-1.0824363	2.4260617
C	1.8116881	-2.2774333	1.6180636
C	1.5006889	-3.5614300	2.0310626
C	2.5326863	-2.1144336	0.4500668
C	1.8866880	-4.6544272	1.2880644
C	2.9226853	-3.2054309	-0.2939314
C	2.5986862	-4.4784278	0.1280677
N	4.0646825	0.4005600	2.2210623
C	5.4376790	0.7205592	1.8080633
Ag	-0.9283049	-1.6014350	-0.2209314
H	-3.6777174	1.2451019	-6.5266980
H	-5.5464180	4.9620926	-1.4073064
H	1.3363148	2.6553828	5.4604014
H	0.4004325	-1.2545553	2.8846961
H	1.2909841	-0.2071371	1.7563554

H	0.9536989	-3.7077497	2.9676285
H	2.8251081	-1.1061582	0.1402411
H	1.6405290	-5.6608019	1.6347464
H	3.5191936	-3.0651818	-1.1996733
H	2.9194578	-5.3452605	-0.4547895
H	2.4131294	-1.5384465	4.2930501
H	5.9843033	1.2558544	2.6011367
H	-4.6565459	0.6721713	-2.1310982
H	-2.6718101	0.6515448	-0.8226770
H	-1.8669685	1.8309153	-1.8510133
H	-2.2108676	-1.1335319	-2.5842498
H	-1.6686055	0.1334045	-3.6747099
H	-0.1761230	-2.4422656	-3.0604197
H	1.4714698	-2.0595193	-2.4612563
H	0.8787761	-1.3259809	-3.9852006
H	-5.2032790	4.6350035	0.3240224
H	-3.8923466	5.1530031	-0.7835761
H	-3.2944800	-0.5055106	-6.4697543
H	-4.9671576	0.0101134	-6.7280932
H	1.6460968	1.8962962	7.0577631
H	2.9713915	2.6806034	6.1917741
H	5.9640331	-0.2212434	1.6087905
H	5.4112932	1.3354911	0.8988272
H	1.3470309	1.1429232	3.7940713
H	3.4036676	1.1678980	2.2130243
H	-4.8262200	2.4379619	-0.3362134
H	-3.5870638	2.0501847	-4.4356098

### **5FFE**

C	-4.8245433	1.1866051	-1.1763808
N	-4.7355435	-0.1143925	-0.7283815
C	-4.0465446	1.9226039	-0.3463821
C	-3.9475448	-0.1603925	0.3296167
N	-3.5165455	1.0616055	0.5816163
C	4.4764411	1.5246047	0.2266169
C	3.5294426	0.7096060	1.1026153
O	3.4744426	0.9056057	2.3186133
N	2.7834438	-0.1993925	0.4796163
C	1.6924456	-0.8863913	1.1616152
C	2.1014450	-2.2353889	1.7306143
O	1.5574460	-2.6743883	2.7356126
C	0.5114477	-1.0883909	0.2076169
C	-0.0305514	0.1776069	-0.3773821
C	0.2054483	1.4516048	0.0556170



C	-0.8815499	0.2946068	-1.5203803
N	-0.4605507	2.3496033	-0.7383815
C	-1.1335496	1.6636045	-1.7153800
C	-1.4595490	-0.6293917	-2.3973788
C	-1.9325481	2.1326037	-2.7543782
C	-2.2565476	-0.1643925	-3.4183771
C	-2.4875473	1.2016051	-3.5893767
N	3.0484435	-2.8993878	1.0786155
C	3.3794429	-4.2773855	1.4296149
Ag	-2.0745479	0.9606057	2.1026137
O	0.0344485	1.1746052	4.2156101
H	5.3649496	1.7697884	0.8206042
H	-0.2647412	-1.6459621	0.7590582
H	0.8226935	-1.7658894	-0.6077861
H	0.8574953	1.7996343	0.8574085
H	-1.2745065	-1.7001833	-2.2784363
H	-2.7032128	-0.8728751	-4.1201297
H	-2.1053962	3.2016418	-2.8991357
H	-3.1129417	1.5348377	-4.4215419
H	1.4007404	-0.2801391	2.0325137
H	2.8633262	-4.5118126	2.3678524
H	-5.1999078	-0.9066627	-1.1578588
H	-3.8378636	2.9880111	-0.3432079
H	-3.7119895	-1.0721307	0.8747316
H	0.9172242	1.4534087	3.9312272
H	0.2043083	0.3315733	4.6570299
H	3.9841650	2.4703988	-0.0493601
H	4.7754622	1.0055623	-0.6956502
H	4.4634900	-4.3926922	1.5738630
H	3.0468229	-4.9762380	0.6459836
H	3.5332203	-2.4477043	0.3147909
H	2.7675188	-0.1846201	-0.5338320
H	-5.4175109	1.4570873	-2.0452255
H	-0.3765274	3.3545854	-0.6779952

### 5KU5

C	5.1451249	1.1688679	1.5067839
C	4.2041259	0.0478691	1.0437844
O	4.3931257	-1.1101293	1.4207840
N	3.2071269	0.3948687	0.2277853
C	2.2841281	-0.5981301	-0.3432140
C	3.0101273	-1.6371289	-1.1962131
O	2.6971276	-2.8251276	-1.1262132
C	1.2051293	0.0688691	-1.2122130

C	0.2331303	0.9608683	-0.4642140
C	0.0401305	0.8768683	0.9237846
C	-0.5488687	1.8618671	-1.1822132
C	-0.8758683	1.7018675	1.5657838
C	-1.4648678	2.6818663	-0.5442138
C	-1.6298675	2.6018663	0.8297847
N	3.9651261	-1.1831293	-2.0052121
C	4.7681253	-2.0801285	-2.8382112
C	-2.1448671	-1.5931289	-2.3612117
N	-1.7918674	-1.3811293	-1.0502132
C	-1.7288675	-2.8451275	-2.6612114
C	-1.2048681	-2.4621280	-0.5682138
N	-1.1568681	-3.3671269	-1.5262128
C	-5.6818631	1.9278671	3.6917815
N	-6.5668620	1.5388675	2.7097826
C	-4.4878643	1.3918677	3.3617818
C	-5.9288627	0.8088683	1.8157836
N	-4.6678642	0.7068685	2.1897832
Ag	-3.3008657	-0.3451304	0.6387848
H	6.1138867	0.7111097	1.7369505
H	0.6428802	-0.7354355	-1.7117733
H	1.6931616	0.6415614	-2.0182719
H	-0.4199285	1.9366935	-2.2660962
H	0.6426580	0.1857575	1.5176784
H	-2.0514291	3.3982955	-1.1245405
H	-0.9819161	1.6500122	2.6527310
H	-2.3398756	3.2620317	1.3342926
H	1.8359558	-1.1934669	0.4662551
H	4.1096876	-2.8374877	-3.2822057
H	-1.7701072	-3.4198883	-3.5838326
H	-0.6691440	-4.2561902	-1.4780937
H	-0.7941044	-2.5904139	0.4313796
H	-7.5503803	1.7847766	2.6881337
H	-3.5275688	1.4504861	3.8667936
H	-6.3882229	0.3716821	0.9317890
H	4.7519799	1.6206926	2.4307868
H	5.2723562	1.9652556	0.7581932
H	5.5359501	-2.5999229	-2.2434385
H	5.2523280	-1.4990977	-3.6332923
H	-2.6445127	-0.8440953	-2.9689429
H	-5.9968044	2.5367097	4.5355075
H	4.2900207	-0.2343213	-1.8662005
H	3.0317092	1.3748910	0.0403340

