

Endohedral Gas Adsorption by Cucurbit[7]uril: A Theoretical Study

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Supporting Information

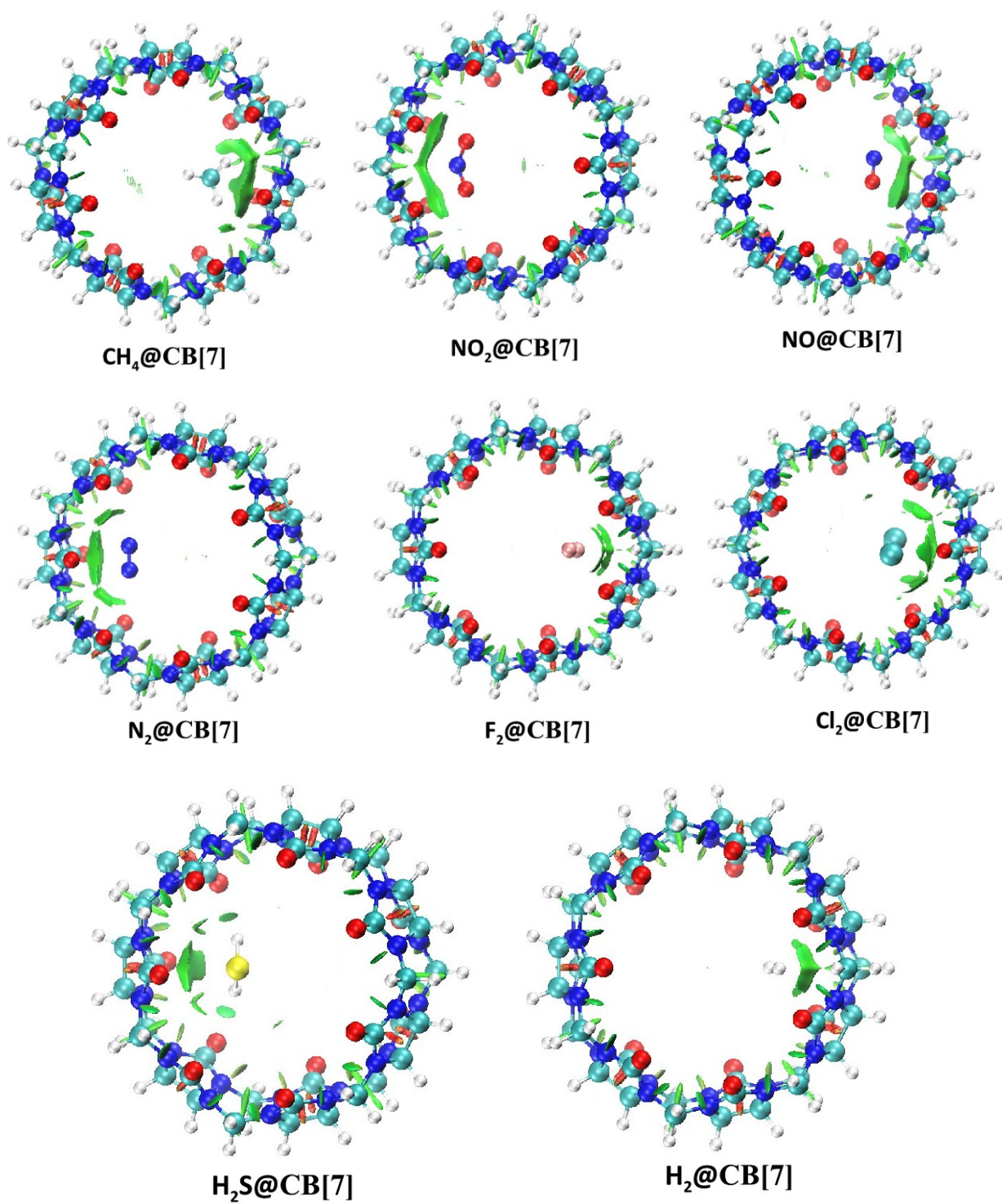


Fig. 1-SI NCI isosurface plots of gas@CB[7] at the ω B97X-D/6-311+G(d,p) level.

The Cartesian coordinates of the systems studied at the ω B97X-D/6-311+G(d,p) level

SO ₂ @Cucurbit[7]uril				CO ₂ @Cucurbit[7]uril			
0 1				0 1			
C	-2.94028300	-4.98559400	-0.13369900	C	-4.72183200	-3.37383800	0.04629700
C	-4.22323800	-4.11457700	-0.01557800	C	-5.40609800	-1.97382300	0.10653500
N	-4.22613400	-3.36359400	-1.23606200	N	-5.05165200	-1.37161400	-1.14854100
C	-3.06036000	-3.52093800	-1.96554600	C	-4.27146200	-2.19796400	-1.94105700
N	-2.24774400	-4.39173200	-1.25474600	N	-4.00869300	-3.33846800	-1.20451300
N	-2.32255700	-4.84544900	1.15260300	N	-3.93720500	-3.41009300	1.24945300
H	-3.14965200	-6.04536100	-0.33745000	H	-5.43837900	-4.20738200	0.04398900
N	-3.99909200	-3.37603000	1.20612300	N	-4.83958200	-1.37348300	1.28658900
H	-5.14668800	-4.70531200	0.06405500	H	-6.49993400	-2.03025800	0.20196000
C	-5.30632800	-2.53364500	-1.69288300	C	-5.65182000	-0.17269700	-1.66829500
O	-2.82199600	-3.03314200	-3.03887300	O	-3.93376100	-1.98263800	-3.07537000
C	-5.02286700	-2.59033700	1.84654700	C	-5.36311600	-0.18249100	1.90071600
C	-2.96093700	-3.91557800	1.95485600	C	-4.03822900	-2.25272900	1.99885900
O	-2.69931600	-3.66190900	3.10044100	O	-3.56586900	-2.06278200	3.08851000
N	-5.17186800	-1.25927100	1.32733700	N	-4.92088400	1.04727900	1.30094500
C	-5.94431900	-0.92205300	0.16484800	C	-5.51930000	1.62025600	0.12423700
C	-4.74030300	-0.14832100	2.03143500	C	-4.15861900	1.96126200	2.01170800
C	-5.98213800	0.63629100	0.19445700	C	-4.92763800	3.06211800	0.07967000
N	-5.35170300	-1.21598300	-1.11525500	N	-5.12036300	1.05271800	-1.13460900
H	-6.94038300	-1.38224600	0.23128000	H	-6.61498600	1.60323800	0.21405000
N	-5.14636200	0.96859800	1.31849300	N	-4.12319500	3.12694600	1.26913600
O	-4.16682300	-0.15162300	3.08807100	O	-3.66641500	1.78807700	3.09543200
N	-5.49527300	1.00615200	-1.10648100	N	-4.23801500	3.09695700	-1.18320500
H	-6.99175700	1.04420000	0.34538000	H	-5.69551600	3.84817000	0.10684100
C	-5.19778500	-0.08644100	-1.90305200	C	-4.41981500	1.94674600	-1.92900200
O	-4.91170800	-0.06257500	-3.07060700	O	-4.08279700	1.77079200	-3.07014900
C	-5.06498700	2.28502600	1.89038900	C	-3.52920600	4.32906500	1.78583500
N	-4.11868100	3.15781000	1.24666000	N	-2.27069000	4.68905500	1.18997100
C	-4.42881000	3.91587600	0.05601400	C	-2.15789600	5.40662800	-0.05421300
C	-3.08908800	3.73632900	1.97638600	C	-1.11143500	4.74987700	1.94622900
C	-3.19591000	4.85223800	-0.08438900	C	-0.64388200	5.76594900	-0.12183800
N	-4.44191100	3.19696600	-1.18356900	N	-2.37748000	4.65702300	-1.25766300
H	-5.37668100	4.45646400	0.18707800	H	-2.81371100	6.28912000	-0.03872200
N	-2.53996800	4.73013600	1.18411100	N	-0.14070500	5.34038500	1.15354900
O	-2.76939000	3.46310600	3.10258800	O	-0.98474800	4.40742300	3.09195900
N	-2.50571700	4.30224000	-1.23017800	N	-0.18166500	5.03585300	-1.27508300
H	-3.46267800	5.90203300	-0.27135200	H	-0.45832100	6.84099000	-0.25916800
C	-3.30580300	3.42072300	-1.94260400	C	-1.22177300	4.46731700	-1.99466900
C	-5.50818200	2.34377500	-1.63469500	C	-3.67033900	4.28428500	-1.76253600
C	-1.42557000	4.98463900	-1.89472300	C	1.09917100	5.26110100	-1.88737200
C	-1.48679300	5.59020000	1.65406300	C	1.15861700	5.67770700	1.66875400
O	-3.08160800	2.97330500	-3.03624700	O	-1.14367200	3.95714700	-3.08072600
N	-0.14483700	4.83690700	-1.25965000	N	2.19295800	4.56674400	-1.26035700
N	-0.17610700	5.29841600	1.14205000	N	2.24695200	4.88060500	1.16967100
C	0.92392500	4.27690500	-1.94590100	C	2.96867400	3.67714600	-1.98843900
C	0.28244900	5.67182000	-0.16577500	C	2.88554300	5.07420000	-0.10067600
C	1.81692200	5.42038300	-0.10010700	C	4.14674300	4.16516800	-0.01498600
N	2.07221500	4.59444600	-1.24519800	N	4.10641700	3.42364600	-1.24183300
C	0.84570900	4.84244200	1.96107100	C	2.88658300	3.93766500	1.95569500
N	1.99517000	4.81024000	1.19112700	N	3.93245900	3.42175700	1.20353900
C	3.38334400	4.33854300	-1.77913800	C	5.16462300	2.58232700	-1.72819000
C	3.28388200	4.54922700	1.77396100	C	4.95571700	2.62248700	1.82643200
O	0.75671600	4.58023500	3.13132600	O	2.61941200	3.65838300	3.09425000
O	0.86451400	3.67671900	-2.98729400	O	2.72659000	3.24706500	-3.08498200
N	4.10093000	3.25710100	-1.16663800	N	5.21116700	1.26404800	-1.15142700
N	3.94700300	3.37558500	1.27922900				

