

SUPPLEMENTARY MATERIALS FILE 2

Systematic Functional and Computational Analysis of Sugar-Binding Residues in *Thermoanaerobacterium xylanolyticum* Family GH116 β -Glucosidase

Meng Huang^{1,2}, Salila Pengthaisong^{1,2}, Ratana Charoenwattanasatien³, Natechanok Thinkumrob⁴, Jitrayut Jitonnorn^{4*}, James R. Ketudat Cairns^{1,2*}

¹School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

²Center for Biomolecular Structure, Function and Application, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

³Research Facility Department, Synchrotron Light Research Institute (Public Organization), Nakhon Ratchasima 30000, Thailand

⁴Unit of Excellence in Computational Molecular Science and Catalysis, and Division of Chemistry, School of Science, University of Phayao, Phayao 56000, Thailand

*Corresponding authors

Cartesian Coordinates

Glc_wt				ONfOM: extrapolated energy = -3352.681214 au									
N	-1	3.09416500	-7.63267500	2.22942500	L	H	4	C	0	-1.25000200	5.14851700	0.95312300	H
C	-1	1.92871500	-6.78322300	2.12646800	L			O	0	-1.40945200	4.09033600	0.34227500	H
C	-1	2.28680600	-5.54113900	1.26490100	L			N	0	-1.89091200	6.30429400	0.60951300	H
C	0	1.21879600	-4.48347000	1.07482100	H			C	-1	-2.90356400	6.37429200	-0.50741600	L
C	0	1.59827900	-3.46960200	-0.06535200	H			C	-1	-4.01451500	7.35778200	-0.13523400	L
O	0	2.78577700	-3.03119600	-0.09264200	H			C	-1	-4.78675000	6.93459100	1.12117100	L
O	0	0.66228200	-3.12685500	-0.84528800	H			C	-1	-5.04113300	7.29862800	2.38666900	L
C	-1	0.79592000	-7.54821200	1.42836600	L			C	-1	-6.18721300	6.15060100	3.40579500	L
O	-1	-0.38484400	-7.44659400	1.85149700	L			O	-1	-6.88652100	5.77098000	4.54697200	L
N	-1	1.46350000	-7.20474700	-4.93727200	L			C	-1	-6.64680600	5.78910700	2.16087700	L
C	-1	2.47859400	-6.20747600	-4.66355000	L			C	-1	-5.93414400	6.17393000	1.02295300	L
C	-1	1.85488100	-4.91641000	-4.09491800	L			C	-1	-2.13593000	6.80545200	-1.75598400	L
C	-1	0.54802100	-4.45598400	-4.72009700	L			O	-1	-2.17503700	7.98022600	-2.16242900	L
C	-1	0.37889000	-4.40089900	-6.09482400	L			N	-1	-1.45119800	5.83812200	-2.36602000	L
C	-1	-0.81109600	-3.94304600	-6.65219400	L			C	-1	-0.38482000	5.10512000	-3.36555200	L
C	-1	-1.82854900	-3.50033900	-5.82476800	L			C	0	0.52374400	4.87025400	-3.46206800	H
O	-1	-3.01797800	-3.04231400	-6.33113500	L			C	0	-0.12511300	3.53984200	-3.98645900	H
C	-1	-1.67571300	-3.53910800	-4.45162200	L			O	0	-1.37594000	3.42189100	-4.03170800	H
C	-1	-0.49150500	-4.00524400	-3.91263400	L			O	0	0.72924500	2.64851500	-4.28503800	H
C	-1	3.43031200	-6.83950400	-3.66024600	L			C	-1	-0.86979200	6.54989200	-4.73410500	L
O	-1	3.23987200	-6.68123900	-2.42644900	L			O	-1	-0.02995900	6.67223200	-5.66323300	L
N	-1	5.99545800	-7.17444700	-1.62332600	L			N	-1	-8.93813600	5.69319100	-5.35205600	L
C	-1	6.90918400	-6.40081200	-0.79022500	L			C	-1	-8.74912800	5.32728400	-3.93698100	L
C	-1	6.55435400	-4.91831100	-0.84180500	L			C	-1	-7.32733500	5.63044400	-3.49345100	L
C	-1	6.43615200	-4.39469000	-2.24949400	L			C	-1	-6.30915600	4.67141000	-4.10319400	L
C	-1	7.47827200	-4.60933900	-3.15802700	L			C	-1	-4.89562700	4.95454600	-3.67980800	L
C	-1	7.38700700	-4.17302200	-4.45919600	L			O	-1	-4.56608900	6.06323400	-3.23805500	L
C	-1	6.24539400	-3.52684600	-4.86449500	L			N	-1	-4.02974600	3.96426800	-3.81274700	L
O	-1	6.20456100	-3.09327800	-6.16296600	L			C	-1	-9.77098400	6.03210500	-3.03955800	L
C	-1	5.19212300	-3.29980600	-4.00623600	L			O	-1	-10.20562500	5.45645400	-2.00840200	L
C	-1	5.2											

O	-1	-5.25675200	-4.24901700	8.24854000	L	H	-1	-6.29732900	5.86021800	0.03453300	L
C	0	0.61630600	-0.53211500	-2.91714200	H	H	-1	-4.67167500	7.20933500	4.52202900	L
O	0	0.89139500	-0.23596200	-4.25690400	H	H	-1	-7.55303800	5.18152700	2.03667300	L
C	0	1.68840300	0.07713800	-1.96142700	H	H	-1	-7.63588200	5.26566700	4.25799100	L
O	0	2.81155200	-0.78354700	-1.87744100	H	H	-1	-3.35489600	5.34366000	-0.61493400	L
O	0	-0.72247200	-0.04510900	-2.71175400	H	H	0	-1.68573300	7.15345900	1.12763200	H
C	0	-1.16735700	0.31422000	-1.41672500	H	H	0	1.40295200	5.09269000	-4.09850900	H
C	0	-0.15968300	1.20528100	-0.68290900	H	H	0	0.96078000	4.63076700	-2.46794900	H
O	0	-0.63128200	1.50422600	0.63429200	H	H	-1	0.21161000	6.96671000	-2.96544000	L
C	0	1.18254000	0.49837200	-0.57647400	H	H	-1	-1.93879900	4.96450900	-2.49922200	L
O	0	2.14885400	1.39342800	-0.024773400	H	H	-1	-7.26546300	5.56788800	-2.38532800	L
C	0	-2.48095100	1.04135700	-1.64334600	H	H	-1	-7.04797300	6.67780300	-3.73710900	L
O	0	-3.52070400	0.10880100	-2.02799100	H	H	-1	-6.60116000	3.62887900	-3.84433900	L
H	-1	2.63360400	-5.89072100	0.26624600	L	H	-1	-6.36442100	4.72926000	-5.21054100	L
H	-1	3.17276400	-5.05327200	1.72946100	L	H	-1	-4.30166400	3.17996000	-4.38238400	L
H	0	0.23102500	-4.92334800	0.82963200	H	H	-1	-3.01659400	4.04056700	-3.67853000	L
H	0	1.08025200	-3.87143000	2.00139400	H	H	-1	-8.92348800	4.22215800	-3.87871600	L
H	-1	1.61871000	-6.46792100	3.15070800	L	H	-1	-9.88978000	5.54438500	-5.61450400	L
H	-1	3.41980400	-7.90389000	1.32444400	L	H	-1	-8.69900500	6.65177400	-5.50156800	L
H	-1	3.81514100	-7.17374500	2.74452200	L	H	-1	-8.10892700	0.19698200	3.23819800	L
H	-1	1.68521600	-5.01535800	-3.00173000	L	H	-1	-9.12148100	1.64962200	3.31140000	L
H	-1	2.59752100	-4.09413500	-4.20585500	L	H	-1	-9.85399600	0.88551000	-0.11989700	L
H	-1	1.18946700	-4.72744900	-6.75744900	L	H	-1	-8.02853500	1.59291000	-1.74720000	L
H	-1	-0.38348400	-4.01778200	-2.81911300	L	H	-1	-6.04545200	1.90113800	3.17173100	L
H	-1	-0.91396700	-3.91671200	-7.74405600	L	H	-1	-3.96065300	3.00198700	2.29026900	L
H	-1	-2.47030700	-3.19132600	-3.78023600	L	H	-1	-5.58986100	3.00998100	-1.70877800	L
H	-1	-2.95902500	-3.08587400	-7.27817400	L	H	-1	-3.72541800	3.49782700	-0.12117400	L
H	-1	3.01440600	-5.98226300	-5.61821400	L	H	-1	-9.92836400	-0.84007600	1.65649200	L
H	-1	1.88451900	-8.06180300	-5.23063400	L	H	-1	-12.10199300	0.04067500	2.12814300	L
H	-1	0.89441400	-7.36511300	-4.13234000	L	H	-1	-11.46102500	1.37073700	2.82203800	L
H	-1	5.60632700	-4.72590200	-0.29395400	L	H	-1	-6.32579000	-3.83472400	-1.58417800	L
H	-1	7.32874300	-4.31766300	-0.31291200	L	H	-1	-5.07397900	-3.98284300	-0.32389700	L
H	-1	8.40367900	-5.08850100	-2.81074800	L	H	0	-5.73380600	-1.65003800	-1.42633600	H
H	-1	4.45940600	-3.54284400	-1.99845600	L	H	0	-7.10283700	-1.65995300	-0.29309800	H
H	-1	8.23938300	-4.31525400	-5.13772900	L	H	-1	-6.71921500	-4.24007000	1.45577700	L
H	-1	4.29393400	-2.76364600	-4.34602400	L	H	-1	-6.61552900	-5.93452800	-0.68220000	L
H	-1	7.07116300	-3.21436200	-6.53339000	L	H	-1	-8.19271600	-5.84037100	-0.30279400	L
H	-1	7.94964800	-6.58048200	-1.15740000	L	H	-1	-8.57882600	-2.88541000	-6.36651400	L
H	-1	6.05785500	-6.84795800	-2.56783500	L	H	-1	-8.03150500	-2.82706300	-4.68656400	L
H	-1	5.05286500	-7.07588300	-1.29854900	L	H	-1	-6.26345600	-3.78255600	-7.03036400	L
H	-1	3.42040300	-2.96157500	3.17626100	L	H	-1	-5.72661300	-3.51192400	-5.37466000	L
H	-1	3.34452300	-1.04746300	1.52031700	L	H	0	-6.83335100	-1.38381700	-7.34625400	H
H	-1	4.99633300	-0.56903400	1.99614900	L	H	0	-5.12832800	-1.64946100	-7.00035000	H
H	-1	3.67348000	-0.46075000	3.15607400	L	H	0	-7.16272300	-0.49182600	-5.18810700	H
H	-1	4.13768200	-3.30137100	1.07816400	L	H	0	-3.79664000	-1.78786200	-5.19181800	H
H	-1	6.37198700	-2.02410600	3.49212000	L	H	0	-3.42785600	-0.77865800	-3.78596900	H
H	-1	5.04885600	-4.52003800	3.94939000	L	H	0	-6.34790100	1.02695500	-3.67340700	H
H	-1	6.62455100	-4.11825800	4.01744600	L	H	0	-4.84961200	0.51807500	-2.79900400	H
H	0	1.51228700	3.74618800	4.66946900	H	H	-1	-8.02760700	-5.37609500	-6.45557900	L
H	0	3.26480000	4.07149200	4.70465900	H	H	-1	-10.19809100	-4.64152400	-5.87234400	L
H	-1	2.70233300	2.91564900	6.72324100	L	H	-1	-9.83714000	-4.58161800	-4.28153700	L
H	-1	4.27117900	1.48552200	4.78642000	L	H	-1	-5.12090900	-7.48822300	0.45463400	L
H	-1	4.56696100	1.81007900	6.37207600	L	H	-1	-5.46075000	-6.97298700	2.11339200	L
H	-1	1.67865800	-2.44082200	4.59309300	L	H	-1	-2.98700000	-6.66708500	-0.70675500	L
H	-1	-0.29779100	-3.82364300	3.91709100	L	H	-1	-4.33110100	-4.59505100	2.99000000	L
H	-1	-1.39828100	-2.69400300	4.72240300	L	H	-1	-1.58162400	-4.68230400	-1.08339900	L
H	-1	-0.23547900	-3.63748600	5.67491600	L	H	-1	-3.02743100	-3.01926900	2.63906500	L
H	-1	0.57304500	-2.10379000	2.39496300	L	H	-1	-0.96019700	-2.72019200	-0.26661400	L
H	-1	-0.54872900	-0.90665400	3.07403500	L	H	-1	-2.78595400	-8.37698800	1.44034100	L
H	-1	1.18532900	-0.54150900	2.96206200	L	H	-1	-4.61334900	-9.66611300	0.61634100	L
H	-1	-0.47810900	-0.42996600	5.57758100	L	H	-1	-5.28756300	-9.75594300	2.09647000	L
H	-1	2.32794500	-0.12630600	4.92187000	L	H	-1	-5.37015500	-3.28013900	4.96080800	L
H	0	7.04365800	-1.01339000	-2.75737700	H	H	-1	-3.72607000	-3.22368700	4.32134700	L
H	0	8.07768300	0.37320100	-2.45201500	H	H	-1	-4.52564100	-1.83654100	6.95756200	L
H	0	4.90625600	-0.74830900	-3.97956600	H	H	-1	-2.99970700	-1.66536500	6.09232200	L
H	0	7.56477700	2.60618200	-3.57402200	H	H	0	-5.76639300	-0.84289400	4.97754200	H
H	0	3.09229700	0.74814900	-4.63022400	H	H	0	-4.60702200	0.26746200	5.73403100	H
H	0	5.71174500	4.13082200	-4.21745400	H	H	0	-4.50733200	-1.01103100	3.05807900	H
H	0	2.39270100	3.05656000	-4.65797100	H	H	0	-3.23795300	-0.04568800	1.54465200	H
H	-1	7.90059200	-1.30508400	-5.03451900	L	H	0	-1.83534800	0.90509100	1.96642100	H
H	-1	10.27026500	-1.49943700	-4.45737100	L	H	0	-2.41639300	0.75304500	5.44810600	H
H	-1	9.89656100	-1.05129800	-2.92689000	L	H	0	-1.71578100	1.73671200	4.18369400	H
H	-1	7.16775800	8.10657700	2.20330600	L	H	-1	-3.14015100	-3.88515300	6.87437700	L
H	-1	5.51613900	8.56818200	2.63502300	L	H	-1	-3.61718000	-5.38403900	4.53162200	L
H	-1	6.54786900	9.51139800	-0.97647300	L	H	-1	-2.18978600	-4.76947700	5.68142700	L
H	-1	5.53278000	7.86459500	-2.59070100	L	H	0	0.63084500	-1.62035700	-2.79693000	H
H	-1	4.63568100	6.06565100	2.37599800	L	H	0	0.71335700	0.73277000	-4.35490500	H
H	-1	3.27758300	4.18931600	1.44934500	L	H	0	2.04458400	0.99478300	-2.44193300	H
H	-1	3.83007700	5.59545300	-2.57680800	L	H	0	2.59551300	-1.58647300	-1.33558300	H
H	-1	2.90299300	3.95496500	-0.96722300	L	H	0	-1.34309800	-0.58186200	-0.79847700	H
H	-1	5.88163900	10.66084300	1.04043600	L	H	0	-0.02348300	2.13645600	-1.24568500	H
H	-1	8.65919400	9.87576500	1.54540300	L	H	0	-0.81772400	2.46391700	0.68606100	H
H	-1	8.16096200	11.33039800	1.00582900	L	H	0	1.06549300	-0.38835800	0.06544000	H
H	0	-0.26163600	4.70178600	4.22715400	H	H	0	1.92112300	1.66002300	0.90821500	H
H	0	-2.62293600	4.18648800	4.64261300	H	H	0	-2.35324100	1.75693200	-2.46113200	H
H	0	-2.99893200	4.27496200	2.91287300	H	H	0	-2.79378100	1.56632600	-0.73257700	H
H	0	-2.55696600	5.75423700	3.81287600	H	H	0	-3.79858400	-0.37306900	-1.17664600	H
H	0	0.18243500	2.77049000	2.94459500	H	O	-1	7.62349500	11.07135000	3.72246600	L
H	0	0.61198300	4.73570600	1.88574600	H	H	-1	8.49554300	0.81438300	-6.10044700	L
H	0	0.47590900	7.13256000	1.95268000	H	H	-1	7.68969900	-7.04365100	1.24920600	L
H	0	-0.77693200	7.07263900	3.03769400	H	H	-1	1.02063500	-8.17575000	0.55511400	L
H	-1	-4.71829100	7.43502600	-0.98865700	L	H	-1	-2.63024400	-7.74875800	3.80442800	L
H	-1	-3.61209600	8.38116500	0.01186400	L	H	-1	-10.36655300	-1.99814600	3.76834400	L
H	-1	-3.42251600	7.88329500	2.48688700	L	H	-1	-10.11595600	7.04318200	-3.29727800	L