## Cartesian coordinates of the CSD models

### AHIDUQ

N	0.3346306	0.8322808	1.3565874
C	1.5306306	0.2082808	1.4565874
H	2.3345818	0.5995530	0.8251785
C	1.7376306	-0.8637192	2.2935874
H	2.7282170	-1.3202498	2.3331866
C	0.6876306	-1.3417192	3.0465874
H	0.8183104	-2.2048093	3.7038060
C	-0.5543694	-0.7087192	2.9625874
C	-0.6923694	0.3752808	2.1095874
H	-1.6621818	0.8625519	1.9872225
C	4.8456306	2.5922808	0.7035874
F	6.0886306	2.1252808	0.5445874
F	4.9586306	3.8572808	1.0755874
F	4.3026306	1.9322808	1.7185874
S	3.8756306	2.4262808	-0.8354126
O	2.6066306	2.9752808	-0.4354126
O	3.8516306	1.0212808	-1.0904126
O	4.6096306	3.2132808	-1.7834126
N	-0.4043694	4.1262808	-1.3524126
N	0.4036306	-4.1267192	1.3525874
C	1.6436306	-4.6447192	1.5065874
H	2.4366559	-4.1902644	0.9072786
C	1.9076306	-5.6967192	2.3565874
H	2.9254061	-6.0858240	2.4266484
C	0.8796306	-6.2457192	3.0945874
H	1.0638769	-7.0857953	3.7687856
C	-0.3983694	-5.6957192	2.9795874
C	-0.5943694	-4.6507192	2.0885874
H	-1.5860118	-4.2139840	1.9192370
Ag	-0.1023694	-2.5057192	0.0005874
N	-0.3343694	-0.8317192	-1.3564126
C	-1.5303694	-0.2087192	-1.4564126
H	-2.3343949	-0.6001597	-0.8251992
C	-1.7373694	0.8632808	-2.2934126
H	-2.7280742	1.3195860	-2.3329853
C	-0.6873694	1.3422808	-3.0474126
H	-0.8188721	2.2053400	-3.7044752
C	0.5546306	0.7092808	-2.9634126
C	0.6916306	-0.3747192	-2.1094126
H	1.6616308	-0.8616894	-1.9870042

C	-4.8463694	-2.5927192	-0.7034126
F	-6.0893694	-2.1247192	-0.5444126
F	-4.9583694	-3.8567192	-1.0754126
F	-4.3023694	-1.9317192	-1.7184126
S	-3.8763694	-2.4267192	0.8355874
O	-2.6063694	-2.9747192	0.4345874
O	-3.8523694	-1.0217192	1.0905874
O	-4.6093694	-3.2137192	1.7835874
C	-1.6433694	4.6452808	-1.5064126
H	-2.4367282	4.1912311	-0.9071741
C	-1.9073694	5.6962808	-2.3564126
H	-2.9251778	6.0853562	-2.4263447
C	-0.8793694	6.2462808	-3.0944126
H	-1.0635349	7.0864299	-3.7684896
C	0.3986306	5.6952808	-2.9794126
C	0.5946306	4.6502808	-2.0884126
H	1.5860380	4.2130951	-1.9190743
Ag	0.1026306	2.5052808	-0.0004126
H	-1.2457213	-6.0839661	3.5468809
H	-1.4243004	-1.0660882	3.5156023
H	1.2461553	6.0834132	-3.5465621
H	1.4249430	1.0659573	-3.5162388

### AWUTAP

N	-3.5906045	1.2532638	-2.4300236
N	-1.5006051	0.1132641	-2.3270236
C	-2.2446049	1.2592638	-2.2790236
H	-1.7251448	2.2122759	-2.1546558
C	-2.2096049	-1.0017356	-2.5010236
H	-1.6284514	-1.9288308	-2.5221832
C	-3.5686045	-1.0567356	-2.6750235
C	-4.2326043	0.1412641	-2.6180235
H	-5.3223985	0.2034530	-2.7329889
Ag	0.6113943	0.1462641	-1.9940237
N	4.5383932	1.0452638	-0.2310242
N	2.6573937	0.0512641	-1.2940239
C	3.2973935	1.1022638	-0.8420240
H	2.8700217	2.0950113	-1.0268678
C	3.2613936	-1.1597355	-1.1050240
H	2.6966437	-2.0170281	-1.4822430
C	4.4883932	-1.3557355	-0.4960241
C	5.1043930	-0.1987358	-0.0790242
H	6.0863386	-0.2019232	0.4063784

C	-1.1856052	-1.5557354	0.5969756
H	-1.7142199	-2.4920766	0.3854414
C	0.1163944	0.8742639	1.1149754
H	0.6378340	1.8088549	1.3357426
C	-1.2316052	0.8442639	0.8929755
H	-1.8232743	1.7642520	0.9030875
C	0.1283944	-1.5667354	0.8659755
H	0.7153980	-2.4858735	0.9073653
C	-1.9216050	-0.4097357	0.7689755
C	0.7213943	-0.3257358	1.2889754
C	-3.3976046	-0.4577357	0.9669755
H	-3.8379744	-1.3140614	0.4350527
H	-3.8844653	0.4540154	0.5920406
C	2.0153939	-0.4707357	2.1069751
H	2.6721208	0.4010440	1.9648263
H	2.5717269	-1.3591781	1.7763266
C	-0.5156054	0.4752640	4.0619746
H	0.0107280	1.4100909	4.2846235
C	-1.8176050	-1.9547353	3.5439747
H	-2.3409071	-2.8887118	3.3244179
C	-0.4696054	-1.9247353	3.7659747
H	0.1232107	-2.8444197	3.7619069
C	-1.8296050	0.4862640	3.7919747
H	-2.4197435	1.4037497	3.7652405
C	0.2203944	-0.6707357	3.8899746
C	-2.4236049	-0.7547356	3.3699748
C	1.6953940	-0.6217357	3.6919747
H	2.1386892	0.2347507	4.2201952
H	2.1857821	-1.5333551	4.0619440
C	-3.7166045	-0.6097357	2.5509750
H	-4.3707377	-1.4841653	2.6894179
H	-4.2788352	0.2747941	2.8821833
O	0.6163943	1.6572637	-4.4130230
O	0.9143942	3.9612630	-5.4150227
O	2.0223939	3.2462632	-3.3370233
S	1.3873941	2.8042634	-4.5780230
F	3.3883935	1.3562638	-4.9140229
F	2.1783939	2.3052635	-6.8450223
F	3.4943935	3.4372632	-5.7490226
C	2.7723937	2.3152635	-5.6350227
H	-4.0724696	-2.0107468	-2.8339867
H	4.9218645	-2.3494142	-0.3832031