C	4.39805800	2.10514700	-1.86535800	N	5.08945900	1.29480000	1.29450100
C	4.77252600	3.33448000	0.10577400	C	5.02741400	0.13454300	-1.93337300
C	5.48277900	1.94978900	0.21333500	C	5.83604100	0.96728200	0.11189600
N	5.21508800	1.33657700	-1.05771000	C	5.88453500	-0.59066100	0.13384500
O	4.05679200	1.83929000	-2.99026200	N	5.34816800	-0.95985900	-1.14760700
C	5.83250300	0.12850700	-1.53124300	O	4.70247700	0.11182800	-3.09074500
N	4.86200300	1.34637300	1.36295200	C	5.38224200	-2.29229300	-1.68894400
C	4.01862200	2.21609100	2.03257100	N	5.09626400	-0.93281900	1.28851200
O	3.49950300	2.02995900	3.10102200	C	4.70061100	0.17865300	2.01505700
C	5.34879800	0.15163300	1.99716000	O	4.16621200	0.17486300	3.09228900
N	5.26455900	-1.09437000	-1.03277700	C	5.04711500	-2.25125000	1.85846000
N	4.92353300	-1.07800100	1.38743200	N	4.35781400	-3.17874000	-1.20727200
C	4.52944800	-1.93974700	-1.84319800	N	4.10530300	-3.14014400	1.23043100
C	5.56894800	-1.67109500	0.24791600	C	3.25076600	-3.50666000	-1.97152400
C	4.93072600	-3.09234300	0.16870900	C	4.40794700	-3.89199500	0.03570900
N	4.29686200	-3.09415000	-1.12419500	C	3.21212900	-4.88285700	-0.06797900
O	4.20218800	-1.72595500	-2.98303800	N	2.50811200	-4.42265900	-1.24140000
C	3.65453000	-4.23144700	-1.71952900	O	3.00943700	-3.11115400	-3.08112400
N	4.07275100	-3.13524200	1.31956600	C	1.46172300	-5.18037600	-1.87649400
C	4.09590400	-1.96324200	2.05613900	N	2.54242000	-4.72877200	1.19115200
O	3.55345500	-1.77643200	3.11285000	C	3.08491000	-3.72055600	1.96953300
C	3.45597800	-4.32607500	1.83247100	O	2.76724200	-3.43846800	3.09438000
N	2.34312400	-4.54052900	-1.21658700	C	1.50302100	-5.59414700	1.67985300
N	2.19771500	-4.66623100	1.22427000	N	0.16469900	-5.02756200	-1.27595400
C	2.08865600	-5.33204900	-0.04840300	N	0.19003700	-5.34010000	1.15188400
C	1.03750100	-4.75864800	1.97340700	C	-0.26806900	-5.78965000	-0.13253400
C	0.56973300	-5.65215900	-0.14943600	C	-0.82967800	-4.83348000	1.94077500
N	0.06613100	-5.30384500	1.14768800	C	-1.80208600	-5.52598400	-0.08450900
C	1.19735900	-4.26081400	-1.93656700	N	-1.98031800	-4.83927500	1.16907700
N	0.13265900	-4.83187300	-1.25218500	C	-0.89811900	-4.51078700	-2.00204400
O	0.90631900	-4.47482400	3.13467200	N	-2.04895100	-4.77027400	-1.27876000
O	1.13809900	-3.68224300	-2.99002600	O	-0.74262800	-4.50383400	3.09395400
C	-1.23783500	-5.65798200	1.63639900	O	-0.83676400	-3.98733400	-3.08281500
C	-1.13171700	-5.02549500	-1.90768000	C	-3.26826200	-4.57759200	1.75334500
H	-1.34593600	4.55695600	-2.89635000	C	-3.35656500	-4.47500400	-1.79675100
H	-1.66495300	6.05714100	-1.97078500	H	1.03452400	4.89996100	-2.91604400
H	-1.74769300	6.62724400	1.40369300	H	1.31147200	6.34141600	-1.88834900
H	-1.43473200	5.47493700	2.73866000	H	1.36499200	6.73327600	1.44682800
H	3.93958100	5.41584900	1.60834000	H	1.12172200	5.52878500	2.74991100
H	3.12180600	4.40953900	2.84476200	H	5.92338700	3.13689900	1.73555300
H	3.26129000	4.07764200	-2.83233200	H	4.68916500	2.52507100	2.88097100
H	3.97585700	5.25997900	-1.69284700	H	5.00935400	2.45384900	-2.80138000
H	6.89947200	0.15484100	-1.27251400	H	6.12353800	3.08830800	-1.55074000
H	5.71646300	0.11412700	-2.61686200	H	6.36101200	-2.74180100	-1.47578000
H	6.44846600	0.17909400	2.01432300	H	5.24688900	-2.19831800	-2.76837600
H	4.96480300	0.15274500	3.01970100	H	6.05185800	-2.69742300	1.81197600
H	4.29167900	-5.11599700	-1.58448100	H	4.74085600	-2.14432500	2.90138400
H	3.55130000	-4.01143300	-2.78396800	H	1.73445300	-6.24713000	-1.87273700
H	4.15820100	-5.16344100	1.71007900	H	1.38686700	-4.82540300	-2.90663900
H	3.25939700	-4.16452500	2.89437800	H	1.78004700	-6.63372300	1.45960800
H	-1.05176400	-4.58759100	-2.90486100	H	1.44409400	-5.44900000	2.76053300
H	-1.32983300	-6.10563700	-1.99540300	H	-3.24224800	-4.25759300	-2.86078000
H	-1.21174900	-5.54469800	2.72216000	H	-3.99224100	-5.36164300	-1.66598800
H	-1.44373300	-6.70524200	1.37797700	H	-3.10742900	-4.42481700	2.82258600
H	-6.25219700	-3.05328900	-1.49019400	H	-3.91999800	-5.44887800	1.59742700
H	-5.18288900	-2.40088800	-2.76957100	H	-6.73361100	-0.20596000	-1.47694200
H	-4.74484400	-2.50174400	2.89892400	H	-5.46817500	-0.16112400	-2.74476300
H	-5.98853700	-3.10932300	1.76195000	H	-5.02045600	-0.17735400	2.93781900
H	0.02336200	6.72084800	-0.37060500	H	-6.46220100	-0.21911800	1.87371100
H	2.41184800	6.34296200	-0.16537000	H	3.12432600	6.13795300	-0.24257100
H	6.56803400	2.03016600	0.36845500	H	5.08745000	4.73026900	0.05096500
H	5.47090400	4.18308500	0.10974000	H	6.90189300	-0.99290800	0.24374300

H	6.65765000	-1.69203500	0.39896800	H	6.83053500	1.43378700	0.15651900
H	5.66962600	-3.90414800	0.22335100	H	5.38074700	-4.39276200	0.14277000
H	0.36175500	-6.71089500	-0.36217400	H	3.52351900	-5.92859000	-0.20226100
H	-6.06334700	2.74675700	1.86358500	H	-2.40149300	-6.44791600	-0.09480800
H	-4.74075000	2.17226100	2.92731400	H	-4.24179400	5.15588200	1.65443100
H	-5.41505600	2.25344900	-2.71877500	H	-3.34442900	4.16898400	2.85013300
H	-6.46325500	2.82181600	-1.38333200	H	-3.55732800	4.09349000	-2.83176400
H	2.72449000	-6.22925900	-0.05978400	H	-4.36206000	5.12350600	-1.60711800
O	1.94588700	1.22348700	-0.40226300	H	-0.01498700	-6.85068400	-0.27142200
O	1.95220200	-1.24600200	-0.43603100	C	-1.86296600	-0.06093300	-0.13907000
S	1.46698000	-0.00436800	-1.00219000	O	-1.82781900	-1.21737900	-0.13384000
				O	-1.90049200	1.09543600	-0.14331500
CO@Cucurbit[7]uril				C ₂ H ₂ @Cucurbit[7]uril			
O 1				O 1			
C	-5.74554000	1.01133700	0.15132200	C	5.67495200	1.71345600	0.14007400
C	-5.79729800	-0.54699000	0.16667600	C	4.96067400	3.09909700	0.07651500
N	-5.00826100	-0.89664000	1.31740300	N	4.15674600	3.11600300	1.26687700
C	-4.58204800	0.21077000	2.03258500	C	4.24588500	1.94357100	1.99447600
N	-4.96469600	1.33039700	1.31518200	N	5.10086700	1.10138400	1.30882400
N	-5.15912500	1.31135000	-1.12837300	N	5.35865100	1.11893600	-1.12837000
H	-6.73711600	1.47993800	0.22781500	H	6.76510600	1.79086700	0.25579700
N	-5.26111800	-0.91313100	-1.11647900	N	4.25353800	3.05029600	-1.17724100
H	-6.81548600	-0.94733400	0.27556600	H	5.65831700	3.94840500	0.08255200
C	-4.95963600	-2.21717900	1.88317100	C	3.49541500	4.27965900	1.78791100
O	-4.02835000	0.20062500	3.10005200	O	3.72289800	1.72090500	3.05589400
C	-5.30915600	-2.24342200	-1.66343500	C	3.62022200	4.18808600	-1.78703100
C	-4.96708600	0.18437000	-1.90888100	C	4.54204100	1.91361800	-1.91027300
O	-4.65208800	0.16286800	-3.06924500	O	4.19530000	1.68532900	-3.04062800
N	-4.28940100	-3.13844400	-1.19059700	N	2.32334200	4.52035600	-1.26523800
C	-4.33752400	-3.85540200	0.05025900	C	2.10510500	5.28693100	-0.07265100
C	-3.18842900	-3.46963500	-1.96207100	C	1.16671100	4.32475000	-1.99962200
C	-3.14612500	-4.85171900	-0.06218300	C	0.59049900	5.64044500	-0.13887700
N	-4.02793700	-3.10939400	1.24634400	N	2.22750000	4.58476200	1.17947300
H	-5.31206500	-4.35229200	0.15956400	H	2.75818300	6.17198800	-0.07180100
N	-2.45728100	-4.40467800	-1.24798900	N	0.12705700	4.89975200	-1.28452900
O	-2.94742700	-3.06351200	-3.06817800	O	1.08797900	3.80387600	-3.08089500
N	-2.45821100	-4.68993200	1.18650900	N	0.09292300	5.22436200	1.14170000
H	-3.46306000	-5.89748400	-0.18273500	H	0.40062300	6.71377700	-0.28461300
C	-2.99053000	-3.67931800	1.96821800	C	1.07118700	4.65587300	1.94080000
O	-2.65310900	-3.38883400	3.08538000	O	0.95256100	4.33568600	3.09396800
C	-1.41045400	-5.15686600	-1.88569500	C	-1.15186600	5.12804900	-1.90025100
N	-0.10935400	-4.99837700	-1.29367700	N	-2.25282800	4.45607600	-1.26189300
C	0.33776000	-5.75722300	-0.15451300	C	-2.93490100	4.98630200	-0.10553700
C	0.94143900	-4.45659800	-2.01715100	C	-3.04968900	3.58090100	-1.98530800
C	1.87189400	-5.48897600	-0.12032200	C	-4.21156900	4.10026000	-0.01061200
N	-0.10883900	-5.30937900	1.13521600	N	-2.29860800	4.79236500	1.16576700
H	0.08681300	-6.81915800	-0.29061100	H	-3.15534200	6.05281700	-0.25633200
N	2.09972100	-4.70396000	-1.29995700	N	-4.19111900	3.35526300	-1.23562200
O	0.86875200	-3.92092400	-3.09128800	O	-2.81974700	3.14283900	-3.08116300
N	2.06749700	-4.82965800	1.14567100	N	-4.00340100	3.35759300	1.20931700
H	2.47394300	-6.40841700	-0.15972600	H	-5.14170900	4.68216500	0.05846200
C	0.92191300	-4.83287000	1.92734000	C	-2.94805800	3.85981000	1.95637200
C	-1.42054100	-5.55940100	1.66959700	C	-1.20087400	5.57784500	1.66065100
C	3.36406800	-4.61460500	1.73344100	C	-5.02906500	2.56196000	1.83226600
C	3.39891000	-4.38876300	-1.82419300	C	-5.26347300	2.52543500	-1.71146000
O	0.84864000	-4.52966900	3.08861400	O	-2.67987700	3.57974600	3.09451100
N	4.06344200	-3.45420100	1.25551800	N	-5.16368200	1.23318500	1.30348000
N	4.05223600	-3.27198900	-1.19053000	N	-5.31331200	1.20485800	-1.14172600
C	4.15590700	-2.29394000	2.00487800	C	-4.76228100	0.12014000	2.02192400

C	4.81014000	-3.39180200	0.03238100	C	-5.91996700	0.90026100	0.12815200
C	5.54505500	-2.02240400	0.12870000	C	-5.95238800	-0.65856000	0.14785000
N	4.94189900	-1.40690800	1.28514500	N	-5.15775000	-0.99380700	1.29984500
C	4.43375700	-2.16618600	-1.93674700	C	-5.11659600	0.07858400	-1.92445100
N	5.27928200	-1.41093800	-1.14178100	N	-5.41680600	-1.01997800	-1.13642200
C	5.46176800	-0.21797600	1.90543400	C	-5.07883200	-2.31387900	1.86195100
C	5.92049700	-0.21901200	-1.62890200	C	-5.42060100	-2.35397400	-1.67430100
O	4.13109100	-1.93355000	-3.07679700	O	-4.79869300	0.06046600	-3.08370600
O	3.68769300	-2.11155000	3.09718600	O	-4.22085800	0.12046200	3.09552200
N	5.03390300	1.01037200	1.29200400	N	-4.11108700	-3.17482100	1.23488400
N	5.38200500	1.01938200	-1.13367900	N	-4.36620400	-3.21065900	-1.20314300
C	4.30004600	1.94226600	2.01003200	C	-3.06672900	-3.71582500	1.96927100
C	5.68858900	1.59157900	0.14648300	C	-4.38562700	-3.93112800	0.03636900
C	5.06502600	3.01625300	0.06411200	C	-3.15111200	-4.87287700	-0.07346800
N	4.29618600	3.11292800	1.27140000	N	-2.48743300	-4.69989900	1.18644400
O	3.80550300	1.78184800	3.09415900	O	-2.75658100	-3.42510800	3.09404000
C	3.68775600	4.31846700	1.76173300	C	-1.41529800	-5.52550800	1.67098000
N	4.32823800	2.98328000	-1.17598600	N	-2.46664900	-4.37723000	-1.24455000
C	4.62262000	1.85820400	-1.93204000	C	-3.24756200	-3.48903800	-1.96982500
O	4.32173700	1.66956600	-3.08065300	O	-3.02420600	-3.07958900	-3.07797900
C	3.77851600	4.16118400	-1.79634100	C	-1.39617800	-5.09131000	-1.88977600
N	2.42295200	4.64999100	1.15872900	N	-0.11462400	-5.22123300	1.13796200
N	2.49871700	4.57029400	-1.28931200	N	-0.10378500	-4.90289700	-1.28918000
C	1.27172400	4.74407100	1.92676700	C	0.89986300	-4.71433500	1.93317300
C	2.30340100	5.34611100	-0.09794000	C	0.35000000	-5.65662800	-0.14919200
C	0.79314700	5.72428300	-0.15596700	C	1.87707800	-5.35778200	-0.10465400
N	0.29595000	5.31630900	1.12800600	N	2.04885500	-4.68680800	1.15819300
O	1.15679800	4.43620200	3.08335000	O	0.81163300	-4.40712800	3.09262400
C	-0.99514500	5.67676000	1.65055300	C	3.33770700	-4.45112200	1.75348200
N	0.31064300	4.99151200	-1.29885400	N	2.10101300	-4.57480100	-1.28576400
C	1.33433800	4.39323200	-2.01653600	C	0.94324900	-4.34841200	-2.00993400
O	1.23986000	3.86699200	-3.09367100	O	0.86732000	-3.82005200	-3.08764100
C	-0.97282500	5.22654100	-1.90289100	C	3.40170100	-4.28331900	-1.82234700
N	-2.09717400	4.89036900	1.16710600	N	4.04345800	-3.30744900	1.24692500
N	-2.06965400	4.45282100	-1.25979800	N	4.08913000	-3.18564600	-1.19725300
C	-2.74408300	5.08208300	-0.09896700	C	4.82063100	-3.29572100	0.03919400
C	-2.86863400	3.67318900	-1.97588700	C	4.42604100	-2.05377800	-1.91780000
C	-4.01747400	4.19311200	0.00588500	C	5.59456500	-1.94373900	0.11835700
N	-4.00387300	3.44557500	-1.21755800	N	5.29624100	-1.31606500	-1.13772300
C	-2.73657700	3.95364600	1.96185400	C	4.18190700	-2.14871200	1.98849300
N	-3.79893200	3.45263800	1.22475800	N	5.05392000	-1.32602900	1.30087900
O	-2.64500300	3.23399800	-3.07260000	O	4.07534400	-1.78977800	-3.03897000
O	-2.45568600	3.67086900	3.09627700	O	3.68131100	-1.92326600	3.06015800
C	-5.08851800	2.63244000	-1.69391400	C	5.91354500	-0.11165200	-1.62245100
C	-4.81793100	2.65455500	1.85373800	C	5.57340000	-0.12380400	1.89208900
H	3.20870400	-4.48142500	2.80607200	H	-4.76425900	2.46705600	2.88749000
H	3.99248500	-5.49847600	1.55646100	H	-5.99560900	3.07769100	1.73847400
H	4.03854200	-5.27912500	-1.73821900	H	-6.21497400	3.03899800	-1.51830100
H	3.27115500	-4.12928800	-2.87726100	H	-5.12400200	2.40087900	-2.78727800
H	6.98810500	-0.26663700	-1.37801300	H	-6.38377300	-2.83005900	-1.44902400
H	5.79655500	-0.20914300	-2.71376600	H	-5.30033600	-2.25847700	-2.75537600
H	5.10109500	-0.20794500	2.93644600	H	-4.78197100	-2.20576700	2.90744800
H	6.56161700	-0.25956100	1.89890200	H	-6.07168100	-2.78427000	1.80604500
H	4.39080600	5.14982500	1.61204500	H	-1.65375900	-6.57491700	1.45117300
H	3.50515900	4.17897600	2.82926700	H	-1.35777600	-5.37901900	2.75153300
H	4.48577800	4.99484000	-1.68043400	H	-1.63218200	-6.16683600	-1.89920800
H	3.65025200	3.93310700	-2.85662000	H	-1.33542400	-4.72121600	-2.91546400
H	-1.18919000	6.73305700	1.42088900	H	3.96865100	-5.34047800	1.61236400
H	-0.95035500	5.53710900	2.73266300	H	3.16907600	-4.28567200	2.81947700
H	-1.17040900	6.30956200	-1.91386400	H	4.02330600	-5.18711300	-1.74510700
H	-0.92145800	4.85359400	-2.92810200	H	3.26695800	-4.01922900	-2.87331000
H	-4.53951800	2.54967700	2.90450800	H	5.26422600	-0.12223900	2.93953400

