Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

Encapsulating and Decontaminating of Sarin by Heptakis(2,3,6-tri-O-Methyl)-β-Cyclodextrin: MD Simulations and QM Calculations

Fatemeh Mahmoudi, Mehdi Shahraki*

Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan, Zahedan,

Iran, P. O. Box 98135-674, E-mail: mehdishahraki@chem.usb.ac.ir

Number of pages: 23

Number of figures: 3

Number of tables: 3

Table of Contents

List of Figures

List of Tables

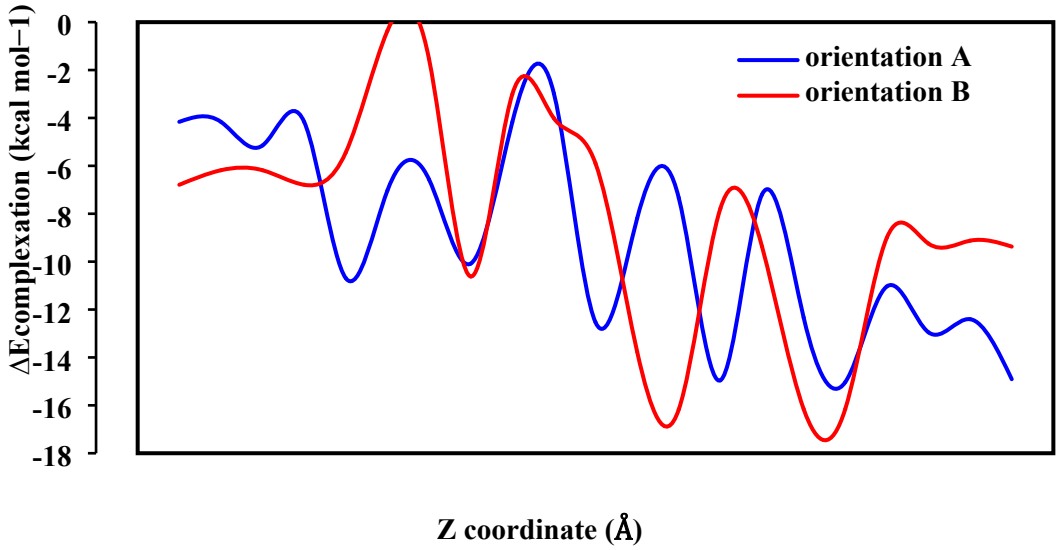

Figure S1. Complexation energies of the M-β-CD@sarin complex at different distances of Z-axis calculated by PM6 method.

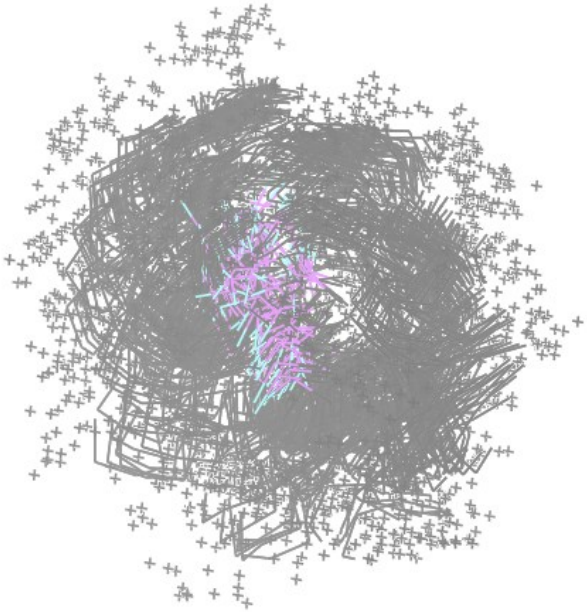

Figure S2. Representation of the superposition of 100 frames extracted from annealing dynamics with NVT ensemble for the M-β-CD@sarin complex (for visual clarity, the frames are shown without oxygens, hydrogens, and lattice).