**CUCSOI**

N	3.5764259	0.0001308	4.2964371
C	3.9204259	0.0001308	5.3884371
C	4.3114259	0.0001308	6.7744371
C	4.4844259	1.2501308	7.4134371
C	4.8314259	1.2291308	8.7834371
C	5.0474259	0.0001308	9.4324371
Ag	2.0074259	0.0001308	2.8444371
C	4.8314259	-1.2288692	8.7834371
C	4.4844259	-1.2498692	7.4134371
N	0.0814259	0.0001308	1.9424371
C	3.9104259	1.2311308	0.4394371
C	2.7394259	1.2381308	-0.3565629
C	2.1984259	0.0001308	-0.7065629
C	4.4484259	0.0001308	0.8614371
N	-0.0855741	0.0001308	-1.9405629
C	0.9324259	0.0001308	-1.4285629
C	2.7394259	-1.2378692	-0.3565629
C	3.9104259	-1.2308692	0.4394371
Ag	-2.0115741	0.0001308	-2.8415629
C	-3.9145741	-1.2308692	-0.4365629
C	-2.7445741	-1.2378692	0.3594371
C	-2.2025741	0.0001308	0.7084371
C	-4.4525741	0.0001308	-0.8585629
C	-0.9365741	0.0001308	1.4314371
C	-2.7445741	1.2381308	0.3594371
C	-3.9145741	1.2311308	-0.4365629
N	-3.5805741	0.0001308	-4.2935629
C	-3.9245741	0.0001308	-5.3855629
C	-4.3155741	0.0001308	-6.7725629
C	-4.4885741	-1.2498692	-7.4115629
C	-4.8355741	-1.2288692	-8.7805629
C	-5.0515741	0.0001308	-9.4305629
C	-4.8355741	1.2291308	-8.7805629
C	-4.4885741	1.2501308	-7.4115629
P	-1.2265741	-3.7008692	-3.7195629
F	-1.3975741	-2.8798692	-2.3635629
F	-1.0485741	-4.4458692	-5.1045629
F	-1.6045741	-2.3678692	-4.5085629
F	-0.8485741	-4.9988692	-2.9095629
F	0.3034259	-3.2678692	-3.7605629
F	-2.7695741	-4.1008692	-3.6985629
P	1.2224259	3.7011308	3.7214371
F	1.3934259	2.8801308	2.3664371

F	1.0444259	4.4461308	5.1074371
F	1.6004259	2.3681308	4.5114371
F	0.8444259	4.9991308	2.9124371
F	-0.3075741	3.2681308	3.7624371
F	2.7654259	4.1011308	3.7014371
H	-5.3429764	0.0005242	-10.4837331
H	-4.3063644	-2.1784159	-6.8667868
H	-4.9742431	2.1666959	-9.3227286
H	-4.3329613	2.1834889	-6.8693329
H	-4.3472252	-2.1729673	-0.7775469
H	-5.3320226	-0.0025587	-1.5069719
H	-4.3747708	2.1714824	-0.7454553
H	-2.2754362	2.1650670	0.6953857
H	-2.2607034	-2.1733474	0.6409959
H	2.2702160	-2.1648128	-0.6923077
H	2.2554569	2.1735552	-0.6380457
H	4.3706670	-2.1714218	0.7476059
H	5.3279975	0.0029467	1.5096595
H	4.3289195	-2.1832933	6.8712873
H	4.3020207	2.1787650	6.8688662
H	4.9708883	-2.1663144	9.3255509
H	5.3388392	-0.0003473	10.4856548
H	4.9648096	2.1678022	9.3246160
H	-4.9691882	-2.1675167	-9.3217564
H	4.3427696	2.1732234	0.7808383

### KAPFOY

C	3.9174262	-3.8427900	-1.6087684
H	4.8616438	-3.9000234	-1.0413604
H	3.8617243	-2.8705918	-2.1280378
C	2.6244274	-3.1467906	0.2902301
C	3.3834267	-2.0557915	0.5772298
H	4.2009807	-1.7557339	-0.0800617
C	3.1004268	-1.2967921	1.7072289
H	3.7345826	-0.4326666	1.9215753
C	2.0754277	-1.6257918	2.5302282
H	1.8702215	-1.0345994	3.4259184
C	1.2914283	-2.7017909	2.2342284
H	0.4732779	-2.9803065	2.9079110
C	1.5224283	-3.4977903	1.1252293
O	2.7924271	-4.0367898	-0.7527690
N	0.7694289	-4.6417893	0.8212296
H	0.4539012	-5.1590331	1.6331737

H	1.2311588	-5.2321195	0.1373071
N	4.1974259	1.3082057	-2.5177676
O	4.2604259	2.1602049	-1.7167683
O	3.3824267	0.4932064	-2.5177676
O	5.0494253	1.3712056	-3.3187669
C	-1.6705690	1.9902051	2.4482283
H	-2.6151712	1.9509123	1.8795427
H	-1.6006087	2.9488400	2.9882728
C	-0.3765702	2.6862045	0.5492298
C	-1.1355696	3.7772036	0.2622301
H	-1.9725497	4.0566596	0.9043285
C	-0.8525699	4.5362029	-0.8677690
H	-1.4752440	5.4100253	-1.0769910
C	0.1724294	4.2072032	-1.6907683
H	0.3985898	4.8117945	-2.5715867
C	0.9554286	3.1312041	-1.3947685
H	1.8357487	2.8826892	-1.9989518
C	0.7254289	2.3352048	-0.2847695
O	-0.5445700	1.7962052	1.5922289
N	1.4784283	1.1912058	0.0182303
C	-2.8975681	-0.9787924	0.3872300
C	-3.7825672	-1.0987923	1.3782292
H	-3.6626371	-1.8684462	2.1446362
C	-4.8815663	-0.2197930	1.4252291
H	-5.5988532	-0.3161343	2.2433857
C	-5.0505663	0.7512061	0.4712299
H	-5.9082750	1.4256364	0.5194734
C	-4.1575669	0.8502061	-0.5697693
H	-4.2840470	1.6151976	-1.3355402
C	-3.0585679	-0.0037932	-0.6097692
C	-2.1095687	1.1362058	-2.5107676
H	-2.0742061	2.1107378	-1.9968169
H	-3.0045262	1.0698537	-3.1503593
N	-1.7390259	-1.8165268	0.2699025
O	-2.0705687	0.0632067	-1.5707684
Ag	0.1544294	-0.6107927	0.1972301
H	-1.7222953	-2.5606338	0.9643459
H	-1.7096016	-2.2597540	-0.6498458
H	2.2601311	1.0826026	-0.6598694
H	1.8888721	1.2545772	0.9503267
H	3.8857657	-4.6542185	-2.3460869
H	-1.2086501	1.0260671	-3.1255060
H	-1.6524935	1.1646966	3.1708762