H	-5.78435600	3.17385800	1.77728100	H	6.67071300	-0.14432000	1.83059100
H	-4.95255200	2.50811900	-2.77020600	H	5.78710400	-0.10304400	-2.70696900
H	-6.03235400	3.15907800	-1.49810100	H	6.98232500	-0.14135000	-1.37411900
H	-5.96679500	-2.65800700	1.84371700	H	4.16839300	5.14214400	1.67568200
H	-4.64388700	-2.11370100	2.92361300	H	3.30393000	4.09973400	2.84769600
H	-5.17838600	-2.14534700	-2.74310100	H	3.49258300	3.95257100	-2.84565300
H	-6.29048100	-2.68642200	-1.44730500	H	4.27576700	5.06396800	-1.67935600
H	5.49565700	-4.24878400	-0.03242700	H	-6.91858300	1.35638100	0.18514700
H	6.62965200	-2.12192500	0.27814600	H	-6.96524400	-1.07114100	0.26028300
H	5.81666800	3.81780700	0.03286200	H	-3.41988000	-5.92950800	-0.21439700
H	6.77696800	1.60229600	0.30134500	H	-5.33777700	-4.47021000	0.14201600
H	2.97075500	6.21997000	-0.10660400	H	0.12055700	-6.72295200	-0.28990500
H	0.62019200	6.80047000	-0.30063700	H	2.49787300	-6.26545200	-0.13358200
H	-4.94879400	4.77260300	0.08038300	H	6.68105800	-2.06944600	0.22566200
H	-1.67673100	-6.22499100	-1.87844200	H	-1.35189300	6.21073700	-1.91998800
H	-1.34312200	-4.80304700	-2.91674700	H	-1.09190800	4.74863300	-2.92255500
H	-1.35421200	-5.41617800	2.75010500	H	-1.16203100	5.43053700	2.74193900
H	-1.70304700	-6.59776300	1.44974100	H	-1.39614000	6.63542700	1.43744300
H	-2.96802900	6.14802200	-0.24863700	H	5.48086100	-4.17406900	0.00976100
C	-1.88360200	-0.80953500	-0.26215500	C	2.03309500	-0.04442200	0.39336300
O	-2.04164700	0.30327600	-0.18975600	H	1.99205700	-0.07883400	1.45990400
				C	2.07313100	-0.00157500	-0.80431500
				H	2.11620400	0.03303200	-1.87089500
C ₂ H ₄ @Cucurbit[7]uril				C ₂ H ₆ @Cucurbit[7]uril			
0 1				0 1			
C	0.81673600	5.63251400	-0.03086900	C	-5.78998800	0.93766900	0.18771100
C	2.30775700	5.20597600	0.08367600	C	-5.84802200	-0.61998400	0.15375100
N	2.56755700	4.55611300	-1.16739200	N	-5.11910600	-1.00535700	1.32915900
C	1.43369600	4.42989100	-1.95218600	C	-4.61710300	0.07372200	2.03502900
N	0.37323600	4.94805000	-1.22231100	N	-4.94877300	1.21503300	1.32283100
N	0.25003400	5.19889300	1.21261700	N	-5.26516200	1.27990700	-1.10499300
H	0.68077400	6.71728100	-0.14783500	H	-6.77446400	1.40634900	0.32841900
N	2.31913000	4.37010300	1.26044400	N	-5.25166800	-0.94650000	-1.11647000
H	2.99545000	6.05355800	0.21662000	H	-6.87120900	-1.01893600	0.20080800
C	3.87891900	4.22247800	-1.65553700	C	-5.05005700	-2.34491200	1.84259700
O	1.38794100	3.99967500	-3.07405400	O	-4.05093100	0.03264200	3.09484700
C	3.53739900	3.94905900	1.90181200	C	-5.27426700	-2.26227900	-1.69902400
C	1.14217200	4.47797100	1.98825900	C	-5.00160400	0.17360400	-1.89277900
O	0.94978500	4.06885500	3.10235100	O	-4.67380600	0.18238300	-3.04965500
N	4.16803000	2.80858300	1.29681300	N	-4.24958300	-3.15534600	-1.23323000
C	5.05717800	2.89626900	0.16731700	C	-4.30706700	-3.90877100	-0.01419000
C	4.30920100	1.61955000	1.99488300	C	-3.11429200	-3.41971700	-1.97951600
C	5.73095700	1.49052300	0.12702900	C	-3.07049800	-4.85004300	-0.11539700
N	4.44190400	3.01080600	-1.12636700	N	-4.06788700	-3.18828400	1.21321200
H	5.77449500	3.71602800	0.31637100	H	-5.26268500	-4.44837500	0.04809800
N	5.20340900	0.83631900	1.29105600	N	-2.36696800	-4.34692200	-1.26997200
O	3.79272900	1.34577000	3.04653400	O	-2.85534400	-2.97049600	-3.06430900
N	5.33228200	0.97232200	-1.15515100	N	-2.42085800	-4.68788300	1.15348800
H	6.82761100	1.53229600	0.18919300	H	-3.33806500	-5.90538600	-0.26848500
C	4.64717400	1.89627300	-1.92216800	C	-3.02719900	-3.73180800	1.95029800
O	4.33732000	1.77955100	-3.07869300	O	-2.74073300	-3.46587600	3.08742800
C	5.67472800	-0.41973600	1.80645300	C	-1.29883400	-5.06394100	-1.91286800
N	5.08324900	-1.58737400	1.21316000	N	-0.01194100	-4.90834300	-1.28861800
C	5.50202200	-2.15957000	-0.04143400	C	0.40823800	-5.69392500	-0.15488100
C	4.27498100	-2.43542100	1.94761500	C	1.06240300	-4.40697800	-2.00859000
C	4.65337400	-3.46397700	-0.13233400	C	1.94168300	-5.43499300	-0.08663500
N	5.14687000	-1.44834700	-1.23578100	N	-0.06068500	-5.26748500	1.13258800
H	6.58532600	-2.34439100	-0.02564300	H	0.15440500	-6.75160100	-0.31636400
N	4.00041600	-3.52987000	1.14485200	N	2.20654400	-4.68969300	-1.28291300

O	3.92117300	-2.28152800	3.08714100	O	1.01502900	-3.87466700	-3.08578700
N	3.80760200	-3.22832200	-1.27644700	N	2.10435500	-4.73719100	1.16479900
H	5.25918900	-4.36722900	-0.29199500	H	2.53826600	-6.35872700	-0.08100200
C	4.15924000	-2.07884900	-1.96766200	C	0.94786800	-4.75640300	1.93151200
C	5.80531500	-0.26352400	-1.71406500	C	-1.37485700	-5.53994300	1.64931900
C	3.04177000	-4.26016500	-1.92082300	C	3.38833500	-4.51096500	1.77672500
C	3.28808800	-4.67498100	1.64067200	C	3.51904900	-4.38744800	-1.78157000
O	3.72636200	-1.72759800	-3.03370400	O	0.85121900	-4.44002500	3.08746700
N	1.77641600	-4.54332600	-1.29668000	N	4.09928000	-3.36347500	1.28628800
N	1.95525400	-4.84136900	1.12466700	N	4.15777600	-3.25484100	-1.16256100
C	0.59664100	-4.45831100	-2.02279900	C	4.19338700	-2.19320900	2.01942400
C	1.65183900	-5.41490300	-0.15481500	C	4.88087100	-3.33632700	0.08328600
C	0.12238800	-5.68897800	-0.07810600	C	5.61379000	-1.96363400	0.16006900
N	-0.38198700	-5.10195100	-1.28539500	N	5.00651800	-1.32921800	1.30280300
C	0.83449500	-4.68627000	1.92325200	C	4.53831000	-2.15810400	-1.92155200
N	-0.26357400	-5.06151600	1.16195900	N	5.35315800	-1.37406800	-1.12258300
C	-1.71693000	-5.28487900	-1.78368800	C	5.51965200	-0.12962700	1.90694400
C	-1.54347800	-5.28555900	1.78428100	C	5.98218100	-0.17984600	-1.61997300
O	0.82172800	-4.34090600	3.07488800	O	4.25815100	-1.95314400	-3.07256000
O	0.46058900	-3.96464300	-3.11067300	O	3.70578900	-1.98696200	3.09887700
N	-2.71387000	-4.44469100	-1.17285100	N	5.07876300	1.08834500	1.28181600
N	-2.61220400	-4.47319300	1.27551500	N	5.42342000	1.05746500	-1.14503000
C	-3.45321100	-3.55269600	-1.93497100	C	4.35156700	2.02690500	1.99775900
C	-3.35378300	-4.75961000	0.07992600	C	5.71954000	1.66003900	0.12277200
C	-4.54189800	-3.75345800	0.14019300	C	5.06334200	3.06785000	0.01506400
N	-4.48752800	-3.09571500	-1.13574100	N	4.33012500	3.18647400	1.24192900
O	-3.26354400	-3.27004900	-3.08809700	O	3.87557200	1.88082700	3.09210900
C	-5.51006300	-2.22110800	-1.64515700	C	3.70317600	4.38967400	1.71488000
N	-4.23873500	-2.95192300	1.29748000	N	4.29096100	2.97691000	-1.20147300
C	-3.15714200	-3.43736000	2.01479300	C	4.61096900	1.84745500	-1.94069300
O	-2.79320300	-3.06637200	3.09906400	O	4.28928600	1.62112700	-3.07671300
C	-5.16917800	-2.02924900	1.88840800	C	3.69142100	4.11996300	-1.84053100
N	-5.45912500	-0.86738400	-1.16270600	N	2.41565700	4.67423500	1.13718000
N	-5.19646400	-0.73058800	1.27087900	N	2.41627400	4.50840900	-1.30651100
C	-4.99496500	0.17271500	-1.94989300	C	1.27676200	4.74063900	1.92542200
C	-5.97999700	-0.42436800	0.09926700	C	2.24347400	5.32297800	-0.13713800
C	-5.88408500	1.12730200	0.00487900	C	0.72572400	5.67381400	-0.16131900
N	-5.12900600	1.33672600	-1.20753400	N	0.26384400	5.25435600	1.13302000
O	-4.60071400	0.08786500	-3.08245900	O	1.19666000	4.45607000	3.09090500
C	-4.98998700	2.62527900	-1.83601600	C	-1.02165600	5.59701500	1.68021400
N	-5.24908600	1.49620300	1.23696700	N	0.22911500	4.93637300	-1.29366900
C	-4.86187100	0.40380900	1.99393400	C	1.24164900	4.32462800	-2.01583300
O	-4.37779600	0.43473400	3.09404700	O	1.13081800	3.78286800	-3.08360400
C	-5.08603600	2.84316100	1.70940800	C	-1.06143700	5.16921200	-1.88257900
N	-3.93184100	3.44136200	-1.31037300	N	-2.12323900	4.80670200	1.20335400
N	-3.97621400	3.55977400	1.13695500	N	-2.15023500	4.49438600	-1.22683800
C	-4.04056700	4.24730500	-0.12740400	C	-2.79774900	5.01313600	-0.04515100
C	-2.92591200	3.99941700	1.92787400	C	-2.97809100	3.64516600	-1.94593800
C	-2.73183300	5.09361800	-0.14486100	C	-4.06878800	4.12408600	0.07753000
N	-2.15145200	4.83868200	1.14461500	N	-4.09826500	3.41323800	-1.16706800
C	-2.76679500	3.67504500	-2.01994600	C	-2.72763100	3.83849900	1.98694600
N	-2.01904100	4.58360000	-1.28720100	N	-3.80725700	3.34904900	1.26711700
O	-2.74954100	3.74369800	3.08946200	O	-2.78680100	3.23215500	-3.05898300
O	-2.48221200	3.21803300	-3.09509900	O	-2.40882100	3.52283000	3.10243600
C	-1.04924000	5.57967600	1.69644600	C	-5.19928600	2.61527000	-1.63355500
C	-0.87995700	5.24018100	-1.86789600	C	-4.79809900	2.52177300	1.90264000
H	2.83199100	-3.92163100	-2.93768400	H	3.20990300	-4.35244800	2.84226100
H	3.64082300	-5.18358300	-1.95553700	H	4.01891300	-5.40002300	1.63526000
H	3.86891200	-5.57952400	1.41408900	H	4.15377700	-5.27590500	-1.65560800
H	3.19905200	-4.55425200	2.72225200	H	3.41815000	-4.15529900	-2.84384100
H	-1.82000100	-6.34370700	1.66917300	H	7.04836800	-0.20677700	-1.36094500
H	-1.42840500	-5.04951600	2.84423000	H	5.86569800	-0.18794100	-2.70566800

