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## CLUSTER EXAMPLE: This ATP induced R1 hexamerization example runs 1.8 days
## on a 16 core (4 quad proc machines) ROCKS Linux cluster.
library(ccems)
topology <- list(
  heads=c("R1X0","R2X2","R4X4","R6X6"),
  sites=list(
    # s-sites are already filled only in (j>1)-mers
    a=list( #a-site thread
      m=c("R1X1"), # monomer 1
      d=c("R2X3","R2X4"), # dimer 2
      t=c("R4X5","R4X6","R4X7","R4X8"), # tetramer 3
      h=c("R6X7","R6X8","R6X9","R6X10","R6X11","R6X12") # hexamer 4
    ), # tails of a-site threads are heads of h-site threads
    h=list( # h-site
      m=c("R1X2"), # monomer 5
      d=c("R2X5","R2X6"), # dimer 6
      t=c("R4X9","R4X10","R4X11","R4X12"), # tetramer 7
      h=c("R6X13","R6X14","R6X15","R6X16","R6X17","R6X18") # hexamer 8
    )
  )
)
g=mkkg(topology,TCC=TRUE)
dd=subset(RNR,(year==2002)&(fg==1)&(X>0),select=c(R,X,m,year))
names(dd)[1:2] <- paste(strsplit(g$id,split="")[[1]],"T",sep="")#i.e. c("RT","XT")
cpusPerHost=c("localhost" = 4,"compute-0-0"=4,"compute-0-1"=4,"compute-0-2"=4)
top10=ems(dd,g,cpusPerHost=cpusPerHost, maxTotalPs=3, ptype="SOCK",KIC=100)
```