## QANZOX

Ag	2.3533554	-0.0770021	-0.0237228
N	3.9313549	0.5559978	1.2832768
N	0.7363558	-0.7860019	-1.2787225
C	4.3283548	1.8129974	1.2182768
H	3.8334213	2.4756799	0.5038994
C	5.3643545	2.3109973	2.0502766
H	5.6615814	3.3573377	1.9539996
C	5.9753543	1.4579975	2.9552763
C	5.4973545	0.1239979	2.9872763
H	5.9257485	-0.6073742	3.6754859
C	4.5233547	-0.2680020	2.1492766
H	4.1657741	-1.3057041	2.1679881
C	0.2143560	0.0509979	-2.1787222
H	0.5809266	1.0799176	-2.2020993
C	-0.7806438	-0.3460020	-3.0347220
H	-1.2056801	0.3811455	-3.7289557
C	-1.2696436	-1.6960016	-2.9787220
C	-0.7146438	-2.5170014	-2.0337223
H	-1.0333640	-3.5562865	-1.9231151
C	0.2623559	-2.0480015	-1.1887225
H	0.7187065	-2.6981348	-0.4321304
P	2.5133553	-4.0120010	1.9382766
F	3.2033551	-5.3800006	1.6062767
F	1.9313555	-4.6620008	3.2042763
F	3.8123549	-3.5400011	2.7662764
F	1.8603555	-2.6360013	2.2442765
F	3.1393551	-3.3540011	0.6482770
F	1.2573557	-4.4750008	1.1152768
Ag	-2.3536433	0.0769979	0.0242771
N	-3.9306429	-0.5560019	-1.2837225
N	-0.7366438	0.7859977	1.2782768
C	-4.3286428	-1.8130016	-1.2177225
H	-3.8338399	-2.4755500	-0.5031407
C	-5.3646425	-2.3110014	-2.0497223
H	-5.6620240	-3.3572816	-1.9532116
C	-5.9756423	-1.4580017	-2.9557220
C	-5.4976424	-0.1240020	-2.9867220
H	-5.9262533	0.6075022	-3.6746968
C	-4.5236427	0.2679978	-2.1497222
H	-4.1658420	1.3056152	-2.1688069
C	-0.2146439	-0.0510021	2.1782765
H	-0.5809341	-1.0800172	2.2015974

C	0.7803558	0.3459978	3.0342763
H	1.2051808	-0.3816535	3.7281486
C	1.2703557	1.6959974	2.9792763
C	0.7143558	2.5169972	2.0342766
H	1.0326921	3.5564008	1.9235571
C	-0.2626439	2.0479973	1.1892768
H	-0.7187940	2.6985012	0.4328754
P	-2.5136433	4.0119968	-1.9377223
F	-3.2036431	5.3799964	-1.6067224
F	-1.9316434	4.6619966	-3.2047219
F	-3.8116429	3.5399969	-2.7667221
F	-1.8606435	2.6359972	-2.2437222
F	-3.1396431	3.3539970	-0.6487227
F	-1.2566436	4.4749967	-1.1157225
H	-6.7765722	-1.7935364	-3.6172151
H	-2.0547842	-2.0310843	-3.6590113
H	2.0557449	2.0306514	3.6594324
H	6.7765424	1.7934740	3.6165287

## QUJJIR

Au	6.4100245	4.0530618	-2.5914429
Ag	1.7230258	1.2060626	1.4565559
Cl	7.8330241	5.8500613	-2.6794429
N	4.2890250	1.9630623	-1.8094432
N	1.3240259	-0.7769369	1.1355560
N	0.7690260	1.1040626	3.2775554
N	2.1430257	3.1660620	1.7565558
N	5.6370247	1.3100625	-3.3224427
C	3.4280253	2.4240622	-0.7404435
C	4.0470251	0.6070627	-2.0024431
C	3.0720254	0.1640629	-1.0304434
C	2.5520255	-1.1279368	-0.9554434
C	1.6610258	-1.5209367	0.0405563
C	0.9830260	-2.7869363	0.0885563
H	1.0697191	-3.5672271	-0.6658870
C	0.2250262	-2.7879363	1.2315560
H	-0.4307892	-3.5740488	1.6018084
C	0.4600261	-1.5389367	1.9105558
C	-0.0369737	-1.2369368	3.1715554
C	0.2130262	-0.0229371	3.8475552
C	-0.0199737	0.2300628	5.2415549
H	-0.4428873	-0.4941131	5.9364079
C	0.3700261	1.5040625	5.4975548

H	0.3332418	2.0374645	6.4464565
C	0.8450260	2.0670623	4.2695551
C	1.2480259	3.3890619	4.0735552
C	1.7280258	3.8890618	2.8525555
C	1.8610257	5.2870614	2.5625556
H	1.6066110	6.0798061	3.2645720
C	2.3150256	5.4050614	1.3025560
H	2.5498750	6.3139464	0.7503898
C	2.5610255	4.0750618	0.8045561
C	3.2580253	3.7770618	-0.3854436
C	2.7600255	1.2900625	-0.2554436
C	4.8960249	0.2090628	-2.9974428
H	5.0457420	-0.7597015	-3.4645791
C	5.2950248	2.3920622	-2.5794430
C	6.6040244	1.2980625	-4.4254424
H	7.0374637	0.2932381	-4.5069650
H	7.3969360	2.0263301	-4.2150909
H	6.1083545	1.5687580	-5.3687779
Au	-6.4099719	-4.0529360	2.5915556
Ag	-1.7229733	-1.2059368	-1.4564433
Cl	-7.8329715	-5.8499355	2.6795556
N	-4.2889725	-1.9629365	1.8095558
N	-1.3239734	0.7760627	-1.1354434
N	-0.7689735	-1.1039368	-3.2784428
N	-2.1429731	-3.1659362	-1.7564432
N	-5.6369722	-1.3099367	3.3225554
C	-3.4279728	-2.4239364	0.7405561
C	-4.0469726	-0.6069369	2.0025558
C	-3.0719729	-0.1639371	1.0305560
C	-2.5519730	1.1280626	0.9545561
C	-1.6609733	1.5210625	-0.0414437
C	-0.9829735	2.7870621	-0.0884436
H	-1.0700607	3.5670739	0.6661879
C	-0.2249737	2.7880621	-1.2314433
H	0.4310400	3.5740599	-1.6018173
C	-0.4599736	1.5390625	-1.9104431
C	0.0370262	1.2370626	-3.1714428
C	-0.2139737	0.0230629	-3.8474426
C	0.0200262	-0.2299370	-5.2414422
H	0.4430533	0.4943067	-5.9362620
C	-0.3699736	-1.5039367	-5.4974421
H	-0.3328193	-2.0374205	-6.4463446
C	-0.8449735	-2.0669365	-4.2694425
C	-1.2479734	-3.3899361	-4.0734425