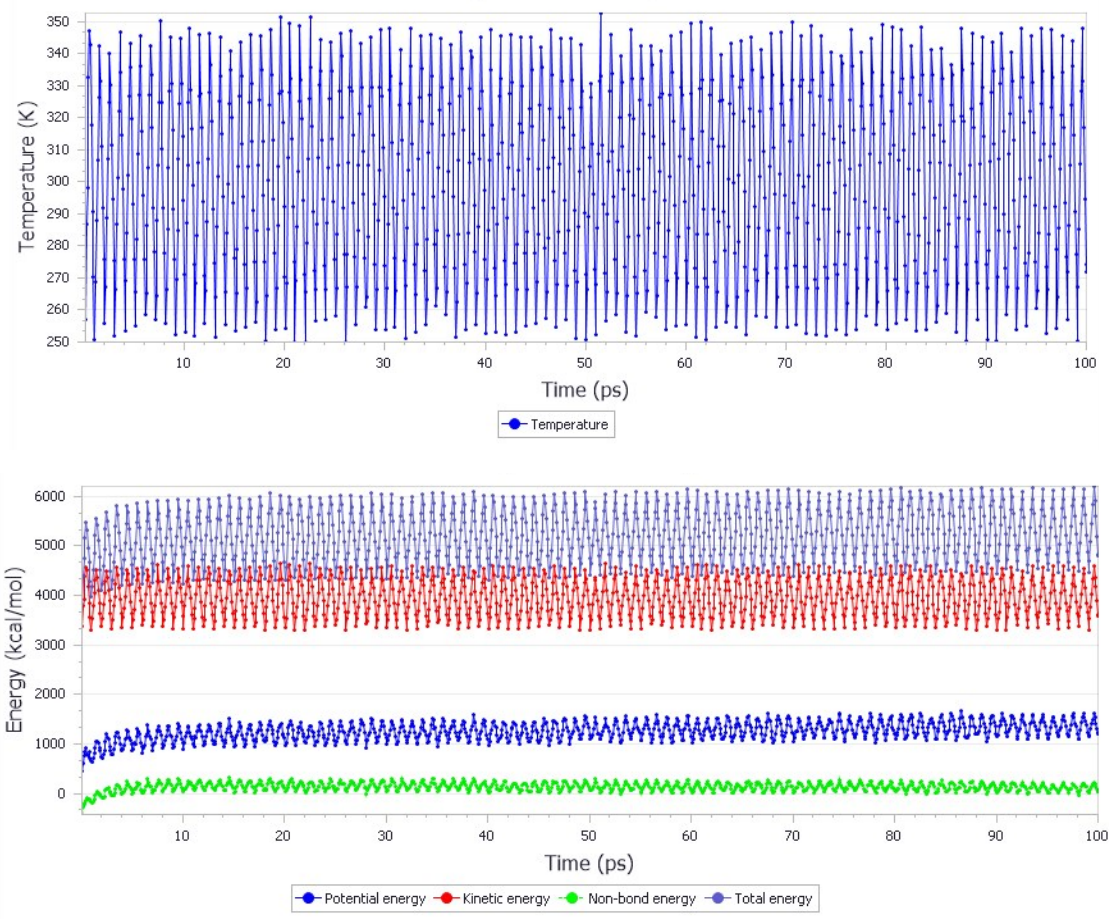

Figure S3. Plots of the potential energy, kinetic energy, non-bond energy, total energy, and temperature of the M-β-CD@sarin complex in an annealing simulation at NVT ensemble as a function of time.

Table S1. Donor-acceptor interactions and stabilization energies, $E^{(2)}$ (kcal mol^{-1}), of the M-β-CD@sarin complex calculated by M06-2X/6-31G(d,p) method

Donor	Acceptor	$E^{(2)}$
M-β-CD donor	sarin acceptor	
LP (1) O2	σ* (1) C216-H221	0.48
LP (2) O2	σ* (1) C216-H221	0.53
LP (1) O15	σ* (1) C218-H226	1.52
LP (2) O15	σ* (1) C218-H226	0.80
LP (1) O17	σ* (1) C218-H226	1.37
LP (2) O17	σ* (1) C218-H226	1.54
LP (1) O25	σ* (1) C217-H223	1.50
LP (2) O25	σ* (1) C217-H223	0.15
LP (1) O30	σ* (1) C216-H220	1.31
LP (2) O30	σ* (1) C216-H220	0.22
LP (1) O35	σ* (1) C216-H221	0.44
LP (2) O35	σ* (1) C216-H221	0.17
sarin donor	M-β-CD acceptor	
LP (1) O214	σ* (1) C67-H150	1.15
LP (2) O214	σ* (1) C67-H150	0.62
LP (1) O214	σ* (1) C68-H153	1.17
LP (2) O214	σ* (1) C64-H145	0.55

Table S2. Topological parameters of the M-β-CD@sarin complex calculated by AIM. All units are in a.u. except distance which is in Å