H	-1	5.61081100	11.27249900	3.41628100	L	C	-1	0.63481200	-1.58867200	7.06371000	L
H	-1	-1.93164400	6.76946400	-4.90615400	L	O	-1	-0.42025400	-1.87328500	7.68773100	L
H	-1	5.58302000	-0.80074300	5.39984400	L	N	-1	9.63315700	-1.19144700	-3.69098100	L
H	-1	4.25970800	-7.46715500	-4.01701700	L	C	-1	8.53796100	-0.41896700	-4.24280100	L H 55
H	-1	-6.57058200	-6.20104100	-4.67597600	L	C	0	7.55325700	0.06002600	-3.17152900	H
H	-1	1.58656100	-1.91350200	7.43595600	L	C	0	6.41952200	0.94522300	-3.68930500	H
H	-1	-5.87769200	-5.44938800	6.70900500	L	C	0	5.16962600	0.41180100	-4.02754200	H
H	-1	-9.01745000	-3.53059000	-0.62766700	L	C	0	4.09019100	1.22059000	-4.38830800	H
N	-1	9.98331700	2.17351600	2.48415900	L	C	0	4.23067600	2.61474700	-4.40039200	H
C	-1	8.62054600	1.65912500	2.21095100	L H 371	O	0	3.21535100	3.47011900	-4.69837200	H
C	0	8.28946500	1.79924600	0.71410300	H	C	0	5.48301000	3.16789300	-4.08970300	H
C	0	6.92894800	1.28467000	0.34315400	H	C	0	6.54891700	2.34398600	-3.73644900	H
N	0	6.76185600	-0.00130700	-0.14248500	H	C	-1	9.02665800	0.79380000	-5.04708200	L
C	0	5.47654400	-0.18208500	-0.44578700	H	O	-1	9.94199000	1.52552000	-4.58846400	L
N	0	4.81161300	0.94200500	-0.16538400	H	N	-1	7.78136000	10.54985300	1.14571200	L
C	0	5.69005800	1.86788800	0.34028200	H	C	-1	6.48089300	10.34124400	1.79840100	L
C	-1	8.54541900	0.17034800	2.65058400	L	C	-1	6.16132300	8.85518800	1.94065000	L
O	-1	7.53336700	-0.24944800	3.21040200	L	C	-1	5.67502900	8.26673400	0.66016300	L
N	-1	9.56541700	-0.60716100	2.29785700	L	C	-1	5.87078300	8.77440600	-0.61400300	L
C	-1	9.56341700	-2.03944400	2.51132100	L H 381	N	-1	5.26436800	7.98674000	-1.53925200	L
C	0	8.82254800	-2.81077700	1.40005900	H	C	-1	4.67199800	6.91836700	-0.90128900	L
C	0	9.37645200	-2.46562800	-0.03298300	H	C	-1	4.92014400	7.05660700	0.48556300	L
O	0	10.20286600	-3.24411900	-0.51859400	H	C	-1	4.39014300	6.09868800	1.36944300	L
O	0	8.92938700	-1.37895100	-0.55122300	H	C	-1	3.66423900	5.04864800	0.83582300	L
C	-1	10.96584500	-2.60860600	2.64047800	L	C	-1	3.45817200	4.91552000	-0.54050900	L
O	-1	11.96456200	-1.88114000	2.40188300	L	C	-1	3.94372800	5.84737500	-1.43032600	L
H	0	9.03348500	1.25004500	0.10310400	H	C	-1	6.39431000	11.07065800	3.13607900	L
H	0	8.34817700	2.86667900	0.42211800	H	N	0	-0.47100400	6.84057200	3.01022200	H
H	0	5.34709800	2.83567900	0.68121900	H	C	0	-0.58514300	5.48606000	2.48470800	H
H	0	3.77126800	1.04747200	-0.20292700	H	C	0	-1.06720300	4.52075800	3.61237400	H
H	0	5.01827500	-1.07690700	-0.83568000	H	O	0	-0.72982200	3.17221100	3.28196000	H
H	-1	7.86254400	2.22287000	2.81294300	L	C	0	-2.55417500	4.63636600	3.95227900	H
H	-1	10.44365000	2.46815500	1.64782500	L	C	0	-1.44385700	5.26204500	1.21672700	H
H	-1	9.93209700	2.93946800	3.11989800	L	O	0	-1.62523600	4.10827700	0.80216300	H
H	0	8.94275100	-3.89926200	1.56328500	H	N	0	-1.96537800	6.36777200	0.64486300	H
H	0	7.73717500	-2.58144000	1.45511500	H	C	-1	-2.97505900	6.36514300	-0.48416100	L H 85
H	-1	9.02390800	-2.26373500	3.46894700	L	C	-1	-4.10681500	7.32675000	-0.11753600	L
H	-1	10.24200800	-0.26358200	1.64617100	L	C	-1	-4.87897700	6.88674600	1.13312700	L
H	-1	11.07852100	-3.66336400	2.91862700	L	C	-1	-4.45625000	7.25672500	2.40204600	L
H	0	7.58967100	-0.69185000	-0.27062200	H	C	-1	-5.14849100	6.85859600	3.54282500	L

G1c_D452A

ON10M: extrapolated energy = -3164.666590 au

N	-1	3.26920900	-7.53066100	2.26792000	L	C	-1	-2.20769900	6.81301200	-1.72700900	L
C	-1	2.08857400	-6.70324100	2.15702400	L	O	-1	-2.26643300	7.98756600	-2.13172100	L
C	-1	2.42860100	-5.45305100	1.30170400	L H 4	N	-1	-1.50084400	5.85992200	-2.33422100	L
C	0	1.34488800	-4.41339500	1.10313300	H	C	-1	-0.43329600	6.14886800	-3.32637400	L H 99
C	0	1.72021300	-3.38378800	-0.02144400	H	C	0	0.51840500	4.94907800	-3.41507100	H
O	0	2.90610800	-2.93701300	-0.04994900	H	C	0	-0.16226800	3.57401000	-3.68230700	H
O	0	0.78510100	-3.02718500	-0.79607400	H	O	0	-1.37983000	3.44302000	-3.35391100	H
C	-1	0.97498700	-7.48828500	1.45213200	L	O	0	0.60437700	2.67421500	-4.12989700	H
O	-1	-0.21019300	-7.40980600	1.86777500	L	C	-1	-0.91777700	6.58684300	-4.69728900	L
N	-1	1.67695400	-7.12076000	-4.90846100	L	O	-1	-0.07444100	6.72673900	-5.62075000	L
C	-1	2.67118700	-6.10494300	-4.62659200	L	N	-1	-8.96429000	5.57864000	-5.36893500	L
C	-1	2.01947200	-4.82694600	-4.05974300	L	C	-1	-8.77750800	5.21382600	-3.95328300	L
C	-1	0.70818000	-4.39022100	-4.69260000	L	C	-1	-7.36460200	5.54305200	-3.50004200	L
C	-1	0.54690000	-4.33586900	-6.06829900	L	C	-1	-6.32452700	4.60457000	-4.10478800	L
C	-1	-0.64793000	-3.89962500	-6.63259600	L	C	-1	-4.91937500	4.91365600	-3.67177900	L
C	-1	-1.67890000	-3.47775600	-5.81103600	L	O	-1	-4.61375500	6.02758700	-3.22603700	L
O	-1	-2.87350400	-3.04142200	-6.32432700	L	N	-1	-4.03370700	3.92219600	-3.80080100	L
C	-1	-1.53421000	-3.51610100	-4.43699600	L	C	-1	-9.81829700	5.89755200	-3.06131500	L
C	-1	-0.34488100	-3.96070300	-3.89113200	L	O	-1	-10.24859100	5.31191500	-2.03396500	L
C	-1	3.62822100	-6.72064600	-3.61810800	L	N	-1	-11.28141600	0.46829500	2.11696600	L
O	-1	3.42686900	-6.56824000	-2.38530600	L	C	-1	-10.08218400	-0.27936500	2.46495500	L
N	-1	6.18607100	-7.01063100	-1.56517900	L	C	-1	-8.87101300	0.63691100	2.66057300	L
C	-1	7.07958700	-6.22133800	-0.72487700	L	C	-1	-8.25604000	1.12473800	1.37216200	L
C	-1	6.69707300	-4.74573000	-0.77626200	L	C	-1	-8.82410200	1.09795000	0.12052000	L
C	-1	6.57804700	-4.22190300	-2.18380500	L	N	-1	-7.96336100	1.67063500	-0.79395800	L
C	-1	7.62988100	-4.41514300	-3.08592700	L	C	-1	-6.83153200	2.09254500	-0.14564700	L
C	-1	7.53875400	-3.97828600	-4.38692500	L	C	-1	-6.97538500	1.75700700	1.21861800	L
C	-1	6.38773900	-3.35311200	-4.79852400	L	C	-1	-5.94545800	2.06850600	2.10418700	L
O	-1	6.34706900	-2.91805400	-6.09650100	L	C	-1	-4.80111600	2.67067600	1.62250600	L
C	-1	5.32484600	-3.14760400	-3.94672600	L	C	-1	-4.66698000	2.97750700	0.23880300	L
C	-1	5.42111600	-3.58431300	-2.62986700	L	C	-1	-5.68162800	2.70282600	-0.64459900	L
C	-1	6.95348700	-6.67936100	0.72373700	L	C	-1	-10.40622200	-1.06114500	3.72262300	L
O	-1	5.81541700	-6.83162700	1.23869700	L	O	-1	-10.79536300	-0.45752900	4.75596200	L
N	-1	5.79609700	-3.71349100	4.37431900	L	N	-1	-7.11174900	-5.75623600	0.00396900	L
C	-1	5.49555000	-2.36346700	3.95100500	L	C	-1	-6.97589000	-4.34716100	0.38063600	L
C	-1	4.44876800	-2.36906200	2.86244800	L	C	-1	-5.97047100	-3.64641600	-0.54459600	L H 131
O	-1	4.94860400	-3.14685000	1.76578600	L	C	0	-5.99271000	-2.12883200	-0.46530800	H
C	-1	4.13181400	-0.95451000	2.39239900	L	C	0	-5.11073000	-1.57262200	0.67192500	H
C	-1	5.01235700	-1.52432200	5.14669100	L	O	0	-5.42539500	-1.82917700	1.85177200	H
O	-1	3.95047200	-1.83579700	5.74581700	L	O	0	-4.11676200	-0.85787500	0.30612100	H
N	-1	3.87298500	1.56496200	5.78791600	L	C	-1	-8.33433500	-3.62380400	0.28166400	L
C	-1	2.63425800	2.38118900	5.84498200	L H 43	O	-1	-8.78963600	-3.00132900	1.27604800	L
C	0	2.48016600	3.31137500	4.63955000	H	N	-1	-9.44469000	-5.14939000	-5.19133200	L
C	-1	1.40529000	1.44475900	5.95266400	L	C	-1	-8.03684400	-4.93307800	-5.52472400	L
O	-1	0.34438400	1.90561300	6.40364300	L	C	-1	-7.72890300	-3.45209300	-5.67367400	L
N	-1	1.57471400	0.18043300	5.56987200	L	C	-1	-6.30221000	-3.21441100	-6.15266100	L H 141
C	-1	0.55525000	-0.87142400	5.70582000	L	C	0	-6.02571800	-1.77940100	-6.59205100	H
C	-1	0.70888800	-1.93431900	4.58483800	L	N	0	-6.14983000	-0.77367400	-5.53777200	H
C	-1	-0.29524000	-3.05591000	4.75512100	L	C	0	-5.23951100	-0.54441600	-4.55252900	H
C	-1	0.50528400	-1.28540800	3.21552600	L	N	0	-4.03892600	-1.10928700	-4.54156500	H