C	-1.7279733	-3.8889360	-2.8524429
C	-1.8609732	-5.2879356	-2.5624430
H	-1.6065465	-6.0807456	-3.2643515
C	-2.3149731	-5.4049356	-1.3024433
H	-2.5498679	-6.3135332	-0.7498356
C	-2.5609730	-4.0749360	-0.8044434
C	-3.2579728	-3.7769360	0.3855562
C	-2.7599730	-1.2899367	0.2555563
C	-4.8959724	-0.2099370	2.9975555
H	-5.0455001	0.7588276	3.4647132
C	-5.2949723	-2.3919364	2.5795556
C	-6.6039719	-1.2979367	4.4255551
H	-7.0373749	-0.2931249	4.5070811
H	-7.3968380	-2.0261935	4.2151465
H	-6.1083019	-1.5686608	5.3688407
H	-2.8073402	1.8579778	1.7235441
H	-0.6049075	-2.0082466	3.6925701
H	1.1277392	4.0944332	4.8962729
H	3.7182660	4.5741288	-0.9707153
H	2.8072702	-1.8576244	-1.7247793
H	0.6050331	2.0082240	-3.6928102
H	-1.1272377	-4.0953744	-4.8960575
H	-3.7181547	-4.5739569	0.9707824

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F	-1.1179887	4.3038603	3.0323700
F	-1.1759887	5.0698603	1.1013700
F	-2.7949887	4.0018603	1.8713700
F	2.0740113	-3.1241397	-2.3366300
F	0.1580113	-3.7371397	-2.1456300
F	1.5870113	-4.1181397	-0.7196300
O	-0.7419887	2.6918603	0.0643700
O	-0.6569887	1.8538603	2.0833700
O	0.6370113	-0.9851397	-1.5866300
O	0.5690113	-1.9501397	0.3783700
C	-0.9239887	2.7208603	1.2543700
C	-1.4739887	4.0318603	1.7943700
C	0.7050113	-1.9241397	-0.8266300
C	1.0820113	-3.2331397	-1.5016300
Ag	0.0260113	-0.2031397	1.6043700
Ag	0.3530113	1.0838603	-1.0136300
O	0.2260113	-3.9831397	3.2773700
O	-3.7199887	-0.1041397	3.0973700

O	4.1320113	-1.5431397	1.2893700
O	1.1060113	1.1268603	5.0783700
O	3.8520113	0.1118603	-3.3796300
O	2.8990113	3.4148603	0.9543700
O	-0.9979887	-1.2871397	-5.0156300
O	-0.0269887	3.7778603	-3.0146300
O	-3.1569887	-3.8041397	-0.7246300
O	-4.1999887	1.5328603	-1.7286300
C	-4.0649887	-2.2971397	1.4363700
H	-4.9281635	-1.8018900	1.9008028
H	-4.3019209	-3.3618449	1.3136485
C	-2.8689887	-2.1611397	2.3573700
C	-1.8859887	-3.1521397	2.4003700
H	-2.0135639	-4.0149950	1.7464152
C	-0.7639887	-3.0261397	3.1993700
C	-0.5859887	-1.8891397	3.9933700
C	-1.5829887	-0.8981397	3.9603700
H	-1.4317188	-0.0087651	4.5732466
C	-2.7089887	-1.0341397	3.1583700
C	0.2110113	-5.0231397	2.3083700
H	0.2288838	-4.6126665	1.2867850
H	-0.6657426	-5.6821054	2.4321615
C	-3.6069887	1.0468603	3.9363700
H	-2.7098368	1.6366114	3.6856516
H	-3.5799384	0.7638916	5.0024833
C	0.6630113	-1.6581397	4.8103700
H	1.0845750	-2.6250789	5.1159761
H	0.4116408	-1.0894096	5.7148366
C	1.6920113	-0.8941397	4.0023700
C	2.4660113	-1.5801397	3.0693700
H	2.3130940	-2.6559440	2.9841424
C	3.3540113	-0.9221397	2.2423700
C	3.4990113	0.4658603	2.3253700
C	2.7330113	1.1488603	3.2593700
H	2.8396380	2.2320878	3.3073701
C	1.8420113	0.4898603	4.0993700
C	4.1590113	-2.9621397	1.2773700
H	3.1720843	-3.3821738	1.0251447
H	4.4941475	-3.3671987	2.2479640
C	1.0660113	2.5508603	5.0543700
H	0.6792823	2.9198567	4.0915667
H	2.0584558	2.9883111	5.2584172
C	4.4730113	1.1888603	1.4243700
H	5.3706790	0.5680392	1.3010642