Interaction	$\rho(r)$	$\nabla^2\rho(r)$	$\lambda_{(1)}$	$\lambda_{(2)}$	$\lambda_{(3)}$	Distance
O15···H226	0.0140	0.0474	−0.0148	−0.0126	0.0749	2.31
O214···H145	0.0087	0.0284	−0.0071	−0.0069	0.0424	2.60
O25···H223	0.0106	0.0357	−0.0106	−0.0098	0.0560	2.44
O35···H221	0.0062	0.0239	−0.0053	−0.0048	0.0340	2.71
O17···H226	0.0119	0.0375	−0.0122	−0.0115	0.0612	2.38
O214···H153	0.0125	0.0428	−0.0120	−0.0116	0.0665	2.35
O30···H220	0.0090	0.0297	−0.0085	−0.0079	0.0460	2.53
O2···H221	0.0060	0.0215	−0.0056	−0.0055	0.0327	2.70
O214···H150	0.0118	0.0390	−0.0117	−0.0114	0.0619	2.38

Table S3. Contributions to total energy calculated for the interaction energy (kcal mol^{-1})

M-β-CD@sarin	
Total energy	956.731
Valence energy (diag. terms)	1127.139
Bond	653.975
Angle	585.334
Torsion	-112.170
Inversion	0.000
Valence energy (cross terms)	-70.231
Stretch-Stretch	0.530
Stretch-Bend-Stretch	-12.874
Stretch-Torsion-Stretch	-0.162
Separated-Stretch-Stretch	0.000
Torsion-Stretch	-1.153
Bend-Bend	-0.171
Torsion-Bend-Bend	-26.309
Bend-Torsion-Bend	-30.092
Non-bond energy	-100.177
van der Waals	-100.177
Electrostatic	0.000
M-β-CD	
Total energy	983.350
Valence energy (diag. terms)	1122.397

Bond	649.365
Angle	579.655
Torsion	-106.623
Inversion	0.000
Valence energy (cross terms)	-69.267
Stretch-Stretch	0.596
Stretch-Bend-Stretch	-12.647
Stretch-Torsion-Stretch	0.224
Separated-Stretch-Stretch	0.000
Torsion-Stretch	-1.076
Bend-Bend	-0.173
Torsion-Bend-Bend	-25.990
Bend-Torsion-Bend	-30.202
Non-bond energy	-69.779
van der Waals	-69.779
Electrostatic	0.000

sarin

Total energy	1033.892
Valence energy (diag. terms)	1054.256
Bond	612.367
Angle	447.436
Torsion	-5.547
Inversion	0.000
Valence energy (cross terms)	-10.702
Stretch-Stretch	0.487
Stretch-Bend-Stretch	-10.518
Stretch-Torsion-Stretch	-0.386
Separated-Stretch-Stretch	0.000
Torsion-Stretch	-0.077
Bend-Bend	0.002
Torsion-Bend-Bend	-0.319
Bend-Torsion-Bend	0.110
Non-bond energy	-9.662
van der Waals	-9.662
Electrostatic	0.000

XYZ coordinates of the optimized geometry of sarin:

0 1

P	1.10874900	-0.19008700	-0.09849700
F	1.12495100	1.20119900	-0.85910800
O	-0.39811400	-0.67233800	-0.28513600
O	2.09552500	-1.14428200	-0.60543900
C	-1.55571900	-0.05505100	0.32057900
C	-1.78972900	1.33951300	-0.23871900
C	-2.71127100	-0.99591700	0.03575500
C	1.30874900	0.35059800	1.60498100
H	-1.38625100	-0.00531300	1.40448900
H	-2.72599000	1.74091700	0.15731300
H	-0.98289100	2.02876400	0.01833800
H	-1.86132300	1.28998100	-1.32838100
H	-3.62245600	-0.62803400	0.51358600
H	-2.49033600	-1.99578500	0.41330100
H	-2.87897200	-1.05987700	-1.04239300
H	2.32657900	0.72544400	1.72279300
H	0.60538400	1.14354700	1.86642800
H	1.16899600	-0.50103100	2.27298800

XYZ coordinates of the optimized geometry of M-β-CD:

0 1

O	-6.25258100	0.49717000	-0.85126700
O	-5.91895300	0.87204000	2.72452300
O	-5.76045700	-1.93802800	2.37432400
O	-6.69419400	-1.88979000	-2.67452100
O	-4.45176700	-2.63650300	-0.09974800