N	0	-5.57840600	0.29645200	-3.56742800	H	H	-1	8.00160800	-1.10010400	-4.95408600	L
C	-1	-7.15526800	-5.54932400	-4.42014800	L	H	-1	10.37076900	-1.25059400	-4.36192600	L
O	-1	-7.33487100	-5.22496000	-3.21760800	L	H	-1	9.97878500	-0.81237200	-2.83314700	L
N	-1	-4.20965100	-9.68515900	1.58494100	L	H	-1	7.04395800	8.28292400	2.29465200	L
C	-1	-3.59085100	-8.40731000	1.94179200	L	H	-1	5.38114200	8.71239400	2.71643600	L
C	-1	-4.46066600	-7.25228800	1.40267100	L	H	-1	6.41807200	9.68148800	-0.88670900	L
C	-1	-3.65641000	-5.99270500	1.15783500	L	H	-1	5.44479000	8.01867400	-2.51024600	L
C	-1	-2.83702800	-5.85861800	0.02499700	L	H	-1	4.54994200	6.19411100	2.44750600	L
C	-1	-2.06153400	-4.74149200	-0.16462600	L	H	-1	3.23363800	4.29407200	1.50892100	L
C	-1	-2.08892600	-3.73362500	0.76608400	L	H	-1	3.78533000	5.71767700	-2.51119900	L
O	-1	-1.32242500	-2.62438700	0.59153800	L	H	-1	2.87913800	4.05702900	-0.91041300	L
C	-1	-2.88231100	-3.84252600	1.89572500	L	H	-1	5.71719800	10.81447300	1.12777100	L
C	-1	-3.67233500	-4.96453000	2.06478200	L	H	-1	8.50581700	10.08121800	1.64940000	L
C	-1	-3.35948600	-8.28147200	3.45167600	L	H	-1	7.98360200	11.52712700	1.10905600	L
O	-1	-4.19829800	-8.75958000	4.25875500	L	H	0	-0.46946400	4.77684500	4.49173200	H
N	-1	-3.18856700	-5.45407100	5.48281100	L	H	0	-2.77737200	4.03303400	4.83784300	H
C	-1	-3.85197600	-4.38754800	6.21654200	L	H	0	-3.17475000	4.25583000	3.12579000	H
C	-1	-4.23865800	-3.22405500	5.27931800	L	H	0	-2.85703400	5.67158700	4.16865100	H
C	-1	-4.04593700	-1.87944000	5.93804700	L	H	0	-1.04048800	3.04424900	2.36496900	H
C	0	-4.65930200	-0.72407900	5.14952300	H	H	0	0.42550300	5.15305100	2.22183600	H
N	0	-4.04032500	-0.52355500	3.84214000	H	H	0	0.05453300	7.46123400	2.40168000	H
C	0	-3.01900900	0.29020500	3.55471300	H	H	0	-1.36723600	7.26211400	3.24149500	H
N	0	-2.38253500	0.99570800	4.51513900	H	H	-1	-4.80641500	7.39219100	-0.97536800	L
N	0	-2.68056700	0.45884400	2.27347000	H	H	-1	-3.72481500	8.35730000	0.03388700	L
C	-1	-5.04688600	-4.79983600	7.08460200	L	H	-1	-3.54179300	7.85864600	2.50924500	L
O	-1	-5.18293700	-4.31659400	8.23849000	L	H	-1	-6.36189500	5.78592400	0.03492100	L
C	0	0.64702100	-0.58617900	-2.95580800	H	H	-1	-4.79104900	7.15748500	4.53511600	L
O	0	0.88576700	-0.20898600	-4.27946700	H	H	-1	-7.61739800	5.07996900	2.02774100	L
C	0	1.71112400	0.02854700	-1.98851100	H	H	-1	-7.71613600	5.15851800	4.24861400	L
O	0	2.86685200	-0.77752600	-1.91177000	H	H	-1	-3.40607200	5.32634300	-0.59634200	L
O	0	-0.72150900	-0.19183900	-2.70628600	H	H	0	-1.76485000	7.26345100	1.08443900	H
C	0	-1.16340100	0.23287000	-1.42912000	H	H	0	1.30040600	5.12373400	-4.17887500	H
C	0	-0.13165000	1.14547500	-0.76687100	H	H	0	1.08574600	4.83241500	-2.46468500	H
O	0	-0.55387400	1.58663400	0.54543200	H	H	-1	0.14411300	7.02087200	-2.92095700	L
C	0	1.16617000	0.38376000	-0.61001200	H	H	-1	-1.97093700	4.97747500	-2.47204700	L
O	0	2.12749400	1.21899900	0.05184900	H	H	-1	-7.30870000	5.47968000	-2.39164900	L
C	0	-2.47986200	0.95132300	-1.67261200	H	H	-1	-7.10356900	6.59595100	-3.74012400	L
O	0	-3.51036600	0.00821900	-2.02840600	H	H	-1	-6.59839000	3.55623200	-3.84958300	L
H	-1	2.78839000	-5.79420200	0.30473000	L	H	-1	-6.37374000	4.66336100	-5.21237100	L
H	-1	3.30214500	-4.94933400	1.77281300	L	H	-1	-4.28738100	3.15190500	-4.37347400	L
H	0	0.36928700	-4.86898400	0.84029500	H	H	-1	-3.02341000	4.03541800	-3.65986300	L
H	0	1.17939500	-3.81296300	2.03302200	H	H	-1	-8.93127100	4.10549300	-3.89800700	L
H	-1	1.76604400	-6.39571600	3.18158200	L	H	-1	-9.91123300	5.41231500	-5.63779300	L
H	-1	3.60575400	-7.79402800	1.36461300	L	H	-1	-8.74240500	6.54184700	-5.51528300	L
H	-1	3.97802600	-7.05909100	2.78844800	L	H	-1	-8.08648200	0.08363300	3.21725800	L
H	-1	1.84467000	-4.93106000	-2.96784500	L	H	-1	-9.12682700	1.51670500	3.28634100	L
H	-1	2.74710000	-3.99055800	-4.16448400	L	H	-1	-9.82260300	0.74505000	-0.15091000	L
H	-1	1.36777200	-4.64581600	-6.72620700	L	H	-1	-8.00042200	1.48982200	-1.76516100	L
H	-1	-0.24369400	-3.97316300	-2.79695600	L	H	-1	-6.05527900	1.82667200	3.16702500	L
H	-1	-0.74424200	-3.87327500	-7.72505600	L	H	-1	-3.98607200	2.96838800	2.30093700	L
H	-1	-2.33956100	-3.18463800	-3.77018700	L	H	-1	-5.58933200	2.95274300	-1.70855900	L
H	-1	-2.80763500	-3.08215000	-7.27103600	L	H	-1	-3.74473900	3.47294100	-0.10809100	L
H	-1	3.20877700	-5.86790300	-5.57728500	L	H	-1	-9.87571200	-0.98483600	1.62205700	L
H	-1	2.11601700	-7.96916000	-5.20053000	L	H	-1	-12.06863300	-0.14625200	2.08109700	L
H	-1	1.10583200	-7.29332500	-4.10750300	L	H	-1	-11.45746500	1.19445500	2.78136500	L
H	-1	5.74206000	-4.57229500	-0.23424100	L	H	-1	-6.19623700	-3.90488300	-1.60023700	L
H	-1	7.45651900	-4.13148200	-0.24135400	L	H	-1	-4.94999300	-4.03154600	-0.33212300	L
H	-1	8.56194300	-4.87732200	-2.73346700	L	H	0	-5.64566200	-1.70511500	-1.42238700	H
H	-1	4.58393700	-3.40809300	-1.94414300	L	H	0	-7.02000500	-1.74830400	-0.29901300	H
H	-1	8.39802700	-4.10312900	-5.06016000	L	H	-1	-6.60149600	-4.32308800	1.43642000	L
H	-1	4.41886900	-2.62793600	-4.29142300	L	H	-1	-6.45194800	-6.01142000	-0.70368600	L
H	-1	7.21817900	-3.02203900	-6.46150700	L	H	-1	-8.03304800	-5.94782800	-0.33434800	L
H	-1	8.12561300	-6.38061200	-1.08560500	L	H	-1	-8.43598400	-2.98977600	-6.39546600	L
H	-1	6.24835700	-6.68131600	-2.50871400	L	H	-1	-7.90070500	-2.92410600	-4.71196000	L
H	-1	5.23970600	-6.93051900	-1.24635000	L	H	-1	-6.09980200	-3.84172100	-7.04581000	L
H	-1	3.50078000	-2.85593600	3.22470100	L	H	-1	-5.57886500	-3.56396000	-5.38621000	L
H	-1	3.39932300	-0.94062100	1.57152100	L	H	0	-6.72394700	-1.47945700	-7.39304600	H
H	-1	5.03867100	-0.43186000	2.05884700	L	H	0	-5.01568300	-1.69325700	-7.03104700	H
H	-1	3.70655600	-0.35073500	3.21035900	L	H	0	-7.09824500	-0.53922100	-5.27633300	H
H	-1	4.23789000	-3.17830600	1.13071100	L	H	0	-3.73453900	-1.83444300	-5.19996800	H
H	-1	6.43197600	-1.86331900	3.56125000	L	H	0	-3.40665600	-0.85520800	-3.76475700	H
H	-1	5.15345100	-4.38467700	4.00574200	L	H	0	-6.33930200	0.94762300	-3.70215500	H
H	-1	6.72077900	-3.95325700	4.08468000	L	H	0	-4.85450300	0.44513000	-2.81214100	H
H	0	1.56055100	3.91574200	4.72613200	H	H	-1	-7.83711200	-5.46941300	-6.48514500	L
H	0	3.33473100	4.00984600	4.55696200	H	H	-1	-10.02483800	-4.77712400	-5.91474900	L
H	-1	2.64864400	3.00023100	6.77683100	L	H	-1	-9.67534700	-4.71326400	-4.32153900	L
H	-1	4.25675300	1.60356200	4.84781300	L	H	-1	-4.93551800	-7.53858400	0.44019200	L
H	-1	4.53610700	1.93080000	6.43589500	L	H	-1	-5.29574400	-7.03286800	2.09757800	L
H	-1	1.74038600	-2.37081200	4.63109400	L	H	-1	-2.81010800	-6.67509500	-0.70596600	L
H	-1	-0.20511200	-3.78958800	3.93997900	L	H	-1	-4.21702300	-4.63555400	2.98548200	L
H	-1	-1.33197400	-2.68244200	4.74004200	L	H	-1	-1.44019000	-4.66338300	-1.07016000	L
H	-1	-0.15766800	-3.60545500	5.69848000	L	H	-1	-2.94120700	-3.03473900	2.64565000	L
H	-1	0.64277600	-2.05081100	2.42641700	L	H	-1	-0.86132600	-2.69133200	-0.24606900	L
H	-1	-0.50583100	-0.87635700	3.10022000	L	H	-1	-2.59054500	-8.38475400	1.43951000	L
H	-1	1.22168400	-0.47824200	3.00009700	L	H	-1	-4.38783900	-9.70676100	0.60152200	L
H	-1	-0.46039200	-0.40293400	5.60496800	L	H	-1	-5.06975600	-9.81201100	2.07710000	L
H	-1	2.34357300	-0.04501400	4.96796100	L	H	-1	-5.29347900	-3.34410700	4.95099800	L
H	0	7.12173700	-0.82717100	-2.67671600	H	H	-1	-3.64667600	-3.25538300	4.32302500	L
H	0	8.10075200	0.60541600	-2.38075600	H	H	-1	-4.48935800	-1.88838100	6.95633300	L
H	0	5.00665000	-0.66594500	-3.97473000	H	H	-1	-2.96139700	-1.68678300	6.10128600	L
H	0	7.50159900	2.80020800	-3.46442600	H	H	0	-5.73077400	-0.91554300	4.95943900	H
H	0	3.13252800	0.76192600	-4.61672400	H	H	0	-4.60411600	0.21672300	5.73035200	H
H	0	5.58627400	4.25113400	-4.09313300	H	H	0	-4.46835700	-1.05242700	3.04821400	H
H	0	2.32477900	3.04906200	-4.57784500	H	H	0	-3.21919800	-0.04793800	1.54319900	H

H	0	-1.76094300	0.78908900	1.98680900	H	C	-1	6.48617300	-4.32545400	-2.25658800	L
H	0	-2.39940400	0.68431500	5.47559700	H	C	-1	7.52850600	-4.52865800	-3.16750600	L
H	0	-1.67615200	1.68194300	4.24060400	H	C	-1	7.43078900	-4.09052500	-4.46759600	L
H	-1	-3.06479700	-3.91024000	6.87868100	L	C	-1	6.28253200	-3.45402800	-4.86942500	L
H	-1	-3.49823300	-5.41366200	4.53036800	L	O	-1	6.23527500	-3.01818600	-6.16691700	L
H	-1	-2.09017900	-4.77425700	5.69042800	L	C	-1	5.22884000	-3.23843200	-4.00873500	L
H	0	0.72009000	-1.67546800	-2.89035000	H	C	-1	5.33183300	-3.67647300	-2.69282800	L
H	0	0.66602000	0.75324200	-4.32160500	H	C	-1	6.86187900	-6.78736900	0.64714600	L
H	0	2.02936400	0.97295100	-2.44432300	H	O	-1	5.72671600	-6.92869100	1.17155400	L
H	0	2.70041300	-1.57578800	-1.34267700	H	N	-1	5.76398200	-3.81149900	4.30795400	L
H	0	-1.33240700	-0.63219100	-0.76720100	H	C	-1	5.47309400	-2.45847600	3.88747700	L
H	0	0.03214200	2.02739500	-1.39362600	H	C	-1	4.41725700	-2.45352400	2.80769800	L
H	0	-0.96611100	2.46119300	0.42613300	H	O	-1	4.90035000	-3.23578600	1.70667700	L
H	0	0.99444700	-0.52995200	-0.02317900	H	C	-1	4.11020500	-1.03579800	2.34063900	L
H	0	1.68077800	1.53786100	0.85415900	H	C	-1	5.00810500	-1.61503400	5.08735000	L
H	0	-2.34744900	1.65906800	-2.49454200	H	O	-1	3.94827000	-1.91632700	5.69524900	L
H	0	-2.79824800	1.49494700	-0.77173500	H	N	-1	3.90431300	1.48501400	5.73878400	L
H	0	-3.77877600	-0.45648000	-1.16115100	H	C	-1	2.67412600	2.31326100	5.80637900	L H 43
O	-1	7.43364200	11.25305000	3.82171500	L	C	0	2.48648700	3.25307200	4.61553700	H
H	-1	8.56315500	1.03216700	-6.01257300	L	C	0	2.78477200	2.63253900	3.23206700	H
H	-1	7.85898100	-6.85296000	1.31848400	L	O	0	3.82080700	2.91005100	2.64518800	H
H	-1	1.21717400	-8.10987900	0.57930100	L	C	-1	1.43702200	1.38882800	5.92410200	L
H	-1	-2.46200600	-7.75795400	3.80560900	L	O	-1	0.38446300	1.85986300	6.38402800	L
H	-1	-10.30548400	-2.15480200	3.72907600	L	N	-1	1.59090600	0.12303000	5.53961300	L
H	-1	-10.18069500	6.90237900	-3.31956400	L	C	-1	0.56240000	-0.91887800	5.68382300	L
H	-1	5.41952300	11.41660500	3.50283700	L	C	-1	0.69630300	-1.98286900	4.56135100	L
H	-1	-1.98246700	6.78658100	-4.87584400	L	C	-1	-0.31726100	-3.09466800	4.73975100	L
H	-1	5.60769300	-0.65855700	5.46587700	L	C	-1	0.48761600	-1.33157400	3.19393800	L
H	-1	4.47164200	-7.33183500	-3.97055300	L	C	-1	0.64629300	-1.63729400	7.04083600	L
H	-1	-6.37622000	-6.26983100	-4.69753000	L	O	-1	-0.40625300	-1.91180000	7.67357700	L
H	-1	1.61999400	-1.85045900	7.47418300	L	N	-1	9.55801000	-1.32446100	-3.78851400	L
H	-1	-5.77108800	-5.52572800	6.69294900	L	C	-1	8.46583300	-0.54116500	-4.33099200	L H 57
H	-1	-8.8928400	-3.65349500	-0.66067300	L	C	0	7.49202100	-0.06940500	-3.24614400	H
N	-1	9.96955500	2.40373300	2.58376100	L	C	0	6.36655700	0.83862200	-3.73830300	H
C	-1	8.61853800	1.86413900	2.30086700	L H 368	C	0	5.09489700	0.33963300	-4.05122400	H
C	0	8.28693600	2.01652100	0.80107400	H	C	0	4.03324400	1.17937600	-4.39729200	H
C	0	7.00135600	1.36508700	0.37197500	H	C	0	4.21653300	2.57065700	-4.42242600	H
N	0	6.95197200	0.02221000	0.03864400	H	O	0	3.23193900	3.45346800	-4.71800900	H
C	0	5.70247700	-0.22009000	-0.33420400	H	C	0	5.48979500	3.08589700	-4.12915900	H
N	0	4.95195700	0.89926600	-0.26325100	H	C	0	6.53490700	2.23303100	-3.78934000	H
C	0	5.75561500	1.91673400	0.18817800	H	C	-1	8.95960700	0.66703100	-5.13904200	L
C	-1	8.56882700	0.37340900	2.73750300	L	O	-1	9.88582800	1.38964700	-4.68791300	L
O	-1	7.56131600	-0.06648300	3.29004600	L	N	-1	7.86125800	10.43282000	1.06619900	L
N	-1	9.60561800	-0.38401000	2.39008100	L	C	-1	6.56431100	10.23669700	1.72967400	L
C	-1	9.62937700	-1.81645500	2.60112300	L H 218	C	-1	6.23145900	8.75378400	1.87424100	L
C	0	8.87943700	-2.61228600	1.51357900	H	C	-1	5.72877800	8.17050200	0.59772200	L
C	0	9.53830000	-2.45190500	0.12745700	H	C	-1	5.91883300	8.67664100	-0.67791600	L
O	0	10.39496400	-3.22132500	-0.25859900	H	N	-1	5.29706300	7.89521600	-1.59825200	L
O	0	9.14724500	-1.40522000	-0.59364900	H	C	-1	4.69964600	6.83247000	-0.95561500	L
C	-1	11.04147700	-2.35919400	2.73840500	L	C	-1	4.96069500	6.96784900	0.42914900	L
O	-1	12.02774900	-1.61251800	2.50750800	L	C	-1	4.42877100	6.01486600	1.31720100	L
H	0	9.10532500	1.59334800	0.18235500	H	C	-1	3.68823300	4.97212100	0.78941500	L
H	0	8.23513500	3.09545500	0.55334300	H	C	-1	3.46939000	4.84144800	-0.58518200	L
H	0	5.37957500	2.92598200	0.31392800	H	C	-1	3.95657400	5.76879700	-1.47880200	L
H	0	3.94158900	0.93042100	-0.41445300	H	C	-1	6.49601400	10.96650200	3.06819800	L
H	0	5.29209100	-1.17249800	-0.64012400	H	N	0	-0.08750600	6.62884300	2.75574600	H
H	-1	7.84615300	2.41234200	2.89888700	L	C	0	-0.37322900	5.29321300	2.23856600	H
H	-1	10.42959900	2.70855400	1.75092700	L	C	0	-0.94403800	4.42831100	3.40397500	L
H	-1	9.89973200	3.16743700	3.22044600	L	O	0	-0.83596200	3.03682900	3.12864700	H
H	0	8.90946100	-3.68907900	1.75928900	H	C	0	-2.41154500	4.68125600	3.73069500	H
H	0	7.81564400	-2.29777700	1.48470000	H	C	0	-1.26401000	5.16762500	0.98456500	H
H	-1	9.08805600	-2.05265100	3.55485500	L	O	0	-1.34724600	4.09827100	0.37600800	H
H	-1	10.27976500	-0.02650600	1.74337400	L	N	0	-1.93779600	6.29556100	0.64240100	H
H	-1	11.17232100	-3.41212900	3.01550500	L	C	-1	-2.94869200	6.35371200	-0.47479100	L H 87
H	0	8.31124100	-0.93598600	-0.25058000	H	C	-1	-4.06792000	7.32619400	-0.09850000	L
H	0	2.41016600	2.75325700	3.68729400	H	C	-1	-4.83387100	6.89335000	1.15846300	L
G1c_D452N											
ONIOM: extrapolated energy = -3333.362694 au											
N	-1	3.18248900	-7.60318400	2.22183800	L	C	-1	-6.68137300	5.72870100	2.19926100	L
C	-1	2.00909400	-6.76425600	2.12099400	L	C	-1	-5.97441800	6.12238900	1.06080900	L
C	-1	2.35416000	-5.51716500	1.26314700	L H 4	C	-1	-2.18740200	6.79446800	-1.72389100	L
C	0	1.25576400	-4.48573500	1.10075200	H	O	-1	-2.23805500	7.96966600	-2.12782800	L
C	0	1.62385500	-3.40490100	0.03210800	H	N	-1	-1.49496900	5.83472100	-2.33720500	L
O	0	2.73254500	-2.80939000	0.14643800	H	C	-1	-0.43297300	6.11355400	-3.33817200	L H 101
O	0	0.74612200	-3.16005100	-0.85581600	H	C	0	0.48297300	4.88651300	-3.44062200	H
C	-1	0.88206100	-7.53818200	1.42524200	L	C	0	-0.16427400	3.56479500	-3.97751600	H
O	-1	-0.29878700	-7.44828000	1.85078400	L	O	0	-1.40697000	3.46323500	-4.09855000	H
N	-1	1.53446800	-7.17552400	-4.94090400	L	O	0	0.68975600	2.64958000	-4.21977300	H
C	-1	2.54087900	-6.16953900	-4.66711000	L	C	-1	-0.92458400	6.55666400	-4.70489100	L
C	-1	1.90641500	-4.88542600	-4.09454300	L	O	-1	-0.08766000	6.68861900	-5.63532800	L
C	-1	0.59420900	-4.43573600	-4.71632800	L	N	-1	-8.98587400	5.62718500	-5.30956900	L
C	-1	0.42199000	-4.37938100	-6.09062000	L	C	-1	-8.79085100	5.26012300	-3.89561000	L
C	-1	-0.77319600	-3.93133000	-6.64482100	L	C	-1	-7.37106700	5.57541300	-3.45410500	L
C	-1	-1.79310800	-3.49968500	-5.81458400	L	C	-1	-6.34527900	4.62702300	-4.06773100	L
O	-1	-2.98764200	-3.05156200	-6.31778000	L	C	-1	-4.93361300	4.92225600	-3.64639600	L
C	-1	-1.63733700	-3.53987000	-4.44180800	L	O	-1	-4.61343300	6.03301300	-3.20296200	L
C	-1	-0.44789200	-3.99621700	-3.90599600	L	N	-1	-4.05876600	3.92225500	-3.78304700	L
C	-1	3.50024600	-6.79486200	-3.66679400	L	C	-1	-9.81744000	5.95368600	-2.99482500	L
O	-1	3.31068600	-6.64088700	-2.43231900	L	O	-1	-10.24483600	5.37195100	-1.96405500	L
N	-1	6.07219100	-7.11042100	-1.63536000	L	N	-1	-11.29017500	0.53733000	2.19422900	L
C	-1	6.98034600	-6.33014200	-0.80236300	L	C	-1	-10.09543100	-0.22209800	2.53202000	L
C	-1	6.61182700	-4.85085900	-0.85021000	L	C	-1	-8.87379000	0.68226200	2.71773200	L