H	4.7671516	2.1333061	1.9023018
C	3.8980113	1.4938603	0.0523700
C	4.1600113	0.6578603	-1.0216300
H	4.7611435	-0.2300342	-0.8366690
C	3.6290113	0.9228603	-2.2826300
C	2.8360113	2.0468603	-2.4906300
C	2.5900113	2.8908603	-1.4106300
H	1.9698757	3.7711287	-1.5836930
C	3.1100113	2.6188603	-0.1546300
C	4.6370113	-1.0561397	-3.1476300
H	4.1528091	-1.7248841	-2.4180729
H	5.6539520	-0.8000121	-2.8051967
C	2.3660113	4.7078603	0.7513700
H	1.3272793	4.6697991	0.3808143
H	2.9789940	5.2930670	0.0437153
C	2.2070113	2.3278603	-3.8396300
H	2.1721089	3.4141047	-4.0014104
H	2.8277866	1.8801778	-4.6259827
C	0.8020113	1.7688603	-3.9306300
C	0.5640113	0.4998603	-4.4556300
H	1.4236113	-0.0694773	-4.8089951
C	-0.7109887	-0.0471397	-4.4816300
C	-1.7919887	0.6528603	-3.9426300
C	-1.5639887	1.9328603	-3.4386300
H	-2.4114554	2.4721592	-3.0188319
C	-0.2909887	2.4928603	-3.4476300
C	0.0620113	-1.9901397	-5.6666300
H	0.8599827	-2.2622139	-4.9546959
H	0.4924536	-1.3969933	-6.4916236
C	-1.1339887	4.5708603	-2.5636300
H	-1.5951409	4.1299710	-1.6674796
H	-1.8836633	4.6956149	-3.3630724
C	-3.1839887	0.0558603	-3.8526300
H	-3.2958510	-0.7191363	-4.6215157
H	-3.9267353	0.8426813	-4.0418138
C	-3.4419887	-0.5541397	-2.4846300
C	-3.1819887	-1.8951397	-2.2506300
H	-2.7934591	-2.4912901	-3.0772800
C	-3.3799887	-2.4651397	-0.9966300
C	-3.8309887	-1.6901397	0.0643700
C	-4.0849887	-0.3441397	-0.1676300
H	-4.4320013	0.2581379	0.6726912
C	-3.9079887	0.2198603	-1.4236300
C	-2.9779887	-4.6771397	-1.8276300

H	-2.0475128	-4.4662516	-2.3763408
H	-3.8301472	-4.6212101	-2.5275086
C	-4.6629887	2.3818603	-0.6906300
H	-3.9150837	2.4959753	0.1117812
H	-5.6077620	2.0138988	-0.2543273
H	1.1216166	-5.6122343	2.4785684
H	0.3769631	2.8476862	5.8553608
H	2.3719345	5.2043110	1.7307083
H	4.8769754	-3.2497733	0.4982398
H	-2.9208268	-5.6915246	-1.4109817
H	-0.3862276	-2.9057515	-6.0730473
H	-4.8406640	3.3623251	-1.1513681
H	-0.7122757	5.5504257	-2.3051100
H	-4.5024333	1.6513720	3.7447601
H	4.7039816	-1.5728210	-4.1136287

## SUDLUA

Au	4.4345175	-0.7170108	-3.5183983
S	-2.9104618	-2.0640070	-3.0783997
O	-0.2694692	-2.9690043	-5.2103937
N	-4.0594585	-2.4890059	-5.3823933
H	-4.0969137	-2.5031748	-6.3922925
N	-2.2164637	-1.1500095	-5.5803927
N	2.9555218	0.5099860	-4.2573963
N	2.3125235	2.7859794	-4.4743959
N	0.0615298	3.3759779	-4.5963953
H	-0.9078583	3.0837678	-4.3527337
C	-5.0554558	-3.2690036	-4.6733953
H	-4.6031404	-4.1421751	-4.1782238
H	-5.8054699	-3.6104546	-5.3978303
H	-5.5496405	-2.6606572	-3.9019495
C	-3.0324615	-1.8820075	-4.8073949
C	-0.9074675	-0.7280107	-5.1673939
C	0.1185298	-1.7000080	-4.9983943
C	1.3835262	-1.2830090	-4.6593953
H	2.1967173	-1.9886935	-4.4861419
C	1.6745253	0.0829870	-4.5523953
C	0.6645282	1.0449843	-4.7643951
C	-0.6424682	0.5969857	-5.0783942
H	-1.4701050	1.3090870	-5.1666242
C	3.1915211	1.7999821	-4.2943963
H	4.2230605	2.1202396	-4.0627527
C	1.0165272	2.4249804	-4.6193953

C	-2.4774629	-1.0270100	-7.0293886
H	-2.2816587	-1.9779878	-7.5556903
H	-1.8050623	-0.2621912	-7.4307124
H	-3.5128778	-0.6976891	-7.2066176
C	0.7245281	-4.0300015	-5.1353941
H	1.0491898	-4.1328715	-4.0853707
H	1.6023176	-3.7410688	-5.7386945
C	0.0715298	-5.2479980	-5.6553923
H	-0.8194055	-5.4983568	-5.0605253
H	0.7605935	-6.1045217	-5.6152765
H	-0.2397891	-5.1088706	-6.7011045
Au	-1.2964663	-0.7170108	-2.2744021
S	6.0495131	-2.0640070	-2.7144007
O	3.4085205	-2.9690043	-0.5824067
N	7.1975098	-2.4890059	-0.4114072
H	7.1820805	-2.5673595	0.5970300
N	5.3545151	-1.1500095	-0.2134078
N	0.1825295	0.5099860	-1.5364042
N	0.8255278	2.7859794	-1.3184046
N	3.0765213	3.3759779	-1.1964051
H	4.0530445	3.0835796	-1.4515532
C	8.1935071	-3.2690036	-1.1204052
H	7.7483472	-4.1565849	-1.5976770
H	8.9560557	-3.5894129	-0.3990941
H	8.6712191	-2.6621628	-1.9028247
C	6.1705128	-1.8820075	-0.9864053
C	4.0455187	-0.7280107	-0.6254063
C	3.0195215	-1.7000080	-0.7944062
C	1.7555252	-1.2830090	-1.1344052
H	0.9424465	-1.9936617	-1.2856398
C	1.4635260	0.0829870	-1.2414049
C	2.4735232	1.0449843	-1.0284053
C	3.7815195	0.5969857	-0.7144063
H	4.6103108	1.3095683	-0.6311822
C	-0.0534698	1.7999821	-1.4994042
H	-1.0839232	2.1125675	-1.7292760
C	2.1215241	2.4249804	-1.1734052
C	5.6165143	-1.0270100	1.2365881
H	5.2204554	-1.8937907	1.7964410
H	5.0768778	-0.1442410	1.5999355
H	6.6890291	-0.8659207	1.4153279
C	2.4135233	-4.0300015	-0.6584063
H	2.0923540	-4.1251283	-1.7118363
H	1.5372374	-3.7518350	-0.0491605