H	-1.70356500	-5.04303700	-2.84853900	H	5.16347500	-0.10878100	2.93936300
H	-1.99799100	-6.33864100	-1.64642400	H	6.61951800	-0.16417900	1.89578900
H	-6.49322700	-2.64476600	-1.40248600	H	4.38072600	5.23335600	1.52449200
H	-5.38295900	-2.18007700	-2.72902200	H	3.55051500	4.27449500	2.78996800
H	-6.17775200	-2.46737100	1.85253700	H	4.37863400	4.97578900	-1.77133300
H	-4.86826800	-1.88510900	2.92840200	H	3.53875200	3.85626800	-2.88926700
H	-5.93772300	3.17494900	-1.74461300	H	-1.23127700	6.65392100	1.46656300
H	-4.76977700	2.44528700	-2.89039600	H	-0.95642000	5.44515200	2.75959300
H	-6.01461200	3.39668900	1.51371700	H	-1.25859000	6.25241800	-1.89194300
H	-4.90907900	2.78876700	2.78561000	H	-1.02385300	4.79531000	-2.90798500
H	-0.79638200	4.89680800	-2.90125300	H	-4.48330300	2.38430000	2.93936500
H	-1.04922200	6.32792100	-1.85309800	H	-5.77042500	3.03603700	1.87599200
H	-1.05794600	5.40546100	2.77443200	H	-5.09196600	2.52038200	-2.71600000
H	-1.19862600	6.64861400	1.49276100	H	-6.13470900	3.13922600	-1.39767100
H	4.55644600	5.05838700	-1.43475300	H	-6.04158400	-2.80941000	1.74424600
H	3.79671600	4.08928500	-2.73618400	H	-4.77961300	-2.27500800	2.89830500
H	3.28226000	3.67688500	2.92826600	H	-5.12772300	-2.13397600	-2.77344800
H	4.25142000	4.78695200	1.90945600	H	-6.25206600	-2.72582600	-1.51053100
H	2.24804900	-6.32585800	-0.30991300	H	5.56781900	-4.19436300	0.06311700
H	-0.12622700	-6.75983600	-0.04939000	H	6.69782700	-2.05932700	0.31554700
H	-5.51888400	-4.24132400	0.26807200	H	5.79652400	3.88301000	-0.06451100
H	-3.67498700	-5.81131400	0.08188700	H	6.80752700	1.69903700	0.27487100
H	-7.00850100	-0.78996700	0.22923500	H	2.89454800	6.20715900	-0.19701100
H	-6.86403900	1.61894000	-0.07476500	H	0.53114800	6.74726500	-0.29964500
H	-2.91331300	6.17110200	-0.26842400	H	-4.99613500	4.70121100	0.20146900
H	6.76503200	-0.46164600	1.67677400	H	-1.55264700	-6.13500800	-1.94919500
H	5.42953800	-0.44962700	2.87027500	H	-1.21394100	-4.67326500	-2.92917800
H	5.63390300	-0.20598900	-2.79093500	H	-1.32727000	-5.39625100	2.73074200
H	6.88075800	-0.36330800	-1.51564600	H	-1.63384900	-6.58356500	1.42478800
H	-4.95359700	4.85834800	-0.17346100	H	-3.02380600	6.08080200	-0.17816600
C	1.96359800	-0.55127100	0.42264700	C	-1.76000600	-0.72100100	-0.04270800
H	1.90606300	-1.59600100	0.12776600	H	-1.05425600	-1.32545800	-0.61924000
H	1.96863000	-0.34404400	1.48867800	H	-1.47904200	-0.78220400	1.01217800
C	2.01654300	0.41585800	-0.48405300	H	-2.74582200	-1.18055200	-0.14646900
H	2.06251600	1.46083300	-0.18777200	C	-1.77881100	0.72387800	-0.53539700
H	2.01264300	0.20911500	-1.55009300	H	-2.49310100	1.32299700	0.03629400
				H	-0.79670500	1.19217200	-0.42814300
				H	-2.05613100	0.78144300	-1.59160600
CH ₄ @Cucurbit[7]uril				N ₂ @Cucurbit[7]uril			
0 1				0 1			
C	4.00093700	4.16447900	-0.09710800	C	-4.15442200	4.05068800	0.02285200
C	5.02327900	2.99909900	0.02728300	C	-2.90263600	4.96859500	-0.09004300
N	4.85372600	2.27758600	-1.19897100	N	-2.22278500	4.45249000	-1.25395200
C	3.79667400	2.74787700	-1.95860700	C	-3.00828900	3.55885200	-1.96708000
N	3.21647700	3.79031900	-1.25000700	N	-4.13725900	3.31179700	-1.20538900
N	3.32932000	4.15547400	1.17022500	N	-3.90463400	3.30786900	1.23460200
H	4.47466300	5.14254800	-0.26401700	H	-5.09778700	4.60809900	0.11190300
N	4.60935500	2.33285000	1.23905700	N	-2.24453800	4.79303400	1.17240400
H	6.06378500	3.34067000	0.12233100	H	-3.15152600	6.02899200	-0.23958200
C	5.71142000	1.21804700	-1.65582200	C	-1.14336200	5.14813300	-1.90290400
O	3.47745000	2.36100700	-3.05149000	O	-2.78126400	3.12375000	-3.06478200
C	5.38987200	1.30216500	1.87308800	C	-1.16618600	5.61206400	1.65445900
C	3.70903100	3.09250200	1.97235100	C	-2.84929800	3.83219500	1.96517300
O	3.36366100	2.89601600	3.10700200	O	-2.54949800	3.54799500	3.09447300
N	5.19549900	-0.01485300	1.33427900	N	0.13378800	5.29359400	1.12709100
C	5.88214600	-0.53521600	0.18346100	C	0.60824100	5.70978300	-0.16280600
C	4.49618600	-0.98377600	2.03162100	C	1.13515900	4.76704200	1.92540600

C	5.49548200	-2.04724500	0.18656400	C	2.13153400	5.38843500	-0.11073800
N	5.43385200	-0.08101000	-1.10632000	N	0.14610300	4.95120500	-1.29728700
H	6.96307300	-0.36376100	0.28586200	H	0.39562000	6.77793700	-0.31449600
N	4.61680100	-2.16571600	1.32023800	N	2.28471300	4.70889000	1.15116900
O	3.93662400	-0.83925700	3.08616200	O	1.03897700	4.46717000	3.08583100
N	4.90803800	-2.24330900	-1.11150900	N	2.34855700	4.60986500	-1.29616100
H	6.35913900	-2.71572700	0.31176100	H	2.76551000	6.28674700	-0.13117600
C	4.93659300	-1.10327900	-1.89506900	C	1.18781800	4.38593500	-2.01643300
O	4.63931300	-1.02847600	-3.05829700	O	1.10739300	3.84973200	-3.08975200
C	4.20204600	-3.41878600	1.88805200	C	3.56521400	4.43494900	1.75005700
N	3.06228400	-4.01979900	1.24659200	N	4.21958900	3.25030700	1.26822300
C	3.16770900	-4.80238400	0.03888900	C	4.98263000	3.16945700	0.05624400
C	1.92392800	-4.33386800	1.97456600	C	4.25789700	2.08228300	2.01009200
C	1.75740200	-5.44442900	-0.08824900	C	5.65685900	1.76869900	0.14782000
N	3.31663700	-4.07651500	-1.18778800	N	4.23937100	3.09686200	-1.17886800
H	3.97456000	-5.54288300	0.13776400	H	5.70531500	3.99660500	0.01197900
N	1.14104200	-5.14708300	1.17191200	N	5.01881100	1.17069300	1.29430300
O	1.68472700	-4.00715100	3.10667200	O	3.76867800	1.91060200	3.09489000
N	1.20612500	-4.79340100	-1.25243500	N	5.37574000	1.17957600	-1.13019200
H	1.78772300	-6.53253600	-0.24390900	H	6.74348700	1.82016100	0.30642100
C	2.16962200	-4.09207600	-1.96382700	C	4.57821900	1.98078300	-1.92986000
C	4.55581000	-3.52305300	-1.66308700	C	3.64070100	4.24672700	-1.80676300
C	0.00737600	-5.24848400	-1.90504000	C	5.95961600	-0.04094300	-1.61844800
C	-0.07863800	-5.74283900	1.64600600	C	5.48299600	-0.04259700	1.91128300
O	2.04964000	-3.63083900	-3.06753100	O	4.28116600	1.77275900	-3.07609600
N	-1.21348600	-4.79208500	-1.29692900	N	5.35641500	-1.25313200	-1.13284200
N	-1.28894400	-5.16829900	1.12293900	N	5.00210900	-1.24823000	1.29197100
C	-2.11639600	-4.02480400	-2.01768800	C	4.54136600	-2.03701300	-1.93192400
C	-1.83021000	-5.45567400	-0.17556500	C	5.63040600	-1.85108200	0.14248500
C	-3.25314000	-4.82515500	-0.12171600	C	4.93568700	-3.24144900	0.04673400
N	-3.30277400	-4.01555200	-1.30485300	N	4.18677200	-3.15035600	-1.18396900
C	-2.15678100	-4.44217900	1.92093200	C	4.23294600	-2.15285600	2.00775900
N	-3.26159700	-4.13073900	1.14203000	N	4.17871100	-3.31829300	1.26272500
C	-4.48900400	-3.38390400	-1.81108400	C	3.56716500	-4.28720300	-1.81534500
C	-4.45868300	-3.59734200	1.73963700	C	3.50702500	-4.49481900	1.74066600
O	-2.00459000	-4.17810400	3.08404900	O	3.74934200	-1.97866300	3.09466300
O	-1.92315900	-3.50895200	-3.08648700	O	4.24253300	-1.81899000	-3.07583600
N	-4.82530000	-2.13354800	-1.18019600	N	2.27167500	-4.63218600	-1.30060900
N	-4.84659000	-2.29770000	1.26670000	N	2.21962800	-4.74465300	1.14611000
C	-4.90881300	-0.96797700	-1.92802600	C	1.11193000	-4.39504100	-2.01835000
C	-5.56904300	-2.04474200	0.05371600	C	2.04952700	-5.41453700	-0.11855000
C	-5.91512600	-0.52917900	0.15019900	C	0.52156900	-5.71362800	-0.16433600
N	-5.51290200	-0.01380000	-1.12715200	N	0.06570100	-4.95031400	-1.29791200
O	-4.57078200	-0.82688700	-3.07312200	O	1.03490100	-3.85646300	-3.09072300
C	-5.80766100	1.30840300	-1.61092700	C	-1.22756000	-5.13220100	-1.90014900
N	-5.15593700	-0.09142300	1.29597700	N	0.05815400	-5.28891300	1.12697700
C	-4.61751400	-1.15186000	2.00837100	C	1.07182200	-4.78440200	1.92398600
O	-4.09860300	-1.09610400	3.09158400	O	0.98523300	-4.48715800	3.08584900
C	-5.33595800	1.19279000	1.91862700	C	-1.24482200	-5.58760800	1.65846100
N	-4.94584000	2.35174100	-1.12338300	N	-2.29671100	-4.42165600	-1.25027500
N	-4.60061100	2.26330000	1.30116400	N	-2.31227300	-4.75407300	1.17730400
C	-3.98526100	2.94350500	-1.92615800	C	-3.07403800	-3.52163000	-1.96406800
C	-5.07913600	2.99329000	0.15368900	C	-2.97836500	-4.92453700	-0.08153800
C	-4.09148000	4.19407000	0.06039600	C	-4.21640200	-3.98850400	0.03394600
N	-3.38944300	3.94720200	-1.17645200	N	-4.19645400	-3.25680500	-1.19858400
O	-3.74985500	2.67314300	-3.07377000	O	-2.84637400	-3.09439400	-3.06476500
C	-2.54378700	4.92636200	-1.80972300	C	-5.25576800	-2.40620100	-1.66653600
N	-3.32759000	4.09141400	1.27008500	N	-3.94837300	-3.24269000	1.24004300
C	-3.64242500	2.96750000	2.01387700	C	-2.89689300	-3.77868100	1.96741100
O	-3.20586700	2.68541600	3.09814400	O	-2.58566800	-3.49199800	3.09300300
C	-2.41311800	5.08914900	1.75121200	C	-4.92244200	-2.39507800	1.87423900
N	-1.20185900	4.98498000	-1.30198900	N	-5.26650300	-1.07700700	-1.11597300