O	-3.27753700	-3.14497200	-2.02027100
O	-5.31633700	-5.28314200	0.12894500
O	-2.72933700	-6.53466000	0.20610100
O	-0.70792700	-1.33641300	-2.18631900
O	-0.60917100	-4.68741000	-0.07934500
O	1.17250500	-5.56192700	-1.27391000
O	-0.10295700	-6.43080800	2.00901800
O	2.60237700	-5.61981500	2.57411100
O	2.45453900	-3.40671600	-3.09532600
O	3.53027900	-3.62540200	0.75284100
O	5.51865200	-3.24940400	-0.38812600
O	4.78502900	-3.20232400	3.13868700
O	5.74383300	-0.58110400	2.67903900
O	7.06350500	-1.40125000	-2.21701100
O	5.02664200	0.37650800	0.00616500
O	4.57716000	1.35626100	-2.03844800
O	7.05151500	2.28565000	0.47042300
O	5.31338100	4.59318400	0.36068100
O	1.55348300	1.15406700	-2.93664000
O	2.63385800	3.86838900	-0.26219800
O	1.47800700	5.47701900	-1.45148500
O	2.77895000	5.50663000	1.92944000
O	-0.02289300	5.96880400	2.32923600
O	-1.19728100	6.42222400	-2.56814200
O	-1.66826400	4.81651500	0.36288700
O	-3.30834400	4.61699100	-1.27895500
O	-3.52985700	5.91985100	2.12669300
O	-5.58327700	3.91238200	1.98666700
O	-2.66376500	2.37453400	-3.11830800
O	-4.74449200	1.72155100	0.39786300

C	-6.02493800	1.17113300	0.36636600
C	-6.20949200	0.19778800	1.52699200
C	-5.34422100	-1.04746700	1.36641700
C	-5.47300100	-1.65084200	-0.03599000
C	-5.32300700	-0.55833900	-1.10904700
C	-6.77524200	0.55145800	3.80089400
C	-4.85901700	-2.97638900	2.71570900
C	-5.59283400	-1.01501300	-2.54081200
C	-7.95604100	-1.27756200	-2.49994600
C	-4.38697100	-3.47540300	-1.22009000
C	-4.27247900	-4.93058400	-0.74660900
C	-2.95071100	-5.16300900	-0.02834500
C	-1.78831900	-4.64511800	-0.86704300
C	-2.03154900	-3.20793700	-1.32585100
C	-6.58334300	-5.35565900	-0.48907600
C	-3.11517700	-6.97126300	1.49497100
C	-0.95293600	-2.72058600	-2.28709300
C	0.13474100	-1.01341000	-1.09995000
C	0.19302500	-5.81487900	-0.29064100
C	0.87342900	-6.21557200	1.01599800
C	1.86706200	-5.15361600	1.46370100
C	2.83527900	-4.79699300	0.34573900
C	2.07251400	-4.50230600	-0.95015700
C	2.29751200	-4.94491700	3.77939400
C	2.98859700	-4.31064200	-2.14858700
C	1.69592200	-4.03913800	-4.10666900
C	4.92132000	-3.67537100	0.81801200
C	5.40159900	-2.77602500	1.95154300
C	5.10443100	-1.30667500	1.65853300
C	5.58212800	-0.90553300	0.25790200

C	5.12181400	-1.93397300	-0.78847800
C	5.60328700	-3.13963500	4.28914700
C	5.28279700	0.73978200	2.90401900
C	5.68609800	-1.71076800	-2.18827000
C	7.92066300	-2.48091200	-1.90600800
C	5.55747300	1.12910400	-1.05929300
C	6.07203700	2.46809200	-0.52533300
C	4.92208000	3.27392900	0.05889900
C	3.77279600	3.36616500	-0.93803000
C	3.40346800	2.01367200	-1.55400000
C	8.30300900	1.86119400	-0.02609400
C	5.73833900	4.78291000	1.69564400
C	2.46242300	2.20741600	-2.74073400
C	2.16095600	-0.05517000	-3.34481100
C	2.39803800	5.24036500	-0.41433900
C	1.86923300	5.81107400	0.89996500
C	0.48188700	5.26791800	1.21081400
C	-0.44665700	5.44850600	0.01521600
C	0.19066400	4.87390300	-1.25812200
C	2.95857300	6.54964800	2.86501900
C	-0.65450500	5.14564700	3.29270200
C	-0.61572300	5.13595300	-2.52559600
C	-0.28452000	7.46500700	-2.82985800
C	-2.85143600	5.34636000	-0.17173500
C	-3.93951200	5.33327600	0.91575200
C	-4.38493800	3.91149100	1.24501900
C	-4.64188600	3.08037000	-0.00433500
C	-3.51482200	3.23232500	-1.01926100
C	-3.08536300	7.25348900	2.00801100
C	-5.40430400	3.82185300	3.38569600