C	-1	-8.26486300	1.16447400	1.42434600	L	H	-1	3.37105900	-1.01450800	1.52590800	L
C	-1	-8.84358500	1.14361900	0.17748300	L	H	-1	5.01930200	-0.52191100	1.99964900	L
N	-1	-7.98496100	1.70817000	-0.74401600	L	H	-1	3.69769800	-0.42816100	3.16226100	L
C	-1	-6.84370000	2.11881900	-0.10507900	L	H	-1	4.18399500	-3.26013900	1.07765000	L
C	-1	-6.97942800	1.78427200	1.26026200	L	H	-1	6.41106800	-1.96736000	3.49003400	L
C	-1	-5.93915600	2.08543300	2.13727300	L	H	-1	5.11176500	-4.47627100	3.94459900	L
C	-1	-4.79305200	2.67656800	1.64619100	L	H	-1	6.68383200	-4.06018000	4.01054900	L
C	-1	-4.66748600	2.98251100	0.26149200	L	H	0	1.45589600	3.65443500	4.63101500	H
C	-1	-5.69210200	2.71801500	-0.61347200	L	H	0	3.17863100	4.10835800	4.69199300	H
C	-1	-10.41657000	-1.00107600	3.79216800	L	H	-1	2.70232400	2.93184200	6.73822000	L
O	-1	-10.79116800	-0.39401800	4.82886000	L	H	-1	4.28057900	1.52016300	4.79551800	L
N	-1	-7.19920100	-5.72690300	0.04504700	L	H	-1	4.57635500	1.84416400	6.38128900	L
C	-1	-7.04646600	-4.31933800	0.42089500	L	H	-1	1.72384400	-2.42941500	4.59889200	L
C	-1	-6.04202000	-3.62814000	-0.51253800	L	H	-1	-0.24110000	-3.82893400	3.92371300	L
C	0	-6.03996600	-2.10899400	-0.45122400	H	H	-1	-1.35039200	-2.71110300	4.73341500	L
C	0	-5.16257700	-1.54188400	0.68508300	H	H	-1	-0.17718800	-3.64582400	5.68180100	L
O	0	-5.42044900	-1.87190900	1.86165800	H	H	-1	0.61104600	-2.09803400	2.40353000	L
O	0	-4.23569800	-0.74362300	0.32047300	H	H	-1	-0.52038800	-0.91264600	3.08717200	L
C	-1	-8.39856900	-3.58273700	0.33343600	L	H	-1	1.21003200	-0.53136500	2.97272200	L
O	-1	-8.83946200	-2.95616400	1.33173100	L	H	-1	-0.44943000	-0.44047400	5.59156400	L
N	-1	-9.56936800	-5.09322400	-5.13045300	L	H	-1	2.35247900	-0.10971500	4.93125200	L
C	-1	-8.16233400	-4.89302800	-5.47553800	L	H	0	7.05555900	-0.96123800	-2.76321900	H
C	-1	-7.84121700	-3.41506900	-5.62671000	L	H	0	8.05042300	0.45577300	-2.44980900	H
C	-1	-6.41632000	-3.19115900	-6.11753500	L	H	0	4.90402800	-0.73406300	-4.00091600	H
C	0	-6.11316300	-1.75818200	-6.54213800	H	H	0	7.50499600	2.66120200	-3.53414300	H
N	0	-6.16783900	-0.77721200	-5.46162800	H	H	0	3.06090400	0.75245600	-4.62690600	H
C	0	-5.15562200	-0.34765000	-4.66036800	H	H	0	5.62427900	4.16546800	-4.13982500	H
N	0	-3.91632600	-0.82659600	-4.75467800	H	H	0	2.32531400	3.05307500	-4.60143900	H
N	0	-5.42639600	0.62302700	-3.78773600	H	H	-1	7.91694500	-1.21681700	-5.03793200	L
C	-1	-7.27762300	-5.51818700	-4.37850400	L	H	-1	10.28938500	-1.39058800	-4.46560800	L
O	-1	-7.44401100	-5.19246500	-3.17443100	L	H	-1	9.91446700	-0.94904400	-2.93350800	L
N	-1	-4.32246900	-9.68443500	1.60082200	L	H	-1	7.11139400	8.17282900	2.22072900	L
C	-1	-3.68827800	-8.41279300	1.95279100	L	H	-1	5.45642400	8.61836100	2.65648100	L
C	-1	-4.55125500	-7.24917500	1.42121900	L	H	-1	6.47264900	9.57842900	-0.95497100	L
C	-1	-3.73682300	-5.99741800	1.16997000	L	H	-1	5.46967800	7.92569400	-2.57071200	L
C	-1	-2.92565500	-5.87097200	0.03036200	L	H	-1	4.59848600	6.10838800	2.39391400	L
C	-1	-2.14091200	-4.76140200	-0.16546900	L	H	-1	3.25592400	4.22157100	1.46591000	L
C	-1	-2.15070200	-3.75360900	0.76567200	L	H	-1	3.78790300	5.64099000	-2.55834400	L
O	-1	-1.37490500	-2.65184700	0.58498900	L	H	-1	2.87894900	3.98875400	-0.95043500	L
C	-1	-2.93565700	-3.85512100	1.90187100	L	H	-1	5.79969700	10.71756200	1.06555400	L
C	-1	-3.73514900	-4.96942000	2.07725700	L	H	-1	8.58528700	9.95698500	1.56371300	L
C	-1	-3.44310300	-8.28969100	3.46072000	L	H	-1	8.07271000	11.40808700	1.02808300	L
O	-1	-4.27977400	-8.75984900	4.27466300	L	H	0	-0.32845800	4.70036500	4.27456600	H
N	-1	-3.22766800	-5.46472900	5.49101400	L	H	0	-2.68332900	4.15051500	4.64921100	H
C	-1	-3.87449500	-4.39201700	6.23050600	L	H	0	-3.05159300	4.29897300	2.92155300	H
C	-1	-4.25761900	-3.22451400	5.29681300	L	H	0	-2.63221700	5.74650200	3.88413200	H
C	-1	-4.04629900	-1.88204600	5.95422700	L	H	0	0.05067100	2.83054900	2.75924400	H
C	0	-4.66784000	-0.72584200	5.17227400	H	H	0	0.59002600	4.85276200	1.95215400	H
N	0	-4.07132300	-0.52816800	3.85670400	H	H	0	0.36812800	7.22224600	2.06809900	H
C	0	-3.04985500	0.28367600	3.55353200	H	H	0	-0.91039400	7.10351200	3.11953300	H
N	0	-2.41219500	1.00304800	4.50399200	H	H	-1	-4.77398200	7.39872600	-0.95044700	L
N	0	-2.69548900	0.40693300	2.27795100	H	H	-1	-3.67463500	8.35292500	0.04996700	L
C	-1	-5.06608300	-4.79290500	7.10841600	L	H	-1	-3.47583100	7.85173200	2.52359500	L
O	-1	-5.18777900	-4.30872200	8.26351200	L	H	-1	-6.33656900	5.80738600	0.07242100	L
C	0	0.09555400	-0.49277300	-3.24536200	H	H	-1	-4.71491600	7.16215100	4.55966300	L
O	0	0.32083800	-0.10110000	-4.55589900	H	H	-1	-7.58222200	5.11308200	2.07548900	L
C	0	1.30202900	-0.19162000	-2.31057100	H	H	-1	-7.66165100	5.19189400	4.29712700	L
O	0	2.27072100	-1.21152600	-2.43595900	H	H	-1	-3.39074800	5.31920400	-0.58360100	L
O	0	-1.13534900	0.15005400	-2.85021100	H	H	0	-1.77780400	7.14306700	1.17997900	H
C	0	-1.38489100	0.48748700	-1.49167300	H	H	0	1.35891100	5.11675700	-4.07867600	H
C	0	-0.15766000	1.10579200	-0.78325800	H	H	0	0.92631600	4.64403000	-2.44992500	H
O	0	-0.47616100	1.44834400	0.57357400	H	H	-1	0.15627700	6.97975900	-2.93738600	L
C	0	0.90269200	0.02122600	-0.84259600	H	H	-1	-1.97478300	4.95694400	-2.47130800	L
O	0	2.06630900	0.32277200	-0.04645700	H	H	-1	-7.30653600	5.51115100	-2.34623100	L
C	0	-2.59651800	1.39604600	-1.54944700	H	H	-1	-7.10178900	6.62579100	-3.69611300	L
O	0	-3.75441700	0.60579300	-1.85682100	H	H	-1	-6.62721400	3.58132500	-3.81049200	L
H	-1	2.70226000	-5.86150700	0.26313400	L	H	-1	-6.40315900	4.68663800	-5.17485100	L
H	-1	3.23646700	-5.02214900	1.72707800	L	H	-1	-4.32471200	3.15464400	-4.35375100	L
H	0	0.29080900	-4.94931100	0.81495900	H	H	-1	-3.04627100	4.02556100	-3.65050800	L
H	0	1.08671100	-3.92986900	2.05553300	H	H	-1	-8.95495000	4.15332500	-3.83930900	L
H	-1	1.69814400	-6.45392300	3.14828100	L	H	-1	-9.93660500	5.47018700	-5.57054900	L
H	-1	3.50889800	-7.86953800	1.31569100	L	H	-1	-8.75583400	6.58822900	-5.45754000	L
H	-1	3.90019100	-7.13871300	2.73653900	L	H	-1	-8.09007400	0.12118500	3.26771900	L
H	-1	1.73972500	-4.98817300	-3.00124700	L	H	-1	-9.11577800	1.56431300	3.34581800	L
H	-1	2.64126600	-4.05614000	-4.20516100	L	H	-1	-9.84771200	0.80055800	-0.08568200	L
H	-1	1.23428000	-4.69711300	-6.75543100	L	H	-1	-8.03188900	1.52803200	-1.71491800	L
H	-1	-0.33769000	-4.01001600	-2.81270500	L	H	-1	-6.04245600	1.84434900	3.20093500	L
H	-1	-0.87836100	-3.90369900	-7.73643200	L	H	-1	-3.96951600	2.96610500	2.31787200	L
H	-1	-2.43382400	-3.20077900	-3.76822200	L	H	-1	-5.60625600	2.96735300	-1.67810800	L
H	-1	-2.93007800	-3.09263300	-7.26501700	L	H	-1	-3.74338200	3.46903500	-0.09297600	L
H	-1	3.07280200	-5.93745500	-5.62220300	L	H	-1	-9.90289200	-0.92928400	1.68726400	L
H	-1	1.96278200	-8.02807400	-5.23682600	L	H	-1	-12.08362100	-0.06950000	2.16479100	L
H	-1	0.96839500	-7.34276300	-4.13524600	L	H	-1	-11.45358200	1.26496300	2.86024300	L
H	-1	5.66310800	-4.66828900	-0.30019400	L	H	-1	-6.27909400	-3.88406200	-1.56631600	L
H	-1	7.38166600	-4.24421300	-0.32151800	L	H	-1	-5.02360600	-4.02326900	-0.30868100	L
H	-1	8.45892400	-5.00001500	-2.82294600	L	H	0	-5.66645200	-1.70005900	-1.40627400	H
H	-1	4.50217800	-3.49231600	-2.00011200	L	H	0	-7.06500800	-1.71190500	-0.30596600	H
H	-1	8.28315500	-4.22353000	-5.14801000	L	H	-1	-6.66305600	-4.29924800	1.47352100	L
H	-1	4.32512900	-2.70984500	-4.34573600	L	H	-1	-6.54785000	-5.98828700	-0.66815100	L
H	-1	7.10225300	-3.13054600	-6.53920600	L	H	-1	-8.12511700	-5.90939500	-0.28561100	L
H	-1	8.02172100	-6.49949600	-1.17184900	L	H	-1	-8.54975400	-2.94565300	-6.34246500	L
H	-1	6.12981000	-6.78143300	-2.57930500	L	H	-1	-7.99982800	-2.88573400	-4.66342100	L
H	-1	5.12934700	-7.02118400	-1.30862200	L	H	-1	-6.22750400	-3.82013500	-7.01248900	L
H	-1	3.46762300	-2.93124100	3.17773900	L	H	-1	-5.69004800	-3.54798800	-5.35723200	L