N	-1.10690600	5.06092600	1.14474700	N	-5.01896300	-1.07212500	1.32107800
C	-0.81093400	5.69298200	-0.11731200	C	-5.81308400	-0.73569500	0.17008200
C	0.02899400	4.87423700	1.91906000	C	-4.60726600	0.04016500	2.03509700
C	0.74499400	5.66423400	-0.17585700	C	-5.80108300	0.82389800	0.16567800
N	1.11981800	5.16912400	1.11879500	N	-5.01077300	1.15487600	1.32046100
C	-0.12453600	4.49361600	-2.01892000	C	-5.01244200	0.03219800	-1.90454500
N	1.01988200	4.80629900	-1.30076700	N	-5.23949300	1.14902000	-1.11848600
O	0.05926900	4.56671000	3.08110700	O	-4.04748100	0.03846900	3.09945600
O	-0.17027300	3.94687000	-3.08891100	O	-4.70094000	0.02701000	-3.06600600
C	2.45906900	5.19775400	1.64310700	C	-4.89552400	2.47881500	1.86760800
C	2.31818500	4.70119600	-1.90941100	C	-5.20645300	2.47517000	-1.67558400
H	0.02866300	-4.85869500	-2.92507500	H	5.84259300	-0.03854400	-2.70411600
H	0.00490500	-6.34937800	-1.93066000	H	7.02643000	-0.05009600	-1.36026400
H	-0.06088200	-6.81449400	1.40644000	H	6.58357300	-0.05010900	1.90807700
H	-0.10482300	-5.60766000	2.72921400	H	5.11893500	-0.04127100	2.94117300
H	-5.29086400	-4.29424900	1.56854200	H	4.15968500	-5.36234000	1.57049700
H	-4.26686900	-3.50888700	2.81102600	H	3.34232200	-4.36212200	2.81195000
H	-4.31875600	-3.17185600	-2.86870400	H	3.44205100	-4.03728800	-2.87104700
H	-5.33012800	-4.08369000	-1.70521500	H	4.22791300	-5.16061300	-1.71827300
H	-6.84527500	1.55564400	-1.35193300	H	-1.46521100	-6.20725200	-1.91761500
H	-5.69470600	1.28250500	-2.69675400	H	-1.16509300	-4.75467000	-2.92303300
H	-6.40738400	1.44475200	1.91997600	H	-1.48895800	-6.63485000	1.43452300
H	-4.97838100	1.10569200	2.94701800	H	-1.18583900	-5.44586500	2.73959600
H	-3.00123100	5.92093200	-1.70723400	H	-6.21577400	-2.89354100	-1.45050900
H	-2.48165800	4.65772700	-2.86637900	H	-5.13177900	-2.29850200	-2.74605400
H	-2.86467200	6.07932600	1.59663800	H	-5.91093100	-2.87428100	1.81818400
H	-2.27110000	4.91283200	2.81944400	H	-4.62358900	-2.29013900	2.91944500
H	2.17147000	4.32882400	-2.92556800	H	-5.07819600	2.36044100	-2.75387900
H	2.77978500	5.70032600	-1.94574900	H	-6.16043600	2.97775000	-1.46727700
H	2.37878200	5.08363700	2.72607300	H	-4.60395500	2.37426400	2.91488200
H	2.91382500	6.16853300	1.40509000	H	-5.87610000	2.97291000	1.80399200
H	6.75085400	1.49097200	-1.43067500	H	-1.36777900	6.22597500	-1.92330900
H	5.57768000	1.13557700	-2.73641500	H	-1.08301600	4.76766600	-2.92482600
H	5.08878600	1.27387500	2.92258500	H	-1.11252700	5.47152500	2.73603800
H	6.45698300	1.55737000	1.80072200	H	-1.39423700	6.66231900	1.42788500
H	-1.84334000	-6.54220700	-0.34405900	H	6.71631800	-1.91909100	0.29966900
H	-4.05985000	-5.57173400	-0.14411700	H	5.64612800	-4.07862200	-0.00644200
H	-6.98525300	-0.33744300	0.31262000	H	0.29307500	-6.77885100	-0.31370100
H	-6.45699000	-2.69095200	0.00461200	H	2.67029500	-6.32182100	-0.14747800
H	-6.12300700	3.29954100	0.31200300	H	-3.24295700	-5.98175600	-0.22638600
H	-4.59616500	5.16971500	0.01637800	H	-5.16692900	-4.53200800	0.13205200
H	1.19265000	6.65498100	-0.34149600	H	-6.80288500	1.26677300	0.25982500
H	5.04884700	-4.12076800	1.85486000	H	4.23295700	5.29254400	1.58791900
H	3.92233200	-3.23153000	2.92700500	H	3.39379000	4.29884800	2.81985600
H	4.45679600	-3.38451500	-2.74172600	H	3.51627500	4.00422700	-2.86427600
H	5.36002200	-4.24098000	-1.45304400	H	4.31489300	5.10884400	-1.70218400
H	-1.22853500	6.70993400	-0.13389800	H	-6.82078600	-1.16269700	0.27423900
C	2.09223600	-0.08668800	-0.48461500	N	-2.03904100	0.51657300	-0.26938300
H	2.35836900	-1.10858900	-0.20505300	N	-2.04615100	-0.57619300	-0.25815800
H	2.29621100	0.06839600	-1.54536700				
H	1.03094500	0.07199000	-0.29262200				
H	2.67696600	0.61449400	0.11352700				
NO ₂ @Cucurbit[7]JuriI				NO@Cucurbit[7]JuriI			
O 2				O 2			
C	-4.85328300	3.17273400	0.07350700	C	4.53528300	3.63307000	0.00751500
C	-5.48882600	1.75175600	0.14886200	C	5.34927300	2.30900500	0.10630600
N	-4.85513000	1.16321500	1.30188600	N	5.11193700	1.67858100	-1.15979200
C	-4.09315500	2.07928700	2.01211100	C	4.19315200	2.36051300	-1.93792200
N	-4.06346800	3.24588800	1.27058000	N	3.77386700	3.46035100	-1.20548800
N	-4.14399900	3.14947000	-1.18065300	N	3.79645500	3.66173000	1.23730200

H	-5.59753600	3.98156900	0.06779800	H	5.16877200	4.52822700	-0.06940400
N	-5.16633500	1.17155400	-1.12395900	N	4.79044900	1.66761300	1.27288300
H	-6.57915300	1.77139200	0.28841600	H	6.42703100	2.47075600	0.24942500
C	-5.31780600	-0.04922200	1.92287300	C	5.77814700	0.49568300	-1.63158600
O	-3.59545900	1.90659400	3.09309800	O	3.86616100	2.08276200	-3.06145000
C	-5.73173600	-0.05050200	-1.62940800	C	5.39288600	0.52421700	1.90680900
C	-4.40997000	2.01277600	-1.92357800	C	3.96126100	2.51465100	1.99274100
O	-4.09040400	1.81110600	-3.06554100	O	3.51281100	2.31310700	3.09032300
N	-5.13889300	-1.25916100	-1.12283600	N	5.03246800	-0.74044600	1.32848900
C	-5.45732200	-1.85085200	0.14591100	C	5.66697900	-1.29903000	0.16432500
C	-4.36547900	-2.08433700	-1.92293800	C	4.28468300	-1.66965100	2.03119100
C	-4.79576100	-3.26003900	0.06805600	C	5.11294800	-2.75552000	0.11572400
N	-4.84024200	-1.25652300	1.30452800	N	5.28093600	-0.74872000	-1.10595200
H	-6.54782900	-1.89100700	0.27955100	H	6.75984100	-1.25277300	0.27558200
N	-4.08416500	-3.22003600	-1.18439500	N	4.28957100	-2.83915400	1.29104300
O	-4.04476800	-1.87221600	-3.06271500	O	3.77054300	-1.50714100	3.10632400
N	-4.00755800	-3.32251900	1.26689900	N	4.44025100	-2.81128900	-1.15539100
H	-5.52529500	-4.08214400	0.05814400	H	5.90011400	-3.52182300	0.15671300
C	-4.06065800	-2.15906300	2.01224500	C	4.61789300	-1.66282800	-1.90809800
O	-3.56766800	-1.98026300	3.09441600	O	4.30347700	-1.50667600	-3.05837900
C	-3.45967300	-4.36523700	-1.79104000	C	3.74548800	-4.06153500	1.81462000
N	-2.15877600	-4.69507900	-1.27824700	N	2.51837400	-4.49026700	1.19726500
C	-1.92580100	-5.46982500	-0.09336500	C	2.47260300	-5.22043900	-0.04497200
C	-1.00444600	-4.45708000	-2.00406300	C	1.36166000	-4.64595700	1.94531800
C	-0.39887800	-5.77127400	-0.15108200	C	0.98680400	-5.67846400	-0.13292000
N	-2.08146300	-4.79195800	1.16810600	N	2.66030900	-4.46083100	-1.24745800
H	-2.54807000	-6.37641400	-0.11066400	H	3.18545500	-6.05695600	-0.01550700
N	0.04761700	-5.00888600	-1.28904700	N	0.44580100	-5.30650700	1.14339600
O	-0.93536300	-3.92253100	-3.07897500	O	1.20100700	-4.31888000	3.09119800
N	0.07600100	-5.34618200	1.13566800	N	0.48873600	-4.96278500	-1.28118600
H	-0.17280500	-6.83679600	-0.30164100	H	0.87295000	-6.76112700	-0.28697500
C	-0.92769100	-4.82542300	1.93557900	C	1.50038700	-4.33444600	-1.99187100
C	-3.36020500	-4.50642400	1.76128900	C	3.93542600	-4.02189200	-1.74534700
C	1.38445600	-5.63942300	1.65554000	C	-0.77159600	-5.25970200	-1.90681900
C	1.33869900	-5.18603400	-1.89615600	C	-0.83481300	-5.73057000	1.64178500
O	-0.82869700	-4.51400700	3.09273700	O	1.40131200	-3.82340300	-3.07586500
N	2.44353100	-4.79577400	1.17182700	N	-1.91075400	-4.64347800	-1.28005900
N	2.40513700	-4.46134600	-1.25662200	N	-1.96578200	-4.99440900	1.14414000
C	3.01607400	-3.81120000	1.95918800	C	-2.73145400	-3.78817400	-2.00017500
C	3.10321700	-4.95250100	-0.09218300	C	-2.58054300	-5.20927700	-0.13453500
C	4.32414100	-3.99325200	0.01608200	C	-3.89687400	-4.38211800	-0.04782100
N	4.04577400	-3.24667000	1.22038300	N	-3.88875200	-3.61636800	-1.26055600
C	3.16671600	-3.55522200	-1.97998600	C	-2.67537200	-4.11284800	1.94169000
N	4.28670100	-3.26654600	-1.21934400	N	-3.74454900	-3.65127100	1.18719600
C	5.01433200	-2.39069600	1.85472400	C	-4.99063400	-2.83029400	-1.74153600
C	5.32678000	-2.39498600	-1.69342400	C	-4.82134900	-2.92597900	1.81105100
O	2.92853400	-3.13914600	-3.08271500	O	-2.43922700	-3.84092600	3.08876100
O	2.71295500	-3.53654700	3.08981200	O	-2.50509000	-3.32515800	-3.08650000
N	5.09697700	-1.06698700	1.30250900	N	-5.11401300	-1.52544400	-1.14485800
N	5.31677000	-1.06827400	-1.13671800	N	-5.02959300	-1.59877100	1.30272300
C	4.69099800	0.04421600	2.02274900	C	-5.02976200	-0.37908000	-1.92043600
C	5.87737200	-0.72729400	0.14354000	C	-5.77351800	-1.28925700	0.11515800
C	5.86363700	0.83159200	0.14155200	C	-5.90648500	0.26239100	0.16550200
N	5.08173500	1.16057800	1.30233500	N	-5.43324500	0.67993300	-1.12476500
O	4.14910100	0.04065000	3.09615000	O	-4.71670100	-0.32199200	-3.07982700
C	4.97651200	2.48386400	1.85180300	C	-5.55042000	2.01629000	-1.64369300
N	5.29224800	1.15927700	-1.13762100	N	-5.10033800	0.62837200	1.30214000
C	5.06214000	0.04250700	-1.92445300	C	-4.66765100	-0.47382800	2.02330900
O	4.75235200	0.03855100	-3.08621400	O	-4.12768600	-0.45794800	3.09749800
C	5.27757800	2.48494400	-1.69692400	C	-5.11563700	1.93833700	1.89454200
N	3.99042500	3.32053600	1.21870000	N	-4.56392800	2.95020200	-1.17176900
N	4.22347200	3.33880500	-1.22187400	N	-4.24522300	2.89147300	1.25831900