C	-3.83072100	2.59769800	-2.36482600
C	-2.04081000	1.14717200	-2.79823900
H	-6.78095900	1.95960600	0.43036600
H	-7.26354600	-0.12207700	1.50568000
H	-4.29082500	-0.75882800	1.51497800
H	-6.46191400	-2.12402700	-0.12991600
H	-4.29378700	-0.17178500	-1.05706000
H	-6.45148700	1.15842100	4.64928200
H	-7.81812300	0.80664300	3.56451100
H	-6.71443800	-0.50928500	4.05908200
H	-5.10478300	-3.28031400	3.73633400
H	-4.95668000	-3.83111100	2.04023200
H	-3.82105000	-2.61896300	2.69101300
H	-5.74530200	-0.11242500	-3.15119600
H	-4.72082800	-1.54962900	-2.92364600
H	-8.70528100	-1.99736000	-2.83511900
H	-8.14326000	-1.01054200	-1.45402600
H	-8.03450100	-0.36365100	-3.10270300
H	-5.26690300	-3.35136800	-1.85557500
H	-4.29442800	-5.57347700	-1.64255400
H	-2.95222500	-4.60191700	0.91863100
H	-1.67281800	-5.28082400	-1.75926800
H	-2.06877000	-2.55599700	-0.44327900
H	-7.28065400	-5.73506100	0.25861900
H	-6.93479200	-4.37455000	-0.83531200
H	-6.56428800	-6.04213500	-1.34651500
H	-2.81927100	-8.02012600	1.57197900
H	-2.58722200	-6.39850100	2.26705600
H	-4.19693000	-6.88213800	1.63528100
H	-0.02475900	-3.28223700	-2.12069200

H	-1.30044600	-2.91415400	-3.30709500
H	0.28539500	0.06700000	-1.12395200
H	-0.30163300	-1.31220200	-0.13663200
H	1.11055400	-1.50727500	-1.21199000
H	-0.41091900	-6.64587000	-0.66347800
H	1.42751400	-7.14455700	0.81158600
H	1.30403900	-4.24457300	1.71984700
H	3.53909500	-5.62982600	0.19625100
H	1.51464100	-3.57282300	-0.78075800
H	2.91736400	-5.39594600	4.55771300
H	2.54530400	-3.88126900	3.70023200
H	1.23867700	-5.06976900	4.04167600
H	3.94343500	-3.90760800	-1.81034100
H	3.17729700	-5.29478100	-2.60193300
H	1.24892100	-3.24964400	-4.71452200
H	2.33746200	-4.66339300	-4.74370300
H	0.90243500	-4.66745100	-3.68472600
H	5.26309700	-4.70293800	0.98317100
H	6.49488800	-2.89491500	2.01507400
H	4.01310000	-1.15906200	1.70164100
H	6.68096700	-0.85129000	0.26430200
H	4.02327200	-1.88444300	-0.85304600
H	5.00674900	-3.53019700	5.11628500
H	6.49639500	-3.76915000	4.17111700
H	5.91264100	-2.11396500	4.50529700
H	5.48781000	0.97146500	3.95243000
H	5.80378100	1.45284100	2.26060600
H	4.20207800	0.81550400	2.72781100
H	5.48000400	-2.60988000	-2.78753700
H	5.16925100	-0.86742000	-2.65364900

H	8.92773100	-2.17957500	-2.20051500
H	7.90652000	-2.72305500	-0.83762700
H	7.63366200	-3.38228500	-2.46282300
H	6.36164700	0.58241700	-1.55728800
H	6.49338500	3.02954600	-1.37549900
H	4.54029800	2.76648700	0.95638600
H	4.06876300	4.04963300	-1.74983100
H	2.91195200	1.39539400	-0.79009200
H	8.98675400	1.82782800	0.82287500
H	8.25475200	0.86222900	-0.48044300
H	8.68915200	2.56698700	-0.77365200
H	5.87060100	5.85866800	1.83314300
H	4.97061600	4.43120000	2.39578400
H	6.68348500	4.26594900	1.88950100
H	1.86384300	3.10692500	-2.57180100
H	3.08465300	2.36415200	-3.63676500
H	1.35418800	-0.76711600	-3.52751800
H	2.75331900	0.09136300	-4.25929600
H	2.82241800	-0.46231600	-2.56904400
H	3.32175400	5.75476300	-0.69299400
H	1.78699100	6.90141100	0.76496100
H	0.57629500	4.19498800	1.43396700
H	-0.61556600	6.52566200	-0.13365100
H	0.30831000	3.78649400	-1.13233100
H	3.67155300	6.18779100	3.60922900
H	3.37819700	7.44440200	2.38304400
H	2.01673400	6.81524100	3.35400500
H	-1.01549100	5.80764700	4.08302900
H	-1.50664600	4.61392000	2.86158500
H	0.06346600	4.43323700	3.72119600