H	0	-6.83047400	-1.42620200	-7.31483900	H	0	2.00586800	1.47883800	1.71067800	H
H	0	-5.11613700	-1.69180500	-7.01170500	H	0	1.22360800	1.26183300	3.19207700	H
H	0	-7.09136200	-0.56537400	-5.11072800	H					
H	0	-3.67258900	-1.67050800	-5.28407300	H					
H	0	-3.17424900	-0.42442800	-4.17103700	H					
H	0	-6.32971200	1.07552200	-3.81734200	H					
H	0	-4.76946100	0.78253800	-2.95497000	H					
H	-1	-7.97586700	-5.43098300	-6.43771800	L					
H	-1	-10.15189900	-4.71757200	-5.84891600	L					
H	-1	-9.78851700	-4.65762300	-4.25866400	L					
H	-1	-5.03689400	-7.53052500	0.46267200	L					
H	-1	-5.37832400	-7.02184000	2.12312500	L					
H	-1	-2.91280300	-6.68744300	-0.70099000	L					
H	-1	-4.26889900	-4.63543800	3.00254900	L					
H	-1	-1.52641500	-4.68907200	-1.07614200	L					
H	-1	-2.98041000	-3.04703400	2.65244900	L					
H	-1	-0.92148200	-2.72300900	-0.25645400	L					
H	-1	-2.69202700	-8.39983600	1.44218000	L					
H	-1	-4.50906200	-9.70399000	0.61892000	L					
H	-1	-5.17963400	-9.80304800	2.10011500	L					
H	-1	-5.31626500	-3.33417200	4.97728400	L					
H	-1	-3.67397300	-3.26131400	4.33560400	L					
H	-1	-4.48127600	-1.88698800	6.97617300	L					
H	-1	-2.95860800	-1.70003100	6.10844400	L					
H	0	-5.74335700	-0.91525400	5.00233800	H					
H	0	-4.60499800	0.21506200	5.75252400	H					
H	0	-4.49816700	-1.06798500	3.06982600	H					
H	0	-3.26859600	-0.05523500	1.54278700	H					
H	0	-1.83635800	0.86114100	1.97420200	H					
H	0	-2.47412600	0.74762100	5.47742700	H					
H	0	-1.73636500	1.70909000	4.20975300	H					
H	-1	-3.07719900	-3.92261600	6.88616100	L					
H	-1	-3.54486300	-5.42100300	4.54119900	L					
H	-1	-2.12100700	-4.79572300	5.68961100	L					
H	0	-0.05902500	-1.58235100	-3.24651400	H					
H	0	0.35630300	0.89352700	-4.54364100	H					
H	0	1.76678100	0.73359900	-2.66726500	H					
H	0	1.91540800	-1.99410300	-1.95021900	H					
H	0	-1.65894800	-0.41240500	-0.91312800	H					
H	0	0.17673100	2.00375000	-1.31744300	H					
H	0	-0.76163600	2.38570700	0.57602500	H					
H	0	0.47348500	-0.90426800	-0.44728200	H					
H	0	2.47074900	-0.56345000	0.12106900	H					
H	0	-2.45720400	2.12113700	-2.35584800	H					
H	0	-2.75004700	1.93682700	-0.60311900	H					
H	0	-4.00769000	0.05792700	-1.04889500	H					
O	-1	7.54276100	11.13853400	3.74517600	L					
H	-1	8.49040900	0.91020900	-6.10057500	L					
H	-1	7.77056800	-6.96997600	1.23427300	L					
H	-1	1.11088000	-8.16183500	0.55027500	L					
H	-1	-2.53763600	-7.77506100	3.80726900	L					
H	-1	-10.32645500	-2.09566500	3.79752500	L					
H	-1	-10.17216300	6.96208000	-3.24980600	L					
H	-1	5.52774300	11.32182300	3.44316200	L					
H	-1	-1.98872800	6.76682900	-4.87450500	L					
H	-1	5.61450100	-0.75521500	5.40175700	L					
H	-1	4.33469500	-7.41413600	-4.02641100	L					
H	-1	-6.50798200	-6.24617000	-4.66254800	L					
H	-1	1.63226700	-1.90880500	7.44300800	L					
H	-1	-5.80057500	-5.51157800	6.72265400	L					
H	-1	-8.97162700	-3.60662200	-0.60415900	L					
N	-1	9.98181400	2.26530700	2.48403900	L					
C	-1	8.62330800	1.73898600	2.21230900	H					
C	0	8.27373700	1.88866100	0.71644800	H					
C	0	6.95402700	1.29250300	0.30162300	H					
N	0	6.84474600	-0.04207000	-0.05829700	H					
C	0	5.58715700	-0.22231300	-0.43291700	H					
N	0	4.88455700	0.93138100	-0.33379300	H					
C	0	5.73456900	1.90390800	0.13459200	H					
C	-1	8.56267900	0.24868200	2.64899400	L					
O	-1	7.55557900	-0.18153800	3.20982800	L					
N	-1	9.58910300	-0.51870200	2.29275600	L					
C	-1	9.60665300	-1.95138000	2.50325600	L					
C	0	8.82681000	-2.73326100	1.42230300	H					
C	0	9.45201800	-2.55427600	0.02345800	H					
O	0	10.31253300	-3.30715200	-0.38491200	H					
O	0	9.02881200	-1.51184300	-0.68711300	H					
C	-1	11.00848500	-2.50790300	2.62861800	L					
O	-1	12.00003200	-1.77080900	2.38966900	L					
H	0	9.06477600	1.42738100	0.08978900	H					
H	0	8.26215100	2.96643100	0.45984300	H					
H	0	5.39122000	2.91378600	0.32296300	H					
H	0	3.88318700	1.00857000	-0.51752000	H					
H	0	5.13672800	-1.14883100	-0.76500600	H					
H	-1	7.86130100	2.29451000	2.81687900	L					
H	-1	10.43784700	2.56587700	1.64746000	L					
H	-1	9.92476400	3.02944800	3.12145800	L					
H	0	8.86303700	-3.81321400	1.65273700	H					
H	0	7.76196100	-2.41975000	1.42197100	H					
H	-1	9.06502800	-2.18258000	3.46141900	L					
H	-1	10.26128400	-0.16758700	1.64052300	L					
H	-1	11.13136100	-3.56215200	2.90437000	L					
H	0	8.19607000	-1.04890300	-0.33406400	H					
N	0	1.78352100	1.89910700	2.62355900	H					
Glc_H507A										
ONIOM: extrapolated energy = -3126.956553393176 au										
N	-1	3.34360300	-7.56049700	2.21540100	L					
C	-1	2.16469800	-6.72951100	2.11304900	L					
C	-1	2.50267500	-5.47970400	1.25631800	L					
C	0	1.40473500	-4.45063000	1.08026000	H					
C	0	1.74635500	-3.44953900	-0.08571600	H					
O	0	2.91393500	-2.97715300	-0.10510700	H					
O	0	0.79437700	-3.17446800	-0.87925700	H					
C	-1	1.04408900	-7.51075400	1.41507700	L					
O	-1	-0.13803600	-7.42908900	1.83873300	L					
N	-1	1.70439500	-7.14058400	-4.94982100	L					
C	-1	2.70349400	-6.12791200	-4.67390700	L					
C	-1	2.05937900	-4.84841900	-4.10176900	L					
C	-1	0.74516200	-4.40735800	-4.72548500	L					
C	-1	0.57480500	-4.35151400	-6.10003000	L					
C	-1	-0.62249500	-3.91133100	-6.65597100	L					
C	-1	-1.64667200	-3.48703100	-5.82719600	L					
O	-1	-2.84340600	-3.04680200	-6.33213700	L					
C	-1	-1.49287100	-3.52682600	-4.45418800	L					
C	-1	-0.30121000	-3.97535100	-3.91665000	L					
C	-1	3.66545900	-6.74718100	-3.67232100	L					
O	-1	3.47284300	-6.59509700	-2.43808400	L					
N	-1	6.23617400	-7.04622900	-1.63683600	L					
C	-1	7.13764200	-6.26019600	-0.80198700	L					
C	-1	6.75915100	-4.78343000	-0.84973600	L					
C	-1	6.63222000	-4.25821100	-2.25606900	L					
C	-1	7.67739500	-4.45388200	-3.16537800	L					
C	-1	7.57882100	-4.01579300	-4.46541800	L					
C	-1	6.42691900	-3.38692400	-4.86882300	L					
O	-1	6.37881500	-2.95078500	-6.16618300	L					
C	-1	5.37038300	-3.17891300	-4.00975300	L					
C	-1	5.47420600	-3.61688200	-2.69388700	L					
C	-1	7.01992300	-6.71892000	0.64711000	L					
O	-1	5.88489400	-6.86821200	1.16959600	L					
N	-1	5.89584600	-3.75235800	4.30752700	L					
C	-1	5.59645000	-2.40114000	3.88721500	L					
C	-1	4.54236500	-2.40284900	2.80571700	L					
O	-1	5.03262700	-3.18125100	1.70504100	L					
C	-1	4.22644200	-0.98701400	2.33882600	L					
C	-1	5.12378000	-1.56146100	5.08672600	L					
O	-1	4.06502800	-1.87024800	5.69275000	L					
N	-1	3.99787200	1.53069500	5.73782400	L					
C	-1	2.76197100	2.35052200	5.80379600	L					
C	0	2.58082800	3.32903600	4.64111500	H					
C	0	2.83032400	2.26316500	3.27074000	H					
O	0	3.98062500	2.20257900	3.08844900	H					
O	0	1.83499400	2.55733200	2.46439700	H					