C	3.0665215	-5.2479980	-0.1374081
H	3.9731561	-5.4899751	-0.7120163
H	2.3805612	-6.1065064	-0.1898238
H	3.3402610	-5.0867656	0.9165939
Cl	5.9785132	2.7079797	-2.4104013
Cl	-2.8404619	2.7079797	-3.3833989
Cl	2.8405221	-2.7080050	3.3825821
Au	-4.4354575	0.7169851	3.5185817
S	2.9105218	2.0639815	3.0785828
O	0.2695293	2.9689790	5.2105769
N	4.0595187	2.4889802	5.3825767
H	4.0972261	2.5034755	6.3924547
N	2.2165238	1.1499840	5.5805758
N	-2.9554617	-0.5100113	4.2565797
N	-2.3124635	-2.7860050	4.4745789
N	-0.0614698	-3.3760032	4.5965787
H	0.9077483	-3.0836118	4.3526055
C	5.0545158	3.2689780	4.6725787
H	4.6014868	4.1416216	4.1771253
H	5.8048374	3.6113553	5.3962812
H	5.5486468	2.6604739	3.9012229
C	3.0325215	1.8819820	4.8075781
C	0.9075275	0.7279851	5.1675771
C	-0.1184697	1.6999825	4.9985777
C	-1.3834660	1.2829837	4.6595787
H	-2.1966351	1.9886602	4.4861679
C	-1.6744652	-0.0830125	4.5525788
C	-0.6644681	-1.0450099	4.7645783
C	0.6425282	-0.5970110	5.0785774
H	1.4701433	-1.3091136	5.1668557
C	-3.1914609	-1.8000077	4.2945797
H	-4.2230416	-2.1203004	4.0631130
C	-1.0164671	-2.4250060	4.6195787
C	2.4775231	1.0269844	7.0295718
H	2.2816344	1.9779394	7.5558835
H	1.8051901	0.2621031	7.4308892
H	3.5129683	0.6977559	7.2067947
C	-0.7244679	4.0299760	5.1355772
H	-1.0491482	4.1328482	4.0855583
H	-1.6022671	3.7410428	5.7388652
C	-0.0714698	5.2479725	5.6555757
H	0.8194689	5.4983322	5.0607127
H	-0.7605353	6.1044957	5.6154597
H	0.2398541	5.1088456	6.7012868

Au	1.2965263	0.7169851	2.2745852
S	-6.0494529	2.0639815	2.7145839
O	-3.4084605	2.9689790	0.5825899
N	-7.1974498	2.4889802	0.4115907
H	-7.1829710	2.5668288	-0.5969183
N	-5.3544549	1.1499840	0.2135909
N	-0.1824695	-0.5100113	1.5365874
N	-0.8254677	-2.7860050	1.3185878
N	-3.0764613	-3.3760032	1.1965883
H	-4.0534804	-3.0840330	1.4505309
C	-8.1934469	3.2689780	1.1205887
H	-7.7482216	4.1565566	1.5977733
H	-8.9559656	3.5893311	0.3992293
H	-8.6711046	2.6621808	1.9030724
C	-6.1704527	1.8819820	0.9855888
C	-4.0454587	0.7279851	0.6255898
C	-3.0194615	1.6999825	0.7945897
C	-1.7554650	1.2829837	1.1345887
H	-0.9423774	1.9935865	1.2859931
C	-1.4634658	-0.0830125	1.2405881
C	-2.4734630	-1.0450099	1.0285887
C	-3.7814593	-0.5970110	0.7145897
H	-4.6103781	-1.3095257	0.6317745
C	0.0535299	-1.8000077	1.4995877
H	1.0839326	-2.1126591	1.7296239
C	-2.1214639	-2.4250060	1.1735884
C	-5.6164542	1.0269844	-1.2364049
H	-5.2204440	1.8938007	-1.7962238
H	-5.0768173	0.1442489	-1.5998321
H	-6.6889634	0.8658438	-1.4151400
C	-2.4134632	4.0299760	0.6585898
H	-2.0923515	4.1251227	1.7120337
H	-1.5371204	3.7518560	0.0493988
C	-3.0664613	5.2479725	0.1375913
H	-3.9730972	5.4899508	0.7121979
H	-2.3804783	6.1064614	0.1899939
H	-3.3402086	5.0867606	-0.9164127
Cl	-5.9784532	-2.7080050	2.4105848
C	0.2802704	4.8227905	-4.4557766
H	0.3781337	5.0901891	-3.3912458
H	1.1980400	5.1141615	-4.9820774
H	-0.5905313	5.3378154	-4.8807338
C	2.8588144	4.8228442	-1.3380705
H	3.7713111	5.3275429	-0.9973397

H	2.6765753	5.0815609	-2.3935026
H	1.9943919	5.1361607	-0.7380249
C	-2.8587543	-4.8228695	1.3382541
H	-1.9593198	-5.1241199	0.7858640
H	-2.7347515	-5.0876458	2.4006055
H	-3.7461096	-5.3326639	0.9426211
C	-0.2801955	-4.8227173	4.4549277
H	-0.3878328	-5.0883879	3.3909137
H	0.5950695	-5.3372907	4.8710590
H	-1.1928532	-5.1162551	4.9889137

### SUMREA

Ag	-1.2170611	2.9824594	0.2757634
Ag	1.4639389	3.4134594	-0.2362366
O	-0.9860611	1.2344594	-1.0172366
O	1.1719389	1.4224594	-1.1292366
C	0.1719389	-2.7665406	-3.7162366
C	-1.0310611	-2.2635406	-3.2722366
H	-1.9817396	-2.7611777	-3.4562124
C	-0.9400611	-1.1185406	-2.4722366
H	-1.8890490	-0.7173881	-2.0914013
C	0.1389389	-0.4735406	-2.1162366
C	1.2929389	-0.9615406	-2.7462366
H	2.2125323	-0.3840166	-2.5768398
C	1.3839389	-2.0815406	-3.5672366
H	2.3217866	-2.4214680	-4.0045033
C	0.1999389	0.9024594	-1.3732366
O	0.9789389	5.0484594	1.1027634
O	-1.2090611	4.7944594	1.3667634
Ag	-1.2170611	-3.2745406	0.2757634
Ag	1.4639389	-2.8435406	-0.2362366
O	-0.9860611	-5.0225406	-1.0172366
O	1.1719389	-4.8345406	-1.1292366
C	0.1719389	-9.0235406	-3.7162366
C	-1.0310611	-8.5205406	-3.2722366
H	-1.9855035	-9.0079116	-3.4670154
C	-0.9400611	-7.3755406	-2.4722366
H	-1.8909618	-6.9738420	-2.0964810
C	0.1389389	-6.7305406	-2.1162366
C	1.2929389	-7.2185406	-2.7462366
H	2.2154274	-6.6492231	-2.5676356
C	1.3839389	-8.3385406	-3.5672366
H	2.3233488	-8.6796316	-4.0004011