H	0.05782500	4.98845300	-3.38372200
H	-1.43653100	4.42230700	-2.59779100
H	-0.87401600	8.35970900	-3.04110700
H	0.38223100	7.65892000	-1.98067300
H	0.34150400	7.23149600	-3.70177300
H	-2.67268000	6.35572000	-0.55650100
H	-4.80496300	5.87819400	0.50194600
H	-3.57879000	3.41573000	1.80746600
H	-5.58213900	3.41567700	-0.46739700
H	-2.59958900	2.78894900	-0.60278800
H	-3.04991100	7.66838900	3.01719200
H	-2.07697200	7.30160400	1.57928300
H	-3.77917500	7.85322900	1.40196000
H	-6.40317600	3.76259400	3.82456600
H	-4.85238900	2.90965400	3.64295100
H	-4.88175400	4.70073900	3.77643200
H	-4.39553500	1.66743500	-2.21539900
H	-4.45813000	3.29743400	-2.92654800
H	-1.05567600	1.12894600	-3.26717700
H	-1.90768900	1.02403900	-1.71370000
H	-2.63331800	0.29462600	-3.15935100
C	0.13631000	-7.57522900	2.80163500
H	-0.65500100	-7.61223200	3.55342100
H	0.09219700	-8.49193800	2.19696200
H	1.11225900	-7.52183000	3.29674200

XYZ coordinates of the optimized geometry of M-β-CD@sarin complex:

0 1

O	-0.57690200	-6.15519200	-0.56727500
O	-1.09620400	-4.86019400	2.74553600

O	1.81622500	-5.09717400	2.50052700
O	1.75194400	-6.94408700	-2.32475700
O	2.61149100	-4.35209200	-0.16273000
O	3.17494300	-3.49635500	-2.22363400
O	5.17584500	-5.40896400	0.15831600
O	6.67128000	-2.94642100	-0.20669800
O	1.52171500	-0.93106900	-2.75846100
O	4.93867300	-0.75573200	-0.58642600
O	5.60502100	1.00007800	-1.93756300
O	7.03014000	-0.16097100	1.18764800
O	6.06695300	2.47656900	1.87916600
O	3.24605200	2.21556600	-3.50355500
O	3.74455400	3.17465500	0.31474900
O	3.29872000	5.29358500	-0.48622200
O	3.25850900	3.89925100	2.82507400
O	0.71851400	5.36643000	2.59026400
O	1.45622800	7.00377000	-2.17811000
O	-0.33016200	4.80740200	-0.13323900
O	-1.32608400	4.49547800	-2.19267800
O	-2.16871100	6.90130100	0.41247600
O	-4.52761700	5.24032600	0.25477300
O	-1.22090900	1.54203400	-3.25652100
O	-3.94143300	2.58472000	-0.51590900
O	-5.53594000	1.51474200	-1.79869300
O	-5.67313900	2.74266900	1.60935600
O	-6.33447300	-0.03971900	1.89507000
O	-6.48289000	-1.13322400	-3.01148100
O	-5.04928900	-1.66820000	-0.00974100
O	-4.75967000	-3.30614600	-1.64085900
O	-6.26577600	-3.53750000	1.68082800

O	-4.07611700	-5.37868300	1.79344000
O	-2.40575100	-2.73046600	-3.41182700
O	-1.86956500	-4.42784500	0.24060100
C	-1.28613900	-5.66044900	0.54324900
C	-0.35703400	-5.51754700	1.74872900
C	0.96059400	-4.81583100	1.41749500
C	1.56087700	-5.27524400	0.08181000
C	0.47523000	-5.29308800	-1.00470100
C	-0.58691900	-4.94936700	4.06231000
C	2.93387200	-4.24431300	2.67262400
C	0.90913400	-5.81173300	-2.37197900
C	1.10680600	-8.14665300	-1.95363300
C	3.43077700	-4.51606400	-1.28788100
C	4.90127400	-4.46920800	-0.85336300
C	5.27571100	-3.09061500	-0.33069100
C	4.79877400	-1.99191800	-1.27176500
C	3.33813100	-2.18611500	-1.68337800
C	5.12949900	-6.75094900	-0.27922500
C	7.17005700	-3.21662200	1.08902200
C	2.90867700	-1.19369000	-2.75641000
C	1.13959400	-0.05676100	-1.71957200
C	6.01469000	0.04600800	-0.98090300
C	6.58671100	0.77588000	0.23366100
C	5.53141400	1.68979800	0.83788000
C	4.94062600	2.61807600	-0.21273300
C	4.55601200	1.85120400	-1.48061400
C	5.73280800	2.01075000	3.17362300
C	4.19224600	2.78496000	-2.62300300
C	3.82983900	1.55555300	-4.60998600
C	3.74192400	4.53772200	0.61632300