C	-1	-2.87793800	6.35568700	-0.48463800	L H 88	O	0	2.35098500	1.34743800	-0.11049900	H
C	-1	-4.00436900	7.32035900	-0.10971600	L	C	0	-2.33226400	1.07313300	-1.61340800	H
C	-1	-4.76940800	6.88170700	1.14579000	L	O	0	-3.39045100	0.15577000	-2.00395500	H
C	-1	-4.33707600	7.24949800	2.41210600	L	H	-1	2.85473900	-5.82117600	0.25674100	L
C	-1	-5.02281100	6.85256500	3.55722400	L	H	-1	3.38083100	-4.97891600	1.72195700	L
C	-1	-6.15655300	6.06966600	3.42874000	L	H	0	0.42090500	-4.91688200	0.86525500	H
O	-1	-6.84940000	5.67603600	4.56911100	L	H	0	1.27905600	-3.82824300	2.00199600	H
C	-1	-6.61064200	5.70401900	2.18301600	L	H	-1	1.84996500	-6.42180400	3.13996100	L
C	-1	-5.90452500	6.10305600	1.04590800	L	H	-1	3.67329300	-7.82418700	1.30966300	L
C	-1	-2.11763000	6.80221900	-1.73228200	L	H	-1	4.05729000	-7.09140600	2.73149400	L
O	-1	-2.17561500	7.97724000	-2.13574500	L	H	-1	1.89160900	-4.95282800	-3.00879700	L
N	-1	-1.41768900	5.84749800	-2.34492000	L	H	-1	2.78875400	-4.01410300	-4.21079400	L
C	-1	-0.35598200	6.13403200	-3.34401600	L H 102	H	-1	1.39032000	-4.66339200	-6.76366300	L
C	0	0.56059900	4.90390600	-3.45107400	H	H	-1	-0.19273700	-3.98888400	-2.82318900	L
C	0	-0.07361500	3.59153100	-4.04387700	H	H	-1	-0.72606500	-3.88388700	-7.74773900	L
O	0	-1.32709400	3.47668300	-4.11548600	H	H	-1	-2.29274200	-3.19348200	-3.78174400	L
O	0	0.78407900	2.72020700	-4.36944100	H	H	-1	-2.78401500	-3.08701700	-7.27929400	L
C	-1	-0.84836400	6.57445300	-4.71132700	L	H	-1	3.23538400	-5.89175300	-5.62802000	L
O	-1	-0.01084200	6.71254400	-5.64033300	L	H	-1	2.13897900	-7.99005800	-5.24544600	L
N	-1	-8.90215200	5.59047300	-5.32961700	L	H	-1	1.13815900	-7.31205800	-4.14516900	L
C	-1	-8.70694200	5.22406000	-3.91551500	L	H	-1	5.80831600	-4.60758200	-0.30118500	L
C	-1	-7.29005800	5.54878300	-3.47154100	L	H	-1	7.52398200	-4.17182100	-0.31950100	L
C	-1	-6.25684500	4.60768800	-4.08393900	L	H	-1	8.61043400	-4.91906800	-2.81952200	L
C	-1	-4.84790800	4.91230800	-3.66015800	L	H	-1	4.64220300	-3.43871000	-2.00245500	L
O	-1	-4.53601300	6.02500200	-3.21567700	L	H	-1	8.43318000	-4.14267000	-5.14450200	L
N	-1	-3.96605900	3.91835600	-3.79586600	L	H	-1	4.46364900	-2.65632200	-4.34798000	L
C	-1	-9.73969200	5.91019000	-3.01608000	L	H	-1	7.24714300	-3.05706700	-6.53710900	L
O	-1	-10.16480300	5.32506400	-1.98628500	L	H	-1	8.18074600	-6.42228700	-1.16985100	L
N	-1	-11.18402100	0.48143300	2.16799600	L	H	-1	6.29309300	-6.71640000	-2.58053000	L
C	-1	-9.98469200	-0.27001700	2.50738000	L	H	-1	5.29221300	-6.96356300	-1.31159700	L
C	-1	-8.76953400	0.64253800	2.69551500	L	H	-1	3.59540100	-2.88718700	3.17397700	L
C	-1	-8.16179100	1.12950600	1.40335400	L	H	-1	3.48849800	-0.97035600	1.52289900	L
C	-1	-8.73832400	1.10532100	0.15553800	L	H	-1	5.13257800	-0.46679200	1.99956500	L
N	-1	-7.88205800	1.67614300	-0.76429000	L	H	-1	3.80847300	-0.38259400	3.16006000	L
C	-1	-6.74465900	2.09423300	-0.12329400	L	H	-1	4.31733700	-3.21021300	1.07501300	L
C	-1	-6.88033500	1.75811000	1.24166400	L	H	-1	6.53171000	-1.90346600	3.49153900	L
C	-1	-5.84356700	2.06591300	2.12051700	L	H	-1	5.24875900	-4.42137300	3.94279200	L
C	-1	-4.70071300	2.66506700	1.63159000	L	H	-1	6.81784900	-3.99463500	4.01150800	L
C	-1	-4.57496900	2.97252400	0.24724000	L	H	0	1.57927300	3.79514900	4.69682900	H
C	-1	-5.59633500	2.70149200	-0.62952200	L	H	0	3.32826600	4.14241800	4.72793600	H
C	-1	-10.30258100	-1.05177100	3.76663200	L	H	-1	2.78444200	2.96883100	6.73597800	L
O	-1	-10.68298800	-0.44777600	4.80299700	L	H	-1	4.37542600	1.56885700	4.79518900	L
N	-1	-7.04704300	-5.75379700	0.02253800	L	H	-1	4.66640700	1.89409400	6.38159400	L
C	-1	-6.90449800	-4.34540800	0.39929800	L	H	-1	1.84593400	-2.39791800	4.59251700	L
C	-1	-5.90325000	-3.64694500	-0.53215900	L H 134	H	-1	-0.10834300	-3.81043800	3.91346600	L
C	0	-5.92642000	-2.12945400	-0.46662800	H	H	-1	-1.22653100	-2.70056900	4.72188300	L
C	0	-5.04849600	-1.56009700	0.67137600	H	H	-1	-0.04854500	-3.62775000	5.67174200	L
O	0	-5.35212500	-1.84012400	1.85028600	H	H	-1	0.73448900	-2.07304800	2.39549700	L
O	0	-4.08330300	-0.81968400	0.29806900	H	H	-1	-0.40609200	-0.89571200	3.07785000	L
C	-1	-8.26143300	-3.61797500	0.30998100	L	H	-1	1.32187900	-0.50261800	2.96640800	L
O	-1	-8.70820400	-2.99489800	1.30785800	L	H	-1	-0.34243100	-0.42428200	5.58257700	L
N	-1	-9.41302100	-5.13374100	-5.15652900	L	H	-1	2.45823600	-0.07415900	4.92700100	L
C	-1	-8.00682000	-4.92381600	-5.49921900	L	H	0	7.18345200	-0.85491800	-2.72712000	H
C	-1	-7.69551400	-3.44363400	-5.64916600	L	H	0	8.20648400	0.54081100	-2.42815100	H
C	-1	-6.27137800	-3.20980500	-6.13755900	L H 144	H	0	5.02072600	-0.61648700	-3.84003000	H
C	0	-5.97373700	-1.76513000	-6.53702600	H	H	0	7.67689200	2.75779000	-3.67368800	H
N	0	-6.05989100	-0.78741500	-5.45461200	H	H	0	3.20607400	0.82709000	-4.58630500	H
C	0	-5.09948000	-0.50908800	-4.51993200	H	H	0	5.81193300	4.23830700	-4.38359200	H
N	0	-3.88193200	-1.03345400	-4.55931700	H	H	0	2.49678300	3.12011500	-4.74314400	H
N	0	-5.41977300	0.34108700	-3.54111800	H	H	-1	8.04635300	-1.13856900	-5.03360100	L
C	-1	-7.11966900	-5.54347600	-4.40103700	L	H	-1	10.41898300	-1.29648200	-4.45748200	L
O	-1	-7.29023100	-5.21947700	-3.19708300	L	H	-1	10.03857300	-0.85824100	-2.92578700	L
N	-1	-4.14600600	-9.69242900	1.58113700	L	H	-1	7.16513200	8.24186400	2.22817900	L
C	-1	-3.52105200	-8.41667500	1.93474400	L	H	-1	5.50646200	8.67592200	2.66143600	L
C	-1	-4.39105400	-7.25869500	1.40231400	L	H	-1	6.52202200	9.64462600	-0.94789500	L
C	-1	-3.58474400	-6.00130700	1.15298800	L	H	-1	5.53295000	7.98589300	-2.56605500	L
C	-1	-2.77259800	-5.86879700	0.01476700	L	H	-1	4.66604100	6.16030100	2.39628000	L
C	-1	-1.99510000	-4.75382200	-0.17925700	L	H	-1	3.33785600	4.26484700	1.46519100	L
C	-1	-2.01326000	-3.74657000	0.75234500	L	H	-1	3.86673300	5.68980000	-2.55751800	L
O	-1	-1.24468100	-2.63946800	0.57345100	L	H	-1	2.96641700	4.03065600	-0.95188100	L
C	-1	-2.79935900	-3.85396700	1.88721100	L	H	-1	5.83804600	10.77817800	1.07206600	L
C	-1	-3.59154100	-4.97376200	2.06076300	L	H	-1	8.62792700	10.03631900	1.57441600	L
C	-1	-3.27917900	-8.29264000	3.44313000	L	H	-1	8.10636800	11.48416200	1.03863700	L
O	-1	-4.11395900	-8.76887000	4.25548200	L	H	0	-0.17865900	4.69759800	4.22402500	H
N	-1	-3.08627100	-5.46726200	5.47511000	L	H	0	-2.52639700	4.10853900	4.63810500	H
C	-1	-3.74158200	-4.39933100	6.21405200	L	H	0	-2.91004700	4.22870400	2.91130200	H
C	-1	-4.13111700	-3.23400800	5.28028700	L	H	0	-2.49589100	5.69752000	3.84206300	H
C	-1	-3.92999700	-1.89045300	5.93867900	L H 167	H	0	0.32029600	2.79065200	2.93016000	H
C	0	-4.49451200	-0.72097200	5.13490000	H	H	0	0.68554300	4.76471300	1.88402500	H
N	0	-3.86190000	-0.56458900	3.83043800	H	H	0	0.51004700	7.15186300	1.96340200	H
C	0	-2.86009300	0.27708500	3.51994400	H	H	0	-0.75969500	7.07281900	3.02858300	H
N	0	-2.20155000	0.97360800	4.48510900	H	H	-1	-4.70951800	7.38850000	-0.96278100	L
N	0	-2.58154100	0.48405800	2.24055300	H	H	-1	-3.61831800	8.34966700	0.03988100	L
C	-1	-4.93184700	-4.80873800	7.08982400	L	H	-1	-3.42014500	7.84864000	2.51359300	L
O	-1	-5.05871700	-4.32595300	8.24494800	L	H	-1	-6.26291400	5.78607700	0.05677900	L
C	0	0.71396900	-0.51761400	-2.97197300	H	H	-1	-4.65783100	7.14966300	4.54730600	L
O	0	0.94612700	-0.21882700	-4.32311200	H	H	-1	-7.50708100	5.08234900	2.05748000	L
C	0	1.81946700	0.07843900	-2.04698900	H	H	-1	-7.59066700	5.15954200	4.27902300	L
O	0	2.93402400	-0.78409000	-2.06311700	H	H	-1	-3.31278000	5.31825500	-0.59465600	L
O	0	-0.62778500	-0.03268100	-2.73437300	H	H	0	-1.65022600	7.14153900	1.13889100	H
C	0	-1.02582900	0.32335300	-1.42485500	H	H	0	1.45911400	5.14491700	-4.05365400	H
C	0	0.01454200	1.18389300	-0.70099200	H	H	0	0.96746400	4.63215100	-2.45271700	H
O	0	-0.45381800	1.46565600	0.62961000	H	H	-1	0.22670900	7.00402900	-2.94185900	L
C	0	1.36869200	0.47850200	-0.63113100	H	H	-1	-1.89130200	4.96654400	-2.48022100	L

H	-1	-7.22689800	5.48442500	-2.36359400	L	C	0	8.33220900	1.87556500	0.73614800	H
H	-1	-7.02753500	6.60108500	-3.71261200	L	C	-1	8.66956900	0.32756200	2.65506400	L
H	-1	-6.53208100	3.55997200	-3.82765700	L	O	-1	7.66450500	-0.10976800	3.21404900	L
H	-1	-6.31332300	4.66744400	-5.19112400	L	N	-1	9.70176700	-0.43265200	2.30014200	L
H	-1	-4.22584800	3.14921800	-4.36735100	L	C	-1	9.72271800	-1.86531600	2.50997900	L H 376
H	-1	-2.95450700	4.02845800	-3.66160000	L	C	0	9.03482200	-2.64304400	1.37028200	H
H	-1	-8.86360300	4.11614500	-3.86000700	L	C	0	9.81070300	-2.53305100	-0.02725500	H
H	-1	-9.85136600	5.42714000	-5.59222500	L	O	0	10.21392600	-3.62863500	-0.48281800	H
H	-1	-8.67841100	6.55313000	-5.47675700	L	O	0	9.91173500	-1.37242300	-0.49998300	H
H	-1	-7.98291800	0.08653700	3.24651600	L	C	-1	11.13409500	-2.41231900	2.63738300	L
H	-1	-9.01853900	1.52261900	3.32362300	L	O	-1	12.12099500	-1.66838400	2.40040000	L
H	-1	-9.73966400	0.75556700	-0.10943100	L	H	0	8.87476600	1.10919200	0.14651500	H
H	-1	-7.92617600	1.49616000	-1.73535200	L	H	0	8.52229300	2.87514700	0.29521500	H
H	-1	-5.94696000	1.82361600	3.18389400	L	H	-1	7.95402200	2.36849200	2.82277100	L
H	-1	-3.88025600	2.95986700	2.30474800	L	H	-1	10.53056700	2.65793900	1.65769300	L
H	-1	-5.51045000	2.95192400	-1.69389700	L	H	-1	10.01194000	3.11729600	3.13106900	L
H	-1	-3.65361700	3.46549300	-0.10548700	L	H	0	8.94924400	-3.71469600	1.64474100	H
H	-1	-9.78597100	-0.97546800	1.66260400	L	H	0	8.00369500	-2.25331600	1.23398300	H
H	-1	-11.97327200	-0.13076300	2.13697400	L	H	-1	9.18711600	-2.10062300	3.46715900	L
H	-1	-11.35345700	1.20761600	2.83408700	L	H	-1	10.37260800	-0.07665900	1.64917300	L
H	-1	-6.13686400	-3.90396200	-1.58644800	L	H	-1	11.26368700	-3.46584100	2.91283300	L
H	-1	-4.88250900	-4.03523800	-0.32683000	L	H	0	7.25264500	1.66947400	0.61932500	H
H	0	-5.56904600	-1.71320200	-1.42366400	H	G1c_H507Q					
H	0	-6.95614600	-1.74684600	-0.31276100	H	ONIOM: extrapolated energy = -3334.984063883607 au					
H	-1	-6.52294900	-4.32322200	1.45256100	L	N	-1	3.01842500	-7.68957100	2.21919200	L
H	-1	-6.39276700	-6.01040000	-0.68972000	L	C	-1	1.86134000	-6.82885300	2.11368900	L
H	-1	-7.97115600	-5.94242000	-0.30971900	L	C	-1	2.23560700	-5.58416000	1.26470700	L H 4
H	-1	-8.40605900	-2.97870000	-6.36585700	L	C	0	1.16591200	-4.52608300	1.08786700	H
H	-1	-7.85929200	-2.91585700	-4.68588800	L	C	0	1.53965300	-3.52320200	-0.06542300	H
H	-1	-6.07682400	-3.83704700	-7.03249800	L	O	0	2.71650800	-3.07203500	-0.07145900	H
H	-1	-5.54393400	-3.56205300	-5.37623600	L	O	0	0.60208400	-3.22079100	-0.86557900	H
H	0	-6.67703300	-1.43072400	-7.32142200	H	C	-1	0.72570100	-7.57866700	1.40563200	L
H	0	-4.96774500	-1.68080700	-6.98630700	H	O	-1	-0.45651700	-7.46924800	1.82271100	L
H	0	-6.99612800	-0.59744300	-5.12353700	H	N	-1	1.43310500	-7.19721200	-4.95353900	L
H	0	-3.59226300	-1.78225300	-5.19766300	H	C	-1	2.45559000	-6.21113200	-4.66717400	L
H	0	-3.21035700	-0.73515100	-3.83172800	H	C	-1	1.84031800	-4.91841700	-4.09301900	L
H	0	-6.20185100	0.96950600	-3.66320000	H	C	-1	0.54131100	-4.44180900	-4.72242200	L
H	0	-4.66873200	0.51158600	-2.79103500	H	C	-1	0.38062600	-4.37566900	-6.09767500	L
H	-1	-7.81513000	-5.46002400	-6.46134700	L	C	-1	-0.80192900	-3.90316500	-6.65862300	L
H	-1	-9.99692000	-4.76171200	-5.87576400	L	C	-1	-1.82009200	-3.45696400	-5.83395200	L
H	-1	-9.63654800	-4.70006300	-4.28489300	L	O	-1	-3.00238400	-2.98464800	-6.34389400	L
H	-1	-4.87320400	-7.54287600	0.44284100	L	C	-1	-1.67554400	-3.50663000	-4.46026000	L
H	-1	-5.22079300	-7.03732900	2.10297500	L	C	-1	-0.49872800	-3.98724000	-3.91778400	L
H	-1	-2.75300000	-6.68480700	-0.71695000	L	C	-1	3.39573800	-6.85872200	-3.66278500	L
H	-1	-4.12905700	-4.64386400	2.98534000	L	O	-1	3.19961800	-6.70728000	-2.42902200	L
H	-1	-1.37962400	-4.67687400	-1.08888900	L	N	-1	5.94594300	-7.23107500	-1.61363700	L
H	-1	-2.85083100	-3.04656700	2.63809700	L	C	-1	6.86181100	-6.47156900	-0.76995400	L
H	-1	-0.78941100	-2.70714400	-0.26728400	L	C	-1	6.52072100	-4.98558100	-0.81321500	L
H	-1	-2.52408000	-8.39669700	1.42576800	L	C	-1	6.41539400	-4.45117100	-2.21786800	L
H	-1	-4.33086000	-9.71277700	0.59892300	L	C	-1	7.46075600	-4.66899100	-3.12191100	L
H	-1	-5.00315700	-9.81711000	2.07897300	L	C	-1	7.38095800	-4.22286100	-4.42050400	L
H	-1	-5.18846700	-3.35070700	4.95897600	L	C	-1	6.24760100	-3.56354000	-4.82779700	L
H	-1	-3.54566400	-3.26637300	4.32001500	L	O	-1	6.21819300	-3.12063700	-6.12342300	L
H	-1	-4.36660100	-1.89884900	6.95991100	L	C	-1	5.19149100	-3.33288000	-3.97400400	L
H	-1	-2.84382600	-1.70112100	6.09476200	L	C	-1	5.27644500	-3.77909000	-2.65955400	L
H	0	-5.57544800	-0.86734300	4.94905900	H	C	-1	6.72398000	-6.93355800	0.67632900	L
H	0	-4.37969900	0.22253300	5.70156800	H	O	-1	5.58246400	-7.05663600	1.19146500	L
H	0	-4.31321200	-1.07544700	3.04471000	H	N	-1	5.65270300	-3.95585200	4.34352500	L
H	0	-3.14902800	0.00497100	1.52052400	H	C	-1	5.38976400	-2.59571900	3.92760600	L
H	0	-1.68965500	0.87704300	1.91624700	H	C	-1	4.34245500	-2.56623300	2.83994200	L
H	0	-1.91836100	0.47034400	5.32327700	H	O	-1	4.81945000	-3.35190500	1.73884500	L
H	0	-1.52294700	1.66812400	4.13795800	H	C	-1	4.06488700	-1.14089600	2.37764700	L
H	-1	-2.94856800	-3.92483700	6.87123100	L	C	-1	4.93111400	-1.74972900	5.12812500	L
H	-1	-3.40220700	-5.42523300	4.52479900	L	O	-1	3.86135700	-2.03453100	5.72652000	L
H	-1	-1.98451000	-4.79084300	5.67583200	L	N	-1	3.87914100	1.36679600	5.78664400	L
H	0	0.72735700	-1.60661600	-2.85738000	H	C	-1	2.66378600	2.21706100	5.84909300	L H 43
H	0	0.79586500	0.75342600	-4.40762700	H	C	0	2.51934500	3.19880800	4.68310400	H
H	0	2.14640800	1.01444900	-2.51541000	H	C	0	2.77255800	2.50202200	3.31290300	H
H	0	2.82267300	-1.50993400	-1.40103400	H	O	0	3.91987800	2.05863000	3.13519900	H
H	0	-1.20321700	-0.57628100	-0.81033600	H	O	0	1.78259600	2.44008300	2.49960700	H
H	0	0.14773100	2.12767000	-1.24366300	H	C	-1	1.40916400	1.31484200	5.95289900	L
H	0	-0.61154000	2.42587200	0.70376600	H	O	-1	0.36190200	1.80281300	6.40722300	L
H	0	1.25280600	-0.42613000	-0.00966900	H	N	-1	1.54285000	0.04831600	5.56328400	L
H	0	2.13954900	1.58843000	0.81924600	H	C	-1	0.49443600	-0.97529800	5.69456200	L
H	0	-2.21399600	1.80043800	-2.42197900	H	C	-1	0.61745100	-2.03611900	4.56785000	L
H	0	-2.62974200	1.58467300	-0.69054100	H	C	-1	-0.41756100	-3.13005000	4.73308000	L
H	0	-3.66768900	-0.33806200	-1.16522800	H	C	-1	0.43110800	-1.37451100	3.20216200	L
O	-1	7.57383500	11.20969500	3.75473200	L	C	-1	0.55486400	-1.70168300	7.04857700	L
H	-1	8.60707100	0.99282100	-6.09429700	L	O	-1	-0.50730700	-1.95995600	7.67200100	L
H	-1	7.92887500	-6.89562900	1.23563400	L	N	-1	9.55306100	-1.49947000	-3.71167200	L
H	-1	1.27857000	-8.13241200	0.54019100	L	C	-1	8.47952300	-0.69372200	-4.25845500	L H 58
H	-1	-2.37779900	-7.77203200	3.79140100	L	C	0	7.48437200	-0.16207100	-3.21434900	H
H	-1	-10.20503300	-2.14572500	3.77161800	L	C	0	6.38050700	0.69409800	-3.84961700	H
H	-1	-10.10084800	6.91627300	-3.27116300	L	C	0	5.09148200	0.19155000	-4.06108100	H
H	-1	5.55811100	11.37942400	3.44951200	L	C	0	4.05038100	0.99240200	-4.54040700	H
H	-1	-1.91363600	6.77745600	-4.88258100	L	C	0	4.27362700	2.34869900	-4.81320600	H
H	-1	5.72380200	-0.69769200	5.40253000	L	O	0	3.29424900	3.20141400	-5.24338300	H
H	-1	4.50468500	-7.36059300	-4.03086600	L	C	0	5.56792200	2.86197000	-4.64158200	H
H	-1	-6.34463200	-6.26607100	-4.68416700	L	C	0	6.59233000	2.04847600	-4.16125800	H
H	-1	1.74618000	-1.87932000	7.43672600	L	C	-1	9.00140300	0.50913900	-5.05674400	L
H	-1	-5.66080500	-5.53220200	6.70252200	L	O	-1	9.93719100	1.21250900	-4.59506300	L
H	-1	-8.83278500	-3.64530200	-0.62856100	L	N	-1	8.03418100	10.26325200	1.18855900	L
N	-1	10.07522500	2.35386900	2.49338300	L	C	-1	6.72885400	10.08766800	1.84126500	L
C	-1	8.72077600	1.81845600	2.21918300	L H 371						