C	0.1999389	-5.3545406	-1.3732366
O	0.9789389	-1.2085406	1.1027634
O	-1.2090611	-1.4625406	1.3667634
C	-0.2570611	2.7024594	3.9207634
C	0.8619389	2.3294594	3.1237634
H	1.7566079	2.9589521	3.1731039
C	0.8949389	1.2534594	2.3337634
H	1.8251319	1.0234137	1.8040921
C	-0.1010611	0.3964594	2.2657634
C	-1.1600611	0.7344594	2.7037634
H	-2.0560807	0.1274787	2.5681534
C	-1.3470611	1.9294594	3.6087634
H	-2.3400412	2.0981191	4.0317360
C	-0.0810611	-0.8235406	1.5437634
C	-0.2570611	8.9594594	3.9207634
C	0.8619389	8.5864594	3.1237634
H	1.7591576	9.2128145	3.1723954
C	0.8949389	7.5104594	2.3337634
H	1.8213558	7.2946176	1.7935318
C	-0.1010611	6.6534594	2.2657634
C	-1.1600611	6.9914594	2.7037634
H	-2.0571215	6.3852248	2.5718879
C	-1.3470611	8.1864594	3.6087634
H	-2.3391017	8.3498391	4.0369692
C	-0.0810611	5.4334594	1.5437634
H	0.1663916	-9.9474754	-4.3082383
H	-0.2570755	9.8070462	4.6060234
H	0.1676960	-3.6977014	-4.2954428
H	-0.2601019	3.5576846	4.5958797

### **XEBHER**

N	-1.6236663	0.2122504	4.1199989
C	-3.5686657	0.2322504	6.1369984
C	-3.1046659	-0.9637493	5.5959985
H	-3.4794537	-1.9306666	5.9364276
C	-2.1436661	-0.9217493	4.5869988
H	-1.7758365	-1.8536706	4.1484451
C	-2.0686662	1.3702501	4.6439988
H	-1.6384694	2.2975045	4.2447314
C	-3.0366659	1.4092501	5.6449985
H	-3.3524910	2.3844904	6.0202778
Ag	-0.1196667	0.1512504	2.5809994
Ag	0.1193332	-0.1507495	-2.5809992

N	-1.3316664	-0.1647495	-0.9969996
C	-3.2686658	-0.0537495	1.0429998
C	-2.7376660	-1.2757492	0.6119999
H	-3.0615238	-2.2301635	1.0309636
C	-1.7776662	-1.2827492	-0.4009998
H	-1.3630913	-2.2336770	-0.7593464
C	-1.8456662	1.0032502	-0.5829997
H	-1.4631940	1.9165090	-1.0449015
C	-2.7866660	1.1012502	0.4400000
H	-3.1101602	2.0957763	0.7523858
N	1.6233328	-0.2127495	-4.1199988
N	1.3323329	0.1642504	0.9969998
C	3.2693323	0.0542505	-1.0429996
C	2.7373325	1.2762501	-0.6119997
H	3.0611934	2.2306652	-1.0310044
C	1.7783328	1.2832501	0.4010000
H	1.3635075	2.2338920	0.7597944
C	1.8463327	-1.0027493	0.5829999
H	1.4639578	-1.9160405	1.0450447
C	2.7863325	-1.1017492	-0.4399998
H	3.1096957	-2.0962727	-0.7524502
C	3.5683323	-0.2317495	-6.1369982
C	3.1043324	0.9642502	-5.5959983
H	3.4788834	1.9313295	-5.9361609
C	2.1433327	0.9212502	-4.5869986
H	1.7753093	1.8529975	-4.1481878
C	2.0683327	-1.3707491	-4.6439986
H	1.6381264	-2.2979927	-4.2447236
C	3.0363324	-1.4097491	-5.6449983
H	3.3524666	-2.3847602	-6.0205581
P	0.2043332	-4.5827482	-2.3919992
F	-0.4586666	-5.7207479	-3.2729990
F	0.8493330	-5.7487479	-1.5659995
F	1.4683328	-4.5727482	-3.3569990
F	-1.0596664	-4.6157482	-1.4249995
F	-0.4506666	-3.4207486	-3.2279990
F	0.8103330	-3.4467486	-1.5369995
P	-0.2046667	4.5832492	2.3919994
F	0.4583331	5.7202489	3.2729992
F	-0.8496665	5.7482489	1.5659996
F	-1.4686663	4.5722492	3.3569991
F	1.0603330	4.6152492	1.4249997
F	0.4503331	3.4212495	3.2279992
F	-0.8106665	3.4472495	1.5369997

H	-4.0167389	-0.0069073	1.8376005
H	-4.3245644	0.2379476	6.9256447
H	4.3242327	-0.2375008	-6.9256548
H	4.0174540	0.0075422	-1.8375375

## ZEDFOG

Ag	1.2281467	-0.3326495	-0.1013286
N	0.6897835	-2.4336621	0.1443402
C	-0.6168523	-4.2976473	-0.6143284
H	-1.4017191	-4.6547359	-1.2824770
N	1.6381465	1.7933493	-0.2083286
C	-0.2728525	-2.9556480	-0.6293284
H	-0.7768901	-2.2566363	-1.3083521
C	1.8121464	4.5683478	0.0846712
H	1.8823705	5.6527911	0.2013683
C	0.0631473	-5.1236468	0.2366712
H	-0.1565495	-6.1941560	0.2721049
C	1.3101467	-3.2376478	1.0176708
C	2.8121459	3.7453482	0.5616710
H	3.6939159	4.1555866	1.0582442
C	0.6801471	2.6233488	-0.6563284
H	-0.1691559	2.1487443	-1.1634064
C	0.7241470	3.9893480	-0.5393284
H	-0.0980281	4.5804009	-0.9457577
C	2.7091459	2.3793490	0.3936710
C	1.0271469	-4.5906471	1.0786708
H	1.5696832	-5.2232214	1.7840640
C	-1.0188521	1.8373492	2.0156702
C	0.1921473	-0.0116497	3.0396696
H	1.0182378	-0.3552905	3.6713643
C	0.0921473	1.3293496	2.7676698
C	-1.7888516	0.8773498	1.3716706
H	-2.5243825	1.1863153	0.6219599
C	-0.7788521	-0.9206492	2.6456698
C	-1.7058517	-0.4816494	1.6876704
S	-1.6958517	0.2143502	-2.6333272
F	-3.0388509	0.4393500	-4.8783260
F	-0.9528521	1.0283498	-5.0123258
F	-1.5108517	-1.0596491	-4.9073260
O	-2.1048514	1.5793494	-2.3273274
O	-0.2988525	-0.0806496	-2.3663274
C	-1.7448516	0.1723502	-4.3923262
O	-2.5948511	-0.8126492	-2.2373274

H	2.0660285	-2.7844183	1.6637980
H	-2.3902293	-1.1800353	1.2003185
H	0.8334529	2.0240609	3.1719737
H	-0.7290418	-1.9698569	2.9438628
H	-1.1397071	2.9039659	1.8232497
H	3.4904201	1.7071602	0.7564390