C	2.84444500	4.79517000	1.82628100
C	1.34453700	4.70204500	1.52176700
C	0.96404600	5.31706600	0.16605800
C	1.98158300	4.94318600	-0.92021200
C	2.85221400	4.21505300	4.15030600
C	-0.65073100	5.05901600	2.81279200
C	1.76932600	5.63026000	-2.26699800
C	2.53036400	7.83092400	-1.77641200
C	-1.06322100	5.42044200	-1.16691200
C	-2.38260600	5.96080800	-0.61225300
C	-3.22497000	4.81689700	-0.07052500
C	-3.36538300	3.72737400	-1.12683300
C	-2.02821800	3.32824300	-1.76057300
C	-1.69621600	8.15137900	-0.04364700
C	-4.69430600	5.60583600	1.61077600
C	-2.25997500	2.44969200	-2.98625500
C	-0.01875800	2.15511200	-3.67940300
C	-5.31361900	2.40819200	-0.73303900
C	-5.97621700	1.88168400	0.53942200
C	-5.52913100	0.46100600	0.84729000
C	-5.65097600	-0.43741700	-0.37617600
C	-4.98520900	0.20693900	-1.59837000
C	-6.75281200	2.96608200	2.49324900
C	-5.60763100	-0.67086500	2.93273200
C	-5.19185900	-0.57520900	-2.89229500
C	-7.49256000	-0.19619200	-3.31676200
C	-5.54833500	-2.85187400	-0.57316600
C	-5.56407000	-3.92634400	0.52570200
C	-4.13809700	-4.23893600	0.96776100
C	-3.21291900	-4.49555100	-0.21550900

C	-3.38327100	-3.45693100	-1.31787300
C	-7.59726000	-3.12939200	1.45391100
C	-4.15519200	-5.10717000	3.17928600
C	-2.67981000	-3.85157500	-2.60772100
C	-1.18314200	-2.11183400	-3.06991700
H	-2.05946400	-6.39800900	0.77109600
H	-0.09480200	-6.53790100	2.07512600
H	0.77419700	-3.73014600	1.34044100
H	1.96694300	-6.29053800	0.20317300
H	0.09281400	-4.26888700	-1.13305800
H	-1.41780200	-4.71104600	4.73100000
H	-0.22345100	-5.96147500	4.27939800
H	0.23205200	-4.24482500	4.23169000
H	3.22572000	-4.32173700	3.72281000
H	3.76860700	-4.54378400	2.03188600
H	2.66954300	-3.20024300	2.45419300
H	-0.00413200	-6.03877800	-2.94182000
H	1.46088700	-5.03004000	-2.89996000
H	1.80757700	-8.95701800	-2.16308600
H	0.83511800	-8.15728100	-0.89292200
H	0.19221800	-8.29679500	-2.54149200
H	3.22419800	-5.45932100	-1.79565600
H	5.51586300	-4.67646300	-1.74526000
H	4.77821700	-2.93132100	0.63837900
H	5.42426400	-1.99945400	-2.17751400
H	2.70928500	-2.07683700	-0.79029800
H	5.44463100	-7.37008500	0.56134600
H	4.11952800	-7.05477200	-0.58558000
H	5.81330700	-6.91301100	-1.12352200
H	8.24377300	-3.01790600	1.05754000

H	6.70959900	-2.54602300	1.82465600
H	6.99610800	-4.25979600	1.37064600
H	3.47010800	-0.25903100	-2.63510100
H	3.15358300	-1.62556300	-3.73213900
H	0.07007500	0.13887100	-1.82938400
H	1.33457400	-0.49467200	-0.73034200
H	1.68047100	0.89748000	-1.79890000
H	6.79210200	-0.56087100	-1.45388600
H	7.42664900	1.38689700	-0.12966300
H	4.72222400	1.05044600	1.21448000
H	5.66700600	3.41139800	-0.44627700
H	3.67557700	1.25088200	-1.21795300
H	6.14974600	2.72718700	3.88417400
H	4.64529700	1.97584300	3.30566800
H	6.15705700	1.01668300	3.35968600
H	3.75495000	3.69295700	-2.20463200
H	5.11351100	3.06496600	-3.15448100
H	3.02341500	1.04366800	-5.13938800
H	4.30577800	2.27696100	-5.28790800
H	4.57929000	0.82131900	-4.29253900
H	4.75911000	4.87737900	0.83596500
H	3.03182700	5.83489700	2.14278100
H	1.05149600	3.63994900	1.50632400
H	0.92773800	6.41049600	0.27738800
H	1.92128200	3.85460500	-1.08037700
H	3.49445000	3.62528700	4.81010500
H	3.00338900	5.28188800	4.35672400
H	1.80703000	3.95188300	4.31843200
H	-0.85503400	5.31098800	3.85635500
H	-1.29632400	5.64988700	2.15746300