C	-1	6.36790700	8.61040700	1.97594200	L	C	-1	-4.00913000	-4.36933700	6.19053500	L
C	-1	5.86440800	8.04259400	0.69278800	L	C	-1	-4.36376400	-3.19052300	5.25980500	L
C	-1	6.07338100	8.55133600	-0.57884800	L	C	-1	-4.13299700	-1.85534000	5.92545800	L H 167
N	-1	5.44448600	7.78587100	-1.50771700	L	C	0	-4.66324200	-0.66838600	5.12408400	H
C	-1	4.82289700	6.73113100	-0.87489100	L	N	0	-4.01824800	-0.52104500	3.82422300	H
C	-1	5.07581500	6.85501500	0.51245600	L	C	0	-2.99375900	0.29607200	3.52460300	H
C	-1	4.51984700	5.90762800	1.39172300	L	N	0	-2.32308900	0.97078200	4.49675300	H
C	-1	3.76442400	4.88117700	0.85320500	L	N	0	-2.70080800	0.50247000	2.24779400	H
C	-1	3.55372700	4.76118000	-0.52364100	L	C	-1	-5.21448900	-4.75261300	7.05744300	L
C	-1	4.06455400	5.68375900	-1.40894700	L	O	-1	-5.33612800	-4.27187800	8.21398400	L
C	-1	6.66368700	10.81211700	3.18285100	L	C	0	0.61042400	-0.58718700	-2.91314300	H
N	0	0.09173600	6.52768200	2.71998400	H	O	0	0.84648000	-0.29409700	-4.26378600	H
C	0	-0.25601000	5.19549500	2.21530100	H	C	0	1.72487200	-0.00747800	-1.98820100	H
C	0	-0.82291300	4.34232600	3.40332400	H	O	0	2.83470800	-0.87556200	-1.98587800	H
O	0	-0.71269100	2.95988400	3.15576200	H	O	0	-0.71833000	-0.07159600	-2.67631200	H
C	0	-2.28626600	4.62597900	3.73448000	H	C	0	-1.11186300	0.31766300	-1.37577300	H
C	0	-1.19042900	5.12567100	0.99343500	H	C	0	-0.04804000	1.15087200	-0.64977100	H
O	0	-1.35951200	4.07188100	0.38015300	H	O	0	-0.51143300	1.44990200	0.67676800	H
N	0	-1.83282500	6.29124200	0.66787300	H	C	0	1.27546700	0.39237300	-0.57351900	H
C	-1	-2.83634200	6.38997100	-0.45405900	L H 88	O	0	2.29350900	1.21356700	-0.02695800	H
C	-1	-3.94047600	7.38092600	-0.08137400	L	C	0	-2.39277900	1.10698000	-1.58668000	H
C	-1	-4.72375200	6.95608300	1.16761800	L	O	0	-3.46940100	0.22068800	-1.99562100	H
C	-1	-4.28992000	7.30735100	2.43810500	L	H	-1	2.58499700	-5.92994300	0.26561600	L
C	-1	-4.99221500	6.92271100	3.57736700	L	H	-1	3.12326000	-5.10758600	1.73769000	L
C	-1	-6.14442200	6.16905800	3.43868200	L	H	0	0.17284700	-4.96537500	0.86014200	H
O	-1	-6.85371600	5.78791900	4.57317000	L	H	0	1.04773900	-3.90893300	2.01403800	H
C	-1	-6.60007400	5.82038800	2.18866800	L	H	-1	1.54828100	-6.51785600	3.14013900	L
C	-1	-5.87739900	6.20658600	1.05754500	L	H	-1	3.34681400	-7.95746200	1.31421600	L
C	-1	-2.05764200	6.82277300	-1.69518300	L	H	-1	3.74054000	-7.24079400	2.74158800	L
O	-1	-2.08376500	8.00063900	-2.09363900	L	H	-1	1.66345500	-5.02338600	-3.00153400	L
N	-1	-1.37818500	5.85350300	-2.30803400	L	H	-1	2.59100000	-4.10218100	-4.19397300	L
C	-1	-0.30368200	6.11770600	-3.29957500	L H 102	H	-1	1.19202500	-4.70498000	-6.75792300	L
C	0	0.58139400	4.86188700	-3.41350400	H	H	-1	-0.39715500	-4.00831900	-2.82377500	L
C	0	-0.08900300	3.55428900	-3.98123300	H	H	-1	-0.89825100	-3.86833600	-7.75084500	L
O	0	-1.34446000	3.47273000	-4.05378800	H	H	-1	-2.47081900	-3.15629400	-3.79101200	L
O	0	0.74131000	2.65019800	-4.28571700	H	H	-1	-2.93835800	-3.02218100	-7.29086300	L
C	-1	-0.77669600	6.57634100	-4.66773600	L	H	-1	2.99892100	-5.98419600	-5.61706800	L
O	-1	0.06956000	6.69746800	-5.59117700	L	H	-1	1.84803400	-8.05600900	-5.25046500	L
N	-1	-8.84876400	5.79734200	-5.33771400	L	H	-1	0.85795300	-7.35796700	-4.15300900	L
C	-1	-8.67125000	5.41994100	-3.92417000	L	H	-1	5.57132700	-4.78835700	-0.26945700	L
C	-1	-7.24935500	5.70708100	-3.47042300	L	H	-1	7.29745000	-4.39567600	-0.27573000	L
C	-1	-6.23639700	4.74307300	-4.08101900	L	H	-1	8.37976600	-5.15894100	-2.77270500	L
C	-1	-4.82283000	5.01040500	-3.64760300	L	H	-1	4.44499900	-3.58313600	-1.97215700	L
O	-1	-4.48582400	6.11296400	-3.19625000	L	H	-1	8.23591500	-4.36813600	-5.09513400	L
N	-1	-3.96536000	3.99524600	-3.78263400	L	H	-1	4.30017000	-2.78623400	-4.31516600	L
C	-1	-9.69184700	6.12779300	-3.02770100	L	H	-1	7.08578700	-3.27402800	-6.48972900	L
O	-1	-10.13762800	5.54899200	-2.00308500	L	H	-1	7.90270800	-6.65814600	-1.13242600	L
N	-1	-11.30266200	0.71423600	2.12310600	L	H	-1	6.01674500	-6.89863400	-2.55547300	L
C	-1	-10.12458200	-0.06853400	2.46610200	L	H	-1	5.00242200	-7.12619500	-1.29356800	L
C	-1	-8.88809400	0.81243000	2.66550400	L	H	-1	3.38146700	-3.02829900	3.20044400	L
C	-1	-8.26063200	1.28967700	1.37915400	L	H	-1	3.33248200	-1.10215500	1.55748900	L
C	-1	-8.83012100	1.28543800	0.12788100	L	H	-1	4.98578100	-0.64207300	2.04607200	L
N	-1	-7.95434300	1.83864600	-0.78430700	L	H	-1	3.65728800	-0.52979900	3.19915200	L
C	-1	-6.81068000	2.22526500	-0.13475900	L	H	-1	4.10786900	-3.36005100	1.10401700	L
C	-1	-6.96288900	1.88665600	1.22784000	L	H	-1	6.33954500	-2.11991900	3.53968600	L
C	-1	-5.92400700	2.16450100	2.11414700	L	H	-1	4.99125300	-4.60682300	3.97196700	L
C	-1	-4.76360300	2.73695400	1.63465800	L	H	-1	6.57010200	-4.21986900	4.05182200	L
C	-1	-4.62192500	3.04723900	0.25248000	L	H	0	1.52662000	3.68358200	4.72348500	H
C	-1	-5.64450000	2.80575700	-0.63147900	L	O	0	3.28099600	3.99723900	4.78106900	H
C	-1	-10.46947400	-0.84759500	3.71990500	L	H	-1	2.69617100	2.83050600	6.78418600	L
O	-1	-10.84082100	-0.23881100	4.75675400	L	H	-1	4.26316000	1.39962000	4.84642400	L
N	-1	-7.31041400	-5.61328000	-0.02634700	L	H	-1	4.55270800	1.71048500	6.43596900	L
C	-1	-7.13488900	-4.21057800	0.35763600	L	H	-1	1.63635700	-2.50155400	4.61090600	L
C	-1	-6.11091400	-3.5335400	-0.56475200	L H 134	H	-1	-0.34859400	-3.86163000	3.91399700	L
C	0	-6.09386400	-2.01589100	-0.49143500	H	H	-1	-1.44344300	-2.72763300	4.72087300	L
C	0	-5.20709300	-1.47426000	0.65354600	H	H	-1	-0.29474900	-2.68822500	5.67340500	L
O	0	-5.52397900	-1.75164300	1.82960700	H	H	-1	0.54655000	-2.13926800	2.40890300	L
O	0	-4.22134000	-0.75630000	0.28946100	H	H	-1	-0.56824100	-0.93671200	3.08989400	L
C	-1	-8.47262100	-3.44896300	0.26366600	L	H	-1	1.16966900	-0.58658400	2.99037600	L
O	-1	-8.90960100	-2.81926900	1.26171700	L	H	-1	-0.50776400	-0.47803400	5.59706800	L
N	-1	-9.62912000	-4.91134700	-5.21633100	L	H	-1	2.30466300	-0.19537000	4.95952600	L
C	-1	-8.21607900	-4.73524400	-5.54981100	L	H	0	7.03408800	-1.01649900	-2.67730500	L
C	-1	-7.86690500	-3.26268900	-5.69120700	L	H	0	8.01957800	0.43113000	-2.44848200	H
C	-1	-6.43446300	-3.06250000	-6.17017000	L H 144	H	0	4.85932700	-0.83999900	-3.79844600	H
C	0	-6.09653900	-1.62239100	-6.55412100	H	H	0	7.56317500	2.49655300	-3.95752200	H
N	0	-6.16015000	-0.65371200	-5.46110900	H	H	0	3.06100100	0.56151600	-4.65887000	H
C	0	-5.19461400	-0.40116000	-4.52512200	H	H	0	5.73896300	3.91964400	-4.83365400	H
N	0	-3.98986800	-0.95447700	-4.56401000	H	H	0	2.40357100	2.90352200	-4.92538900	H
N	0	-5.49420600	0.45419300	-3.54391600	H	H	-1	7.92380000	-1.35579700	-4.97286100	L
C	-1	-7.35130700	-5.38177300	-4.44927100	L	H	-1	10.28824500	-1.57568300	-4.38356000	L
O	-1	-7.52089400	-5.05889100	-3.24487790	L	H	-1	9.90978300	-1.13477300	-2.85214900	L
N	-1	-4.51831000	-9.63022600	1.53133700	L	H	-1	7.23443000	8.01179100	2.32615200	L
C	-1	-3.86372200	-8.37210900	1.89439300	L	H	-1	5.58459300	8.48539500	2.75164100	L
C	-1	-4.70124700	-7.19035000	1.36213400	L	H	-1	6.64565400	9.44417700	-0.84723600	L
C	-1	-3.86222000	-5.95249200	1.12325500	L	H	-1	5.62503400	7.81789100	-2.47868500	L
C	-1	-3.04022000	-5.83538900	-0.00957000	L	H	-1	4.68302100	5.99283000	2.47013800	L
C	-1	-2.23389300	-4.73941800	-0.19396400	L	H	-1	3.31338600	4.13536200	1.52266300	L
C	-1	-2.23239000	-3.73612800	0.74207700	L	H	-1	3.90180400	5.56428500	-2.49034800	L
O	-1	-1.43525400	-2.64786300	0.57272900	L	H	-1	2.95063100	3.92118400	-0.89756400	L
C	-1	-3.02769700	-3.82876700	1.87181600	L	H	-1	5.97822400	10.58563800	1.17380600	L
C	-1	-3.84870200	-4.92909800	2.03563200	L	H	-1	8.74559600	9.77185700	1.68913600	L
C	-1	-3.62783800	-8.26080500	3.40471900	L	H	-1	8.26367700	11.23466200	1.15688800	L
O	-1	-4.47912600	-8.71951900	4.20999100	L	H	0	-0.19898300	4.64394700	4.25873200	H
N	-1	-3.37636800	-5.45010700	5.45060700	L	H	0	-2.56107300	4.10836900	4.66029700	H