C	2.95224400	3.86730900	1.95913900	C	-3.49451100	3.34841200	-1.95628700
C	4.25131800	4.06903200	0.01172300	C	-4.62181000	3.64121200	0.08363000
C	3.01261800	5.00540100	-0.09482800	C	-3.48773200	4.70025200	-0.03549500
N	2.35877500	4.83873500	1.17099000	N	-2.78352900	4.29024300	-1.22741900
O	2.65753900	3.58973500	3.09126800	O	-3.26002300	2.98527700	-3.07821200
C	1.28529200	5.66351700	1.65568600	C	-1.78523300	5.10496300	-1.86927600
N	2.32065800	4.49959200	-1.25665600	N	-2.78465000	4.57443300	1.20820400
C	3.09636400	3.60547500	-1.98001000	C	-3.24319100	3.52122900	1.98153600
O	2.86271100	3.18253100	-3.08108400	O	-2.87819200	3.24111600	3.09233700
C	1.24130000	5.20521000	-1.89579000	C	-1.78346700	5.48995700	1.68401200
N	-0.01855900	5.34712700	1.13775800	N	-0.47272700	5.00710600	-1.29194800
N	-0.04576000	5.00729300	-1.28657300	N	-0.46599900	5.29808200	1.13929200
C	-0.50293900	5.76310600	-0.14833800	C	-0.04917200	5.77482100	-0.15070400
C	-1.09004700	4.44021700	-2.00101700	C	0.59397200	4.88224500	1.92784700
C	-2.02442700	5.43558500	-0.08756400	C	1.49541400	5.57168800	-0.13088400
N	-2.24734400	4.66137800	-1.27462500	N	1.73314800	4.93724900	1.13986800
C	-1.01061200	4.80484300	1.93789100	C	0.59266500	4.49669000	-2.01716400
N	-2.16473500	4.75059400	1.17205000	N	1.74403100	4.78177800	-1.30361600
O	-1.01387300	3.90699700	-3.07609900	O	0.54362700	4.58086400	3.09081700
O	-0.90370400	4.49275200	3.09416400	O	0.53232000	3.95630700	-3.08970900
C	-3.54300800	4.30851100	-1.78499000	C	3.04313000	4.78684700	1.71761800
C	-3.43669700	4.43999100	1.76719300	C	3.05122700	4.52966800	-1.84318000
H	1.33337700	-5.50388100	2.73790200	H	-0.72181700	-4.88105100	-2.93003900
H	1.63371200	-6.68357000	1.42384300	H	-0.91658500	-6.35092900	-1.92395200
H	1.58498900	-6.25915100	-1.90570900	H	-0.97348100	-6.79338400	1.40320000
H	1.26891000	-4.81746100	-2.92186900	H	-0.81712300	-5.59528200	2.72521500
H	6.29716400	-2.86598100	-1.48702000	H	-5.75572700	-3.49400200	1.69829700
H	5.19186900	-2.28631100	-2.77154600	H	-4.57319300	-2.83342400	2.87046400
H	4.71643300	-2.28994100	2.90062700	H	-4.83850100	-2.67664900	-2.81186400
H	6.00682600	-2.86168200	1.79652200	H	-5.92002800	-3.39275300	-1.57632800
H	5.96022600	2.97224100	1.78912500	H	-6.54654500	2.40795000	-1.40036000
H	4.68411700	2.38007800	2.89894200	H	-5.43571800	1.94609300	-2.72732000
H	6.24011900	2.97326900	-1.49381500	H	-6.14594500	2.32530200	1.88275000
H	5.14201600	2.37190300	-2.77450900	H	-4.77539100	1.83214900	2.92701400
H	1.51556900	6.71186900	1.42346600	H	-2.10688300	6.15739700	-1.84676600
H	1.23835300	5.52735700	2.73815800	H	-1.71192600	4.76611400	-2.90496800
H	1.46968200	6.28226800	-1.90749900	H	-2.11545800	6.51391000	1.46653300
H	1.17618700	4.83388100	-2.92081000	H	-1.70283800	5.34981000	2.76393100
H	-3.26161700	4.29547200	2.83534000	H	2.92166900	4.24912800	-2.89059400
H	-4.12507200	5.28333600	1.61583200	H	3.64244400	5.45490300	-1.77873700
H	-3.42414600	4.08686700	-2.84770800	H	2.90182900	4.64891700	2.79156800
H	-4.21510500	5.16900800	-1.65967100	H	3.62499000	5.70082600	1.53446900
H	-6.41817700	-0.05590800	1.92276700	H	6.84744600	0.58004300	-1.39656900
H	-4.95014000	-0.04610900	2.95145900	H	5.64026800	0.46147500	-2.71422400
H	-5.58102000	-0.04893900	-2.71100300	H	5.05266800	0.51435700	2.94467900
H	-6.80687300	-0.06288400	-1.40460400	H	6.48730000	0.63159900	1.87650300
H	3.38689100	-6.00431500	-0.23989700	H	-2.75215600	-6.28362600	-0.29297400
H	5.28462900	-4.51903800	0.11360000	H	-4.80085600	-5.00646900	-0.00538700
H	6.86585600	1.27537500	0.22870400	H	-6.94056700	0.60506600	0.31383500
H	6.88686400	-1.15329500	0.23550500	H	-6.74211900	-1.80904400	0.13393600
H	5.20237700	4.61244000	0.10488300	H	-5.61794300	4.08506000	0.22267000
H	3.27629800	6.06205600	-0.24508300	H	-3.86261400	5.72693400	-0.15349100
H	-2.66213100	6.33143800	-0.09983300	H	2.05759000	6.51508200	-0.18857200
H	-4.11546200	-5.23886000	-1.67016800	H	4.50007800	-4.85494000	1.71181500
H	-3.34228300	-4.13798000	-2.85273600	H	3.52918200	-3.89585900	2.87215500
H	-3.18992400	-4.36201400	2.83023100	H	3.81790500	-3.82914700	-2.81374600
H	-4.03232000	-5.36202800	1.60573700	H	4.66628400	-4.82808400	-1.59273500
H	-0.29510000	6.83215000	-0.30011100	H	-0.34671100	6.82600000	-0.27581700
O	-1.75373100	1.08580100	-0.13642500	N	2.12702800	0.43907400	-0.33668400
O	-1.76162900	-1.10066100	-0.11473700	O	2.02616000	-0.69514100	-0.23990700
N	-2.18879200	-0.00738300	-0.28282100				

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C	-3.05788700	4.97460000	-0.09470700	C	5.76997000	-0.90911600	0.12651600
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C	-2.97409200	3.83131800	1.95584200	C	4.62560600	-0.18390200	2.04674900
N	-2.39283400	4.80829600	1.16538300	N	5.07140900	-1.27578700	1.32434000
N	-2.37398800	4.47363100	-1.26335500	N	5.10712100	-1.17526100	-1.12689700
H	-3.32747400	6.03027300	-0.24063300	H	6.77109700	-1.36333400	0.12326600
N	-4.27130300	3.30453600	-1.21433400	N	5.32470700	1.04083900	-1.10611300
H	-5.24411300	4.57186000	0.12300900	H	6.80722500	1.05605400	0.35746000
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O	-2.66610400	3.55071200	3.08357400	O	4.10015400	-0.21151100	3.12861600
C	-5.32373100	2.44347000	-1.68053700	C	5.32721800	2.38585800	-1.61246000
C	-3.15214200	3.57774800	-1.98194100	C	4.96887900	-0.03445500	-1.90088800
O	-2.92652600	3.15874500	-3.08596100	O	4.65433200	0.00982500	-3.06104000
N	-5.32400400	1.11709500	-1.12258100	N	4.25580000	3.22759700	-1.15138000
C	-5.88298500	0.78298600	0.16027600	C	4.23590900	3.91605700	0.10532800
C	-5.08743400	0.00303800	-1.91153700	C	3.14407400	3.49889300	-1.92846100
C	-5.88404600	-0.77602200	0.16018400	C	3.01157200	4.86609400	-0.02304000
N	-5.09518500	1.11656000	1.31585800	N	3.91361600	3.12984500	1.27262700
H	-6.88807700	1.21844900	0.25553600	H	5.18672900	4.44601500	0.25783700
N	-5.32517800	-1.11076400	-1.12256900	N	2.34853900	4.37937000	-1.21075500
O	-4.78507700	0.00287500	-3.07504900	O	2.93500500	3.08975600	-3.04073500
N	-5.09700300	-1.11080500	1.31590500	N	2.32115300	4.68789700	1.22058200
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C	-4.69262500	0.00255200	2.03335600	C	2.85827100	3.67046400	1.99188300
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C	-5.32669900	-2.43710400	-1.68062900	C	1.29454900	5.10355800	-1.87144700
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C	-4.29673800	-4.02770800	0.02060500	C	-0.47383400	5.69040300	-0.15793900
C	-3.15661900	-3.57419600	-1.98214200	C	-1.04450200	4.36672200	-2.01504600
C	-3.06388400	-4.27104200	-0.09483200	C	-2.00733000	5.41701700	-0.14436500
N	-4.02183000	-3.27867700	1.22415500	N	-0.04225500	5.24563300	1.13856200
H	-5.24974600	-4.56592400	0.12267400	H	-0.22464500	6.75304600	-0.29263400
N	-2.37940400	-4.47081500	-1.26346100	N	-2.21243300	4.60784400	-1.31221400
O	-2.93029700	-3.15511300	-3.08598900	O	-0.95339500	3.81886900	-3.08172500
N	-2.39868900	-4.80543800	1.16528800	N	-2.22237000	4.78260700	1.13041100
H	-3.33453700	-6.02644000	-0.24077500	H	-2.61190200	6.33311600	-0.21229800
C	-2.97912400	-3.82803900	1.95581600	C	-1.08685800	4.79107600	1.92617600
C	-4.99710200	-2.43474800	1.86450300	C	1.25458000	5.52570900	1.69496500
C	-1.32255800	-5.63130100	1.64166500	C	-3.52755000	4.57499800	1.70150500
C	-1.30459200	-5.17860800	-1.90793600	C	-3.50281200	4.28173700	-1.85123200
O	-2.67072400	-3.54760400	3.08347800	O	-1.03032300	4.50773400	3.09336000
N	-0.02175800	-5.31228600	1.11680300	N	-4.21797700	3.40516400	1.23394800
N	-0.01314500	-4.97874900	-1.30869700	N	-4.16307900	3.17484700	-1.20827900
C	0.97966500	-4.78964100	1.91833200	C	-4.29768900	2.25026700	1.99321500
C	0.45478800	-5.72944900	-0.17227700	C	-4.94253400	3.31401800	-0.00051200
C	1.97569400	-5.39688600	-0.12229300	C	-5.66846800	1.94119600	0.10965600
N	2.12930900	-4.72878900	1.14515900	N	-5.06317100	1.34450000	1.27519600
C	1.02187000	-4.39579200	-2.02355300	C	-4.53476300	2.05902200	-1.94462800
N	2.18364400	-4.60386100	-1.30022800	N	-5.39510500	1.31749200	-1.15298400
C	3.41053700	-4.45994600	1.74473400	C	-5.56655100	0.15171900	1.90147200
C	3.47404800	-4.24582800	-1.81918600	C	-6.01723900	0.11032300	-1.62699600
O	0.93570500	-3.85836700	-3.09562300	O	-4.21437000	1.80967800	-3.07621000
O	0.88262400	-4.49472700	3.07983700	O	-3.83609300	2.08596800	3.09116100
N	4.07143100	-3.27965400	1.26193500	N	-5.11128600	-1.07314200	1.30206900
N	4.08864400	-3.10930100	-1.18295800	N	-5.45501100	-1.11423800	-1.12390100
C	4.12335600	-2.11322500	2.00534100	C	-4.33973200	-1.97187600	2.02174600
C	4.83389500	-3.20430700	0.04946000	C	-5.74793700	-1.68215700	0.16164900