H	-0.83539000	3.98839700	2.67522100
H	2.67810800	5.48611600	-2.86970200
H	0.93519800	5.15312900	-2.78877200
H	2.22235800	8.86077700	-1.96610000
H	2.76991000	7.70692800	-0.71497300
H	3.43399400	7.60880900	-2.35868100
H	-0.49185700	6.22910300	-1.62553600
H	-2.92949900	6.42832600	-1.44810400
H	-2.72393600	4.37627100	0.80476400
H	-4.02504100	4.10245500	-1.92545600
H	-1.42749200	2.77867800	-1.02273000
H	-1.64315500	8.80633200	0.82667600
H	-0.69733000	8.08050500	-0.49524000
H	-2.38409900	8.58566100	-0.78159200
H	-5.75978500	5.80006300	1.75420500
H	-4.39367500	4.78188500	2.26960900
H	-4.11837100	6.50440000	1.85298700
H	-3.16096500	1.85153200	-2.82439600
H	-2.43339900	3.11607400	-3.84662400
H	0.66518500	1.35372200	-3.96577400
H	-0.19773700	2.82058100	-4.53543400
H	0.44589900	2.74263500	-2.87692500
H	-5.77461400	3.35733000	-1.01950600
H	-7.06087200	1.86452700	0.34716600
H	-4.47363900	0.49779900	1.15590200
H	-6.71760200	-0.59345200	-0.59426100
H	-3.90289700	0.28760300	-1.40589200
H	-6.38252900	3.62149600	3.28434300
H	-7.58510500	3.46868700	1.98013100
H	-7.11410700	2.02967700	2.92874300

H	-6.33885600	-0.99759900	3.67556500
H	-5.06601600	-1.54618800	2.56147800
H	-4.91053300	0.03756400	3.40228400
H	-4.98561800	0.10701500	-3.73109700
H	-4.49019300	-1.40886100	-2.93910600
H	-8.38948500	-0.76476000	-3.57058300
H	-7.70944900	0.47195300	-2.47425100
H	-7.20522800	0.42638100	-4.17484100
H	-6.53886700	-2.67919800	-1.00616000
H	-6.01651600	-4.83182800	0.08774800
H	-3.75024600	-3.36013500	1.50309200
H	-3.42739500	-5.49382900	-0.62789000
H	-2.97578600	-2.50155800	-0.95859400
H	-8.09696400	-3.12142100	2.42436000
H	-7.63738000	-2.11589600	1.03600800
H	-8.12342600	-3.82945500	0.78977600
H	-3.86186900	-6.02338300	3.69677800
H	-3.45342400	-4.30943600	3.45349200
H	-5.16989800	-4.82115500	3.47120600
H	-1.76013300	-4.40646300	-2.37094100
H	-3.34959900	-4.50917500	-3.17091700
H	-1.12276500	-1.15979700	-3.60059800
H	-1.11579900	-1.91231800	-1.98839500
H	-0.32625200	-2.73918600	-3.34975300
C	8.28943900	0.15155900	1.74556400
H	8.49706400	-0.60468100	2.50549800
H	9.08060300	0.11594400	0.98424900
H	8.28529100	1.14507800	2.20933400
P	0.90298900	0.89503200	3.07557900
F	1.78158000	0.13346500	4.14023200

O	-0.16020000	-0.26036600	2.79692900
O	0.38669700	2.18422200	3.56682800
C	-1.02010200	-0.23764700	1.62643800
C	-2.04018700	-1.33742000	1.84584000
C	-1.67269600	1.12054600	1.41088700
C	1.99119500	0.99985400	1.65997500
H	-0.38947500	-0.48601100	0.76150400
H	-2.75188100	-1.35720600	1.01303800
H	-1.56953900	-2.32126200	1.93308700
H	-2.59821100	-1.13032000	2.76490200
H	-2.32799400	1.07520700	0.53611400
H	-0.94389100	1.92091300	1.23782700
H	-2.27403800	1.40320100	2.28128500
H	2.73092000	1.77857900	1.86482900
H	2.47422600	0.04202100	1.44748300
H	1.42228300	1.32342500	0.78251700