C	5.53378200	-1.81704900	0.14878000	C	-5.08669500	-3.09103900	0.09334900
N	4.89991600	-1.21234000	1.29401500	N	-4.30315500	-3.14864600	1.29404000
O	3.63271000	-1.93622200	3.08867700	O	-3.84161300	-1.78446800	3.09991700
C	5.37200400	-0.00307700	1.91208000	C	-3.65307100	-4.32816900	1.79261100
N	5.27159800	-1.22062100	-1.12951300	N	-4.36390200	-3.05761500	-1.15462900
C	4.44869700	-1.99608100	-1.92800400	C	-4.68582800	-1.94653400	-1.91977200
O	4.14785200	-1.77221700	-3.07031200	O	-4.39783100	-1.76440300	-3.07268300
C	5.86978200	-0.00331600	-1.60830500	C	-3.78920400	-4.22842400	-1.76549400
N	4.90123600	1.20670100	1.29401200	N	-2.38580800	-4.62838600	1.17868300
N	5.27286300	1.21460500	-1.12949200	N	-2.49242000	-4.59524800	-1.26924000
C	4.12569300	2.10847200	2.00533500	C	-1.22439700	-4.67843200	1.93503300
C	5.53583500	1.81068500	0.14880400	C	-2.26118700	-5.34321200	-0.06698400
C	4.83771800	3.19884400	0.04956700	C	-0.74175400	-5.67893200	-0.13684100
N	4.07517700	3.27498700	1.26195100	N	-0.24397500	-5.24366100	1.13755100
O	3.63479000	1.93202000	3.08864000	O	-1.10397200	-4.34424100	3.08393000
C	3.41578700	4.45608700	1.74482800	C	1.05712000	-5.57035300	1.65532900
N	4.09254600	3.10492700	-1.18297300	N	-0.29142400	-4.94397800	-1.29191700
C	4.45106900	1.99121200	-1.92801100	C	-1.34090400	-4.39161500	-2.00991200
O	4.14992900	1.76778000	-3.07032800	O	-1.27346400	-3.88076400	-3.09641200
C	3.47923500	4.24219800	-1.81909500	C	0.98799000	-5.16100600	-1.91250000
N	2.13490400	4.72652900	1.14526100	N	2.13944000	-4.77331600	1.14577100
N	2.18920400	4.60159500	-1.30012600	N	2.08373600	-4.47445000	-1.28303800
C	1.98212900	5.39483700	-0.12218400	C	2.77285300	-4.98578100	-0.12469600
C	1.02720800	4.39487700	-2.02348400	C	2.85090500	-3.56623100	-1.99718500
C	0.46161500	5.72917800	-0.17220500	C	4.05077600	-4.09893200	-0.04675000
N	-0.00717500	4.97888900	-1.30856300	N	3.99013900	-3.32206500	-1.25095300
C	0.98538600	4.78893700	1.91849100	C	2.81505700	-3.86225600	1.93935400
N	-0.01540700	5.31274100	1.11693900	N	3.88412400	-3.38810900	1.19608700
O	0.94042600	3.85750400	-3.09553000	O	2.60165800	-3.11834000	-3.08491400
O	0.88797000	4.49405100	3.07997100	O	2.55430700	-3.57827600	3.07885800
C	-1.29838300	5.18021400	-1.90783500	C	5.04881100	-2.48019800	-1.73191400
C	-1.31589200	5.63310800	1.64174100	C	4.93126100	-2.61788900	1.81535800
H	-1.26860700	-5.49815300	2.72415800	H	-3.38799900	4.46061900	2.77847500
H	-1.55426400	-6.67900800	1.40806100	H	-4.15468300	5.45422600	1.49954100
H	-1.53246200	-6.25559500	-1.91447300	H	-4.14538200	5.17232600	1.79082600
H	-1.24716800	-4.81032300	-2.93451100	H	-3.35858500	4.00418700	-2.89756800
H	4.14186700	-5.11516400	-1.73174200	H	-7.08428700	0.14261300	-1.37195200
H	3.34170100	-3.98961400	-2.87243800	H	-5.89771500	0.09225000	-2.71222100
H	3.23870400	-4.32194300	2.81415800	H	-5.21395100	0.15792200	2.93532500
H	4.07404700	-5.32118800	1.58421400	H	-6.66675400	0.17207700	1.88578900
H	6.47255800	-0.00365200	1.91158700	H	-4.33120600	-5.18317200	1.66189600
H	5.00592100	-0.00288200	2.94126600	H	-3.46306900	-4.16890700	2.85606000
H	6.93311300	-0.00386100	-1.33695500	H	-4.47138500	-5.07953900	-1.62914300
H	5.76645000	-0.00327500	-2.69523500	H	-3.67989200	-4.01175600	-2.83026800
H	4.08033800	5.31654200	1.58436900	H	1.26696900	-6.62775900	1.44332300
H	3.24373600	4.31825200	2.81424000	H	1.02031600	-5.41125800	2.73503200
H	4.14798100	5.11081000	-1.73155700	H	1.20057300	-6.24121800	-1.92766400
H	3.34663800	3.98621700	-2.87237100	H	0.91735000	-4.78748800	-2.93631400
H	-1.26209300	5.49998400	2.72424500	H	4.69224100	-2.54935400	2.87863200
H	-1.54650500	6.68103700	1.40805000	H	5.88902100	-3.14052000	1.68446500
H	-1.24135000	4.81185800	-2.93440700	H	4.88355900	-2.32761500	-2.80046300
H	-1.52501400	6.25746400	-1.91437800	H	6.00641500	-2.99656400	-1.57539400
H	-5.98042400	2.92317800	1.81020800	H	5.85317000	2.72652900	1.90288800
H	-4.69200500	2.33772400	2.90932000	H	4.52653400	2.11824000	2.94276300
H	-5.19660700	2.33238500	-2.75933400	H	5.23515700	2.31319200	-2.69794000
H	-6.28780600	2.92473900	-1.46864500	H	6.28000300	2.86369500	-1.35221000
H	0.24947200	-6.79955500	-0.32002400	H	-5.63324600	4.16403800	-0.09383500
H	2.61626700	-6.29021800	-0.15410400	H	-6.75400700	2.03501900	0.25516400
H	6.61824200	-1.88947200	0.31346000	H	-5.81684700	-3.91272000	0.08211400
H	5.54131600	-4.04419900	-0.00194700	H	-6.83580700	-1.72075800	0.31536100
H	6.62039200	1.88170800	0.31346300	H	-2.90296900	-6.23601200	-0.05217900
H	5.54618100	4.03787400	-0.00161300	H	-0.54016600	-6.75133200	-0.27265700

H	0.25757300	6.79950800	-0.32008700	H	4.98354900	-4.68039300	-0.02288500
H	-6.29143400	-2.91706800	-1.46877000	H	1.54177600	6.17655900	-1.87982800
H	-5.19942700	-2.32612800	-2.75942100	H	1.24401900	4.73173500	-2.89703400
H	-4.69558700	-2.33270500	2.90921700	H	1.17513200	5.37270200	2.77318400
H	-5.98446900	-2.91641800	1.80973800	H	1.51472200	6.57255100	1.48734100
H	2.62375100	6.28742100	-0.15394700	H	2.99229700	-6.05456500	-0.26074000
F	2.26337000	-0.00111700	-0.67305200	Cl	1.54791600	-0.36094900	0.79107600
F	1.90300500	-0.00529600	0.66579300	Cl	1.71991600	0.35769100	-1.09048500

H ₂ S@Cucurbit[7]uril				H ₂ @Cucurbit[7]uril			
0 1				0 1			
C	-5.75176200	0.83495700	0.24931900	C	5.80173400	-0.79825600	0.16216100
C	-5.76642900	-0.72439200	0.25470000	C	5.80656200	0.76066600	0.16475000
N	-4.92571600	-1.06311000	1.37111300	N	5.01468000	1.09557600	1.31733800
C	-4.48257800	0.04973600	2.06652700	C	4.61149700	-0.01818000	2.03521500
N	-4.91287900	1.16595300	1.36882700	N	5.01467600	-1.13212800	1.31793500
N	-5.24975300	1.15774600	-1.05898000	N	5.24018800	-1.12892300	-1.12062700
H	-6.74809900	1.27963600	0.38657800	H	6.80594200	-1.23633100	0.25533100
N	-5.28065800	-1.06539100	-1.05485600	N	5.25475500	1.09906500	-1.11988500
H	-6.76980500	-1.14956700	0.40196000	H	6.81287400	1.19228400	0.26522900
C	-4.84582300	-2.37763200	1.94418600	C	4.92216300	2.41834400	1.87037500
O	-3.89135300	0.04757000	3.11339900	O	4.06233300	-0.01798000	3.10490700
C	-5.26303300	-2.39480100	-1.59515100	C	5.26473200	2.42585200	-1.67674900
C	-5.02787500	0.04154300	-1.84398500	C	5.01128800	-0.01304600	-1.90936400
O	-4.74169100	0.03512300	-3.01366200	O	4.71067200	-0.01060200	-3.07349800
N	-4.19548600	-3.24259400	-1.13125100	N	4.21904600	3.29494800	-1.21010200
C	-4.21269400	-3.98979100	0.09332800	C	4.24458100	4.02072200	0.02635500
C	-3.07177100	-3.49426200	-1.89231300	C	3.10576100	3.58339100	-1.98057700
C	-2.99534300	-4.94857600	-0.04965400	C	3.02289800	4.97819900	-0.09138800
N	-3.90847100	-3.25968300	1.29971300	N	3.95736600	3.27238100	1.22751500
H	-5.17289800	-4.51408700	0.19863800	H	5.20326800	4.54803200	0.13250500
N	-2.30864100	-4.42489400	-1.20841100	N	2.33594300	4.48662800	-1.26224600
O	-2.82331100	-3.02233500	-2.97394500	O	2.87847000	3.16950900	-3.08633300
N	-2.32311500	-4.82278100	1.21012400	N	2.35313700	4.81920500	1.16703700
H	-3.28020400	-5.99579800	-0.22291700	H	3.30597900	6.03053600	-0.23580500
C	-2.87283100	-3.83845900	2.01636400	C	2.91905000	3.83281100	1.95704900
O	-2.54700900	-3.57780000	3.14365600	O	2.60368200	3.55367900	3.08319000
C	-1.24297900	-5.12559900	-1.87607200	C	1.26810600	5.20502500	-1.90680200
N	0.05141300	-4.95754100	-1.27525200	N	-0.02649900	5.01184200	-1.31262500
C	0.51160100	-5.74972000	-0.16262500	C	-0.49581200	5.75928200	-0.17513300
C	1.09722300	-4.39997900	-1.99607700	C	-1.05822400	4.41931600	-2.02356100
C	2.03736200	-5.44263500	-0.11115900	C	-2.01733900	5.42687800	-0.12806400
N	0.04769100	-5.36312000	1.13938700	N	-0.02096100	5.33893100	1.11400400
H	0.28912000	-6.81178000	-0.34088800	H	-0.29015300	6.82971200	-0.31989900
N	2.25937900	-4.65678100	-1.29078200	N	-2.22054700	4.62312400	-1.29990200
O	1.01502000	-3.84723300	-3.06088100	O	-0.96969700	3.87762700	-3.09346000
N	2.19810400	-4.77550200	1.15679500	N	-2.17597100	4.77048800	1.14465000
H	2.66306000	-6.34647100	-0.14053100	H	-2.65791200	6.31975100	-0.17041300
C	1.05494200	-4.84901200	1.93938400	C	-1.02658600	4.82883700	1.91830700
C	-1.25562700	-5.67246800	1.66390800	C	1.28111100	5.65271600	1.63941700
C	3.48320000	-4.51577500	1.75304000	C	-3.45795100	4.50020700	1.74158000
C	3.55372200	-4.30313300	-1.80330700	C	-3.50872400	4.25624700	-1.81783000
O	0.96735600	-4.57125600	3.10572800	O	-0.93270700	4.54146100	3.08202100
N	4.14486300	-3.33358400	1.27631300	N	-4.11249600	3.31235300	1.26727600
N	4.16602600	-3.16407200	-1.17001400	N	-4.11760300	3.11898800	-1.17665200
C	4.18874400	-2.16779500	2.02184800	C	-4.13628900	2.14312000	2.00731300
C	4.90810200	-3.25231200	0.06497700	C	-4.86860500	3.21962100	0.05237000
C	5.59535200	-1.85895100	0.16514300	C	-5.55464000	1.82712400	0.16072900
N	4.95535700	-1.25816200	1.30933500	N	-4.89334900	1.22525300	1.29389100
C	4.52352200	-2.05121100	-1.91747900	C	-4.48314300	2.00681700	-1.92144500
N	5.32933700	-1.26350900	-1.11298800	N	-5.30933700	1.23529900	-1.12213500
C	5.43106100	-0.05329400	1.93408700	C	-5.35877100	0.01867100	1.92318200
C	5.93706100	-0.05304400	-1.59660200	C	-5.91033700	0.01795500	-1.59795700
O	4.23492700	-1.83728500	-3.06483800	O	-4.18490000	1.78205000	-3.06420500
O	3.70037800	-1.99768200	3.10716600	O	-3.63951100	1.97383900	3.08901700
N	4.97686900	1.16091300	1.31142900	N	-4.90190700	-1.19180800	1.29551300
N	5.35407900	1.16861900	-1.11059200	N	-5.31828200	-1.20310800	-1.12055200
C	4.22186400	2.08037700	2.02370200	C	-4.14725000	-2.11195300	2.00833100
C	5.62909500	1.75419300	0.17036400	C	-5.56696000	-1.79127600	0.16344500
C	4.96771700	3.16040400	0.07427600	C	-4.88960100	-3.18832300	0.05708100
N	4.19828500	3.24867700	1.28120800	N	-4.13041300	-3.28234300	1.26997300

O	3.72712900	1.91484500	3.10684500	O	-3.64734000	-1.94339100	3.08872300
C	3.55854700	4.44135700	1.76168100	C	-3.48309200	-4.47339900	1.74607800
N	4.23152500	3.09347900	-1.16531000	N	-4.14136900	-3.09600100	-1.17415000
C	4.56928100	1.97653100	-1.91576600	C	-4.49904800	-1.98199300	-1.91972800
O	4.28208400	1.77374900	-3.06550500	O	-4.20020000	-1.76086900	-3.06310300
C	3.64568400	4.24801900	-1.79537900	C	-3.54116700	-4.23867500	-1.81375200
N	2.28197900	4.73044600	1.16043500	N	-2.20426900	-4.75406900	1.14710800
N	2.35612300	4.62548500	-1.28774900	N	-2.25428500	-4.61280900	-1.29777200
C	1.13761000	4.82666700	1.93895600	C	-1.05405300	-4.81999400	1.91892700
C	2.14146500	5.40810800	-0.10462700	C	-2.05300000	-5.41472200	-0.12437600
C	0.62169900	5.74269500	-0.16312700	C	-0.53359900	-5.75639400	-0.17442900
N	0.14520200	5.36629400	1.13716100	N	-0.05381300	-5.33946700	1.11389200
O	1.03910600	4.54643100	3.10381800	O	-0.95585400	-4.53127000	3.08194800
C	-1.15363000	5.70146900	1.65729400	C	1.24698300	-5.66170300	1.63733200
N	0.15261400	4.95651800	-1.27654500	N	-0.06199900	-5.01116100	-1.31254700
C	1.19192500	4.38413900	-1.99487100	C	-1.09186700	-4.41458800	-2.02275200
O	1.10415000	3.83141300	-3.05932700	O	-1.00218000	-3.87396200	-3.09311400
C	-1.13748400	5.14329200	-1.88106000	C	1.23065000	-5.21125800	-1.90872100
N	-2.23629100	4.87156900	1.20258100	N	2.32371500	-4.83483800	1.16385100
N	-2.21562900	4.46212500	-1.21341600	N	2.30350500	-4.49975000	-1.26493900
C	-2.89916500	5.00431000	-0.06159600	C	2.98981100	-4.99698900	-0.09617200
C	-2.99059100	3.53985700	-1.89588000	C	3.07655700	-3.59904900	-1.98294700
C	-4.13592500	4.07008400	0.07841200	C	4.21827000	-4.04793300	0.01987700
N	-4.12370400	3.31377300	-1.14080700	N	4.19353700	-3.31907100	-1.21477800
C	-2.81193100	3.90468800	2.01177600	C	2.89963600	-3.85512500	1.95489500
N	-3.85512400	3.34326400	1.29238500	N	3.94014900	-3.30063400	1.22382000
O	-2.74257800	3.05609500	-2.97226900	O	2.84871100	-3.18096400	-3.08701200
O	-2.49877900	3.64466600	3.14282600	O	2.58986700	-3.57678200	3.08277800
C	-5.20383000	2.48340000	-1.60698600	C	5.24231700	-2.45408500	-1.68174300
C	-4.81287100	2.48205200	1.93502400	C	4.91360400	-2.45607600	1.86640000
H	3.31590700	-4.38576300	2.82424700	H	-3.28887500	4.37230300	2.81271700
H	4.14388600	-5.37745400	1.58302600	H	-4.12563400	5.35603400	1.57123800
H	4.21798100	-5.17384400	-1.70661400	H	-4.18129200	5.12249300	-1.73439800
H	3.42918300	-4.05215100	-2.85877700	H	-3.37490900	3.99614800	-2.86998200
H	7.00295200	-0.06455000	-1.33417900	H	-6.97354700	0.02218600	-1.32619600
H	5.82432500	-0.05051400	-2.68272000	H	-5.80767800	0.01675000	-2.68493700
H	5.05476300	-0.05104200	2.95955000	H	-4.97393200	0.01808700	2.94549400
H	6.53178800	-0.06300600	1.94418400	H	-6.45952500	0.02258200	1.94236500
H	4.23775200	5.29027000	1.60028000	H	-4.15711700	-5.32503100	1.57955400
H	3.38333800	4.30860100	2.83128500	H	-3.31086800	-4.34382900	2.81651200
H	4.32695100	5.10445100	-1.69073800	H	-4.21918400	-5.10026400	-1.72680400
H	3.52141500	4.00500200	-2.85274300	H	-3.40782200	-3.98195000	-2.86679400
H	-1.38021300	6.74522900	1.40279500	H	1.47806200	-6.70869300	1.39992700
H	-1.09782800	5.59025100	2.74221800	H	1.19318000	-5.53237700	2.72033300
H	-1.36353000	6.22000000	-1.92270200	H	1.45977600	-6.28787900	-1.91077800
H	-1.08072100	4.74180500	-2.89509600	H	1.17443100	-4.84666500	-2.93671300
H	-4.49148100	2.37023900	2.97284200	H	4.60949000	-2.35403300	2.91037300
H	-5.80516600	2.95610500	1.90405100	H	5.90130200	-2.93748700	1.81403200
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H	-6.14878200	2.99898000	-1.38992900	H	6.20833500	-2.93317900	-1.47315700
H	-5.84660400	-2.83432800	1.92343400	H	5.91360400	2.89269800	1.82314600
H	-4.51474400	-2.26546800	2.97895200	H	4.61365400	2.31492400	2.91294100
H	-5.14981300	-2.29148400	-2.67611100	H	5.13711000	2.31665600	-2.75569700
H	-6.21590300	-2.89116300	-1.36876900	H	6.23252100	2.89934000	-1.46402100
H	5.62291300	-4.08610100	0.01531100	H	-5.58375600	4.05219700	-0.00934800
H	6.68040200	-1.92185200	0.33091700	H	-6.63650800	1.88952900	0.34555400
H	5.69781400	3.98133700	0.03379200	H	-5.60995300	-4.01670500	-0.00030400
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H	2.78355600	6.30055400	-0.12493100	H	-2.69910700	-6.30376200	-0.16284000
H	0.41868400	6.80816700	-0.34396900	H	-0.33458900	-6.82795700	-0.32004600
H	-5.08676800	4.61321700	0.17235900	H	5.17377300	-4.58184600	0.12159700
H	-1.48606900	-6.19875600	-1.91328900	H	1.50331300	6.28033400	-1.90737700

H	-1.18256200	-4.72848400	-2.89162700	H	1.21136600	4.84181900	-2.93525700
H	-1.19415700	-5.56041600	2.74843200	H	1.22476700	5.52340100	2.72228600
H	-1.50335200	-6.71209600	1.41200000	H	1.51933100	6.69826900	1.40269900
H	-3.16247700	6.05608600	-0.24139500	H	3.26539500	-6.05108400	-0.24231600
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S	-1.65983800	-0.01356200	-1.16531700				
Cucurbit[7]uril							
O 1							
C	5.74283400	-1.02041200	-0.07770800				
C	5.26004700	-2.50043200	-0.13507900				
N	4.40107700	-2.52513100	-1.29140900				

C	4.45283700	-1.34501200	-2.01695800
N	5.20912200	-0.44894400	-1.28111900
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N	4.63205200	-2.69670400	1.14158100
H	6.08104800	-3.22062300	-0.26262400
C	3.91570100	-3.73989600	-1.88829400
O	3.97657200	-1.15252900	-3.10407100
C	4.22242700	-3.97490600	1.65962600
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O	4.31177100	-1.48695900	3.08394100
N	2.96319200	-4.46491900	1.16735200
C	2.77988300	-5.12316800	-0.09462800
C	1.82470400	-4.48281300	1.95529100
C	1.32905700	-5.68117400	-0.00459400
N	2.73769000	-4.28292300	-1.26616600
H	3.53996900	-5.90733400	-0.22185200
N	0.82374100	-5.09031100	1.21122100
O	1.73626200	-4.09302800	3.08923500
N	0.72908400	-5.24781900	-1.23321400
H	1.28846700	-6.77754200	0.06690800
C	1.56787600	-4.44989700	-1.99222100
O	1.34399800	-4.02641500	-3.09501500
C	-0.40367200	-5.50898200	1.83744500
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N	-3.48343300	-3.72968800	1.30044200
O	-2.05408300	-3.54075600	3.10762200
N	-3.62325900	-3.90932800	-1.13818200
H	-4.49549500	-5.21259600	0.23658700
C	-2.53241200	-4.23910500	-1.92595600
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C	-4.57297100	-2.98391500	1.86781400
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N	-4.98860700	-1.90120000	-1.20109300
N	-4.82379800	-1.71420900	1.23795000
C	-4.70780900	-0.78825400	-1.97525200
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N	-5.09957600	0.32430800	-1.24601900
C	-4.75588200	-0.53713800	1.96878600
N	-5.32251600	0.45806700	1.19041100
C	-5.19906000	1.61458200	-1.87543100
C	-5.48945000	1.80152300	1.67505900
O	-4.33311500	-0.41305400	3.08744100
O	-4.25996700	-0.79090200	-3.09111800
N	-4.35763400	2.62769900	-1.29950000
N	-4.56963900	2.76824000	1.13687400
C	-3.32655300	3.20259100	-2.02495600
C	-4.72312900	3.40331700	-0.14341900
C	-3.65493600	4.53757300	-0.11616700
N	-2.87844800	4.29335100	-1.29949800
O	-2.93117200	2.85297500	-3.10532300
C	-1.90132000	5.20377100	-1.82747100
N	-2.99165700	4.34219400	1.14745400
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O	-3.38282000	3.14121100	3.08476000

C	-2.09043000	5.30263000	1.72898300
N	-0.60670100	5.12980100	-1.20035600
N	-0.73900700	5.24173700	1.24452800
C	0.52130900	4.82514500	-1.94813200
C	-0.28113800	5.82958900	0.01879300
C	1.26720900	5.68899700	0.10656600
N	1.62221600	5.11313400	-1.15924500
O	0.54168300	4.43635000	-3.08568100
C	2.96644900	4.98979300	-1.65563500
N	1.45705000	4.86232000	1.27305900
C	0.28638500	4.69533600	1.99737100
O	0.18656000	4.21633700	3.09570200
C	2.73914100	4.65816000	1.89280300
N	3.71224600	3.87128900	-1.14424300
N	3.53812700	3.62693600	1.28713600
C	4.37048800	3.84795400	0.13138200
C	3.92452500	2.51044400	2.01269000
C	5.24251700	2.55867700	0.06629100
N	4.90139100	1.86452200	1.27482900
C	4.03127700	2.78071700	-1.93580800
N	4.83463800	1.94528500	-1.17353800
O	3.52637200	2.19196400	3.10166100
O	3.71521900	2.61588300	-3.08403600
C	5.58949900	0.70627700	1.77260300
C	5.54724700	0.85301100	-1.78529700
H	-4.61800400	-3.16904900	-2.76359300
H	-5.66999900	-3.83512200	-1.47538100
H	-5.48591300	-3.59628000	1.82097000
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H	-6.24456800	1.95563500	-1.83714800
H	-2.28949300	6.22872500	-1.73663900
H	-1.76014100	4.95662100	-2.88182700
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H	3.51236800	5.91466500	-1.42693400
H	2.89700300	4.85992500	-2.73762500
H	3.30147100	5.60418900	1.87604300
H	2.55450000	4.36040500	2.92721700
H	5.29862800	0.86516200	-2.84867200
H	6.62763500	1.00953000	-1.65601400
H	5.36648600	0.62764300	2.83872500
H	6.66946100	0.85273900	1.63017900
H	4.71591100	-4.49515800	-1.86463500
H	3.65777900	-3.51264600	-2.92501900
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H	5.00066700	-4.71547600	1.43235000
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H	-4.09178500	5.54584200	-0.15735500
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H	1.78340400	6.65051600	0.23923600
H	6.32226400	2.76493800	0.04430100
H	-0.49701900	-6.60173500	1.75513000
H	-0.33948800	-5.22420900	2.88982400
H	-0.57444400	-5.48892800	-2.79343800
H	-0.64464900	-6.76433300	-1.53762100
H	4.96099900	4.76577500	0.26475800