H	0	-2.93464700	4.24358000	2.93232700	H	0	-2.69110300	1.62810600	-0.66909400	H
H	0	-2.49009700	5.69876800	3.87012500	H	0	-3.77111100	-0.27198400	-1.16532900	H
H	0	0.25688900	2.72706900	2.95820900	H	0	7.70821100	10.96170600	3.86853800	L
H	0	0.67663500	4.70171000	1.92017800	H	-1	8.54406000	0.76550300	-6.02056000	L
H	0	0.56762900	7.08837100	2.01817700	H	-1	7.62468600	-7.13558600	1.26936600	L
H	0	-0.71557000	7.03907600	3.07039700	H	-1	0.94976400	-8.20216000	0.52932000	L
H	-1	-4.63858500	7.47047400	-0.93824200	L	H	-1	-2.71579900	-7.76449800	L
H	-1	-3.52966400	8.39956300	0.07515700	L	H	-1	-10.39939000	-1.94366200	L
H	-1	-3.35889200	7.88286200	2.54768800	L	H	-1	-10.02615700	7.14372600	L
H	-1	-6.23769700	5.90304200	0.06490200	L	H	-1	5.69923200	11.18326400	L
H	-1	-4.62583100	7.20621200	4.57091200	L	H	-1	-1.83550700	6.80674300	L
H	-1	-7.51103800	5.22194900	2.05505500	L	H	-1	5.55068500	-0.90267300	L
H	-1	-7.60594000	5.29145400	4.27639600	L	H	-1	4.22146300	-7.49140300	L
H	-1	-3.29636500	5.36426000	-0.57133800	L	H	-1	-6.59293500	-6.12232400	L
H	0	-1.59334900	7.13705000	1.17611800	H	H	-1	1.53262600	-1.99311800	L
H	0	1.47316700	5.07239800	-4.03814300	H	H	-1	-5.95901200	-5.45586200	L
H	0	1.00119800	4.59169800	-2.42018700	H	H	-1	-9.03885800	-3.45783200	L
H	-1	0.29820500	6.97104800	-2.89006000	L	N	-1	9.99449300	2.05156000	L
H	-1	-1.87289900	4.98530400	-2.45011000	L	C	-1	8.62869900	1.55149400	L
H	-1	-7.19445100	5.63629200	-2.36242900	L	C	0	8.23043900	1.66282900	L
H	-1	-6.95912000	6.75351800	-3.70516900	L	C	-1	8.53758800	0.06045500	L
H	-1	-6.53931700	3.70147300	-3.83111600	L	O	-1	7.51855100	-0.35398700	L
H	-1	-6.28474200	4.80909000	-5.18823300	L	N	-1	9.55251200	-0.72383600	L
H	-1	-4.24091200	3.23539700	-4.35913800	L	C	-1	9.53631500	-2.15748500	L
H	-1	-2.95218800	4.07938300	-3.64196500	L	C	0	8.82605500	-2.98481600	L
H	-1	-8.85594200	4.31606900	-3.87461300	L	C	0	9.62188100	-2.88216700	L
H	-1	-9.80018500	5.65901700	-5.60662300	L	O	0	9.97800600	-4.00651700	L
H	-1	-8.60010500	6.75472400	-5.47916600	L	O	0	9.78070500	-1.73810000	L
H	-1	-8.11895900	0.23446400	3.21857800	L	C	-1	10.93276300	-2.74025700	L
H	-1	-9.11872600	1.69571000	3.29613100	L	O	-1	11.93938600	-2.02026800	L
H	-1	-9.83830600	0.96207100	-0.14454100	L	H	0	8.70137500	0.85323700	L
H	-1	-7.99715100	1.66409400	-1.75641800	L	H	0	8.56158200	2.62646300	L
H	-1	-6.03979100	1.92020500	3.17578800	L	H	-1	7.87239300	2.11793600	L
H	-1	-3.94005700	3.00812800	2.31394800	L	H	-1	10.46229100	2.34779900	L
H	-1	-5.54600900	3.05863000	-1.69418500	L	H	-1	9.94653700	2.81353500	L
H	-1	-3.68642200	3.51849500	-0.09259500	L	H	0	8.68451000	-3.98478700	L
H	-1	-9.93854800	-0.77502800	1.61931100	L	H	0	7.81623400	-2.48973200	L
H	-1	-12.10680100	0.12216500	2.08467600	L	H	-1	8.98927700	-2.38348700	L
H	-1	-11.45783500	1.44150600	2.79148300	L	H	-1	10.23594000	-0.38191900	L
H	-1	-6.34458300	-3.77979800	-1.62154900	L	H	-1	11.03427800	-3.79789700	L
H	-1	-5.10146200	-3.94801800	-0.35520400	L	C	0	6.69650000	1.60567200	L
H	0	-5.72083300	-1.60424800	-1.44451800	H	C	0	6.26559000	2.25855500	L
H	0	-7.11385500	-1.60709000	-0.34046900	H	O	0	7.00486800	3.03470900	L
H	-1	-6.75920800	-4.20259200	1.41320800	L	N	0	5.02444100	1.93696800	L
H	-1	-6.65852500	-5.88307700	-0.73591300	L	H	0	4.70027200	2.34422900	L
H	-1	-8.23695900	-5.77721100	-0.36487200	L	H	0	4.35730600	1.36768600	L
H	-1	-8.56128500	-2.77694000	-6.40993300	L	H	0	6.17587400	2.13225300	L
H	-1	-8.02316600	-2.73520800	-4.72651800	L	H	0	6.32727600	0.57283600	L
H	-1	-6.25033800	-3.69048500	-7.06679400	L					
H	-1	-5.72063500	-3.43621900	-5.40620300	L					
H	0	-6.78775800	-1.26073300	-7.33702400	H					
H	0	-5.08719400	-1.56776600	-6.99907600	H					
H	0	-7.09197000	-0.43909600	-5.13273800	H					
H	0	-3.71881300	-1.71002100	-5.20262300	H	N	-1	3.09209100	-7.65580500	L
H	0	-3.31284400	-0.67577100	-3.83420600	H	C	-1	1.92864100	-6.80331900	L
H	0	-6.25962700	1.10309400	-3.66447100	H	C	-1	2.29092500	-5.55742800	L
H	0	-4.74108800	0.60713500	-2.79466600	H	C	0	1.21419600	-4.50571700	L
H	-1	-8.03213300	-5.27185800	-6.51322400	L	C	0	1.57711000	-3.49569300	L
H	-1	-10.19920900	-4.52163700	-5.93728200	L	O	0	2.74881500	-3.03595400	L
H	-1	-9.84692100	-4.47603400	-4.34406100	L	O	0	0.63085100	-3.19764100	L
H	-1	-5.18462100	-7.45813400	0.39857000	L	C	-1	0.79548100	-7.56215700	L
H	-1	-5.52935500	-6.95132800	2.05891400	L	O	-1	-0.38582600	-7.46027800	L
H	-1	-3.03669600	-6.64841200	-0.74485700	L	N	-1	1.47529100	-7.18613400	L
H	-1	-4.38330300	-4.58989100	2.95852900	L	C	-1	2.49200700	-6.19250900	L
H	-1	-1.61125700	-4.67393200	-1.09961300	L	C	-1	1.87001400	-4.90316900	L
H	-1	-3.06341600	-3.02363600	2.62604700	L	C	-1	0.56526700	-4.43662200	L
H	-1	-0.97682900	-2.73270700	-0.26562000	L	C	-1	0.39873800	-4.37383500	L
H	-1	-2.86353800	-8.37490000	1.39136900	L	C	-1	-0.78926200	-3.91047200	L
H	-1	-4.69774200	-9.64161700	0.54797300	L	C	-1	-1.80726500	-3.47001700	L
H	-1	-5.38127600	-9.73556000	2.02356500	L	O	-1	-2.99480000	-3.00675500	L
H	-1	-5.42176700	-3.27925900	4.93176900	L	C	-1	-1.65699200	-3.51644200	L
H	-1	-3.77357800	-3.23333800	4.30284500	L	C	-1	-0.47476200	-3.98797200	L
H	-1	-4.57576500	-1.85726800	6.94406500	L	C	-1	3.44056400	-6.83191700	L
H	-1	-3.04337300	-1.69398600	6.08876900	L	O	-1	3.24823200	-6.67983600	L
H	0	-5.74601100	-0.78721300	4.93009400	H	N	-1	6.00130800	-7.18321000	L
H	0	-4.52947400	0.26925500	5.69624300	H	C	-1	6.91517000	-6.41598800	L
H	0	-4.47700900	-1.01713200	3.03292400	H	C	-1	6.56358700	-4.93247800	L
H	0	-3.27504300	0.04113100	1.52114400	H	C	-1	6.44904200	-4.40109700	L
H	0	-1.79645500	0.87493500	1.93556600	H	C	-1	7.49234300	-4.61311700	L
H	0	-2.06230700	0.45860300	5.33663700	H	C	-1	7.40435800	-4.16966500	L
H	0	-1.62285500	1.64707800	4.15780500	H	C	-1	6.26485500	-3.51889700	L
H	-1	-3.20842100	-3.91776900	6.85450200	L	O	-1	6.22729000	-3.07831600	L
H	-1	-3.68546700	-5.39599500	4.49866000	L	C	-1	5.21052000	-3.29419300	L
H	-1	-2.25923000	-4.80241600	5.66085700	L	C	-1	5.30372500	-3.73766500	L
H	0	0.60145000	-1.67546400	-2.79586800	H	C	-1	6.78622400	-6.87657200	L
H	0	0.71069200	0.68053600	-4.34852100	H	O	-1	5.64761900	-7.00674100	L
H	0	2.06151900	0.92249600	-2.46284600	H	N	-1	5.70864300	-3.90042400	L
H	0	2.69221400	-1.62110400	-1.34935200	H	C	-1	5.43462300	-2.54282900	L
H	0	-1.32369300	-0.56649300	-0.75010800	H	C	-1	4.38287900	-2.52239200	L
H	0	0.12070700	2.08725600	-1.19525700	H	O	-1	4.86107500	-3.30650700	L
H	0	-0.67752700	2.41052500	0.73728600	H	C	-1	4.09359700	-1.09976800	L
H	0	1.12379000	-0.51236500	0.03796400	H	C	-1	4.97480900	-1.69809600	L
H	0	2.06509700	1.49745200	0.89048700	H	O	-1	3.90941100	-1.98935100	L
H	0	-2.24046000	1.83026400	-2.39314800	H	N	-1	3.90377300	1.41211000	L
						C	-1	2.68279500	2.25401100	L
H	0	-2.69110300	1.62810600	-0.66909400	H	0	-2.69110300	1.62810600	-0.66909400	H
H	0	-3.77111100	-0.27198400	-1.16532900	H	0	-3.77111100	-0.27198400	-1.16532900	H
O	-1	7.70821100	10.96170600	3.86853800	L	O	-1	7.70821100	10.96170600	L
H	-1	8.54406000	0.76550300	-6.02056000	L	H	-1	8.54406000	0.76550300	L
H	-1	7.62468600	-7.13558600	1.26936600	L	H	-1	7.62468600	-7.13558600	L
H	-1	0.94976400	-8.20216000	0.52932000	L	H	-1	0.94976400	-8.20216000	L
H	-1	-2.71579900	-7.76449800	3.76063300	L	H	-1	-2.71579900	-7.76449800	L
H	-1	-10.39939000	-1.94366200	3.72049500	L	H	-1	-10.39939000	-1.94366200	L
H	-1	-10.02615700	7.14372600	-3.28032600	L	H	-1	-10.02615700	7.14372600	L
H	-1	5.69923200	11.18326400	3.55227600	L	H	-1	5.69923200	11.18326400	L
H	-1	-1.83550700	6.80674300	-4.84431000	L	H	-1	-1.83550700	6.80674300	L
H	-1	5.55068500	-0.90267300	5.45136300	L	H	-1	5.55068500	-0.90267300	L
H	-1	4.22146300	-7.49140300	-4.01918500	L	H	-1	4.22146300	-7.49140300	L
H	-1	-6.59293500	-6.12232400	-4.73112900	L	H	-1	-6.59293500	-6.12232400	L
H	-1	1.53262600	-1.99311800	7.45680600	L	H	-1	1.53262600	-1.99311800	L
H	-1	-5.95901200	-5.45586200	6.66259000	L	H	-1	-5.95901200	-5.45586200</	

C	0	2.52064000	3.21780100	4.64726900	H	O	0	-4.20990600	-0.78278100	0.31418800	H
C	0	2.77432700	2.51181500	3.27683400	H	C	-1	-8.43574400	-3.49832700	0.29537200	L
O	0	3.91676700	2.05741700	3.10702000	H	O	-1	-8.87317900	-2.87006300	1.29412600	L
O	0	1.79211100	2.46703400	2.45024500	H	N	-1	-9.60351000	-4.97761800	-5.17769300	L
C	-1	1.43488900	1.34326600	5.93810500	L	C	-1	-8.19304500	-4.79224400	-5.51700400	L
O	-1	0.38604700	1.82468700	6.39576300	L	C	-1	-7.85467700	-3.31753000	-5.66212500	L
N	-1	1.57585300	0.07706800	5.54999700	L	C	-1	-6.42554900	-3.10817100	-6.14703100	L H 144
C	-1	0.53510500	-0.95359100	5.68702800	L	C	0	-6.10279600	-1.67028700	-6.55068400	H
C	-1	0.66107900	-2.01536200	4.56153900	L	N	0	-6.17903700	-0.68731000	-5.47305600	H
C	-1	-0.36564500	-3.11618800	4.73258200	L	C	0	-5.22274000	-0.43354900	-4.52761200	H
C	-1	0.46478900	-1.35728600	3.19553700	L	N	0	-4.01630000	-0.98405700	-4.55832300	H
C	-1	0.60588900	-1.67733600	7.04195400	L	N	0	-5.53578100	0.41852200	-3.54844400	H
O	-1	-0.45200900	-1.94197000	7.66996000	L	C	-1	-7.31949200	-5.43095800	-4.41883900	L
N	-1	9.56022900	-1.43009700	-3.75388200	L	O	-1	-7.48659900	-5.10730500	-3.21430700	L
C	-1	8.47897800	-0.63272000	-4.29772700	L H 175	N	-1	-4.43360300	-9.64989600	1.55737300	L
C	0	7.50984300	-0.11824100	-3.21761800	H	C	-1	-3.78636300	-8.38667300	1.91584300	L
C	0	6.40917100	0.78661100	-3.77909700	H	C	-1	-4.63416600	-7.21162900	1.38499000	L
C	0	5.12539600	0.29508200	-4.04152900	H	C	-1	-3.80471000	-5.96836100	1.14083800	L
C	0	4.09051000	1.12087200	-4.48705400	H	C	-1	-2.98799000	-5.84739100	0.00460600	L
C	0	4.30971200	2.49291000	-4.65991800	H	C	-1	-2.19003300	-4.74614500	-0.18470700	L
O	0	3.33370600	3.36356600	-5.05708400	H	C	-1	-2.19183700	-3.74134900	0.74971800	L
C	0	5.59362000	3.00275400	-4.41876200	H	O	-1	-1.40297000	-2.64786100	0.57549400	L
C	0	6.61407300	2.16261800	-3.97994900	H	C	-1	-2.98205000	-3.83767400	1.88271800	L
C	-1	8.98934800	0.57244000	-5.09998400	L	C	-1	-3.79473400	-4.94341600	2.05151800	L
O	-1	9.92202400	1.28304400	-4.64310900	L	C	-1	-3.54534200	-8.27127800	3.42505000	L
N	-1	7.97879200	10.32973600	1.13347300	L	O	-1	-4.39025700	-8.73458600	4.23439300	L
C	-1	6.67728600	10.14614800	1.79158400	L	N	-1	-3.30541100	-5.45557800	5.46543800	L
C	-1	6.32715200	8.66663500	1.93003900	L	C	-1	-3.94277000	-4.37803000	6.20611900	L
C	-1	5.82259000	8.09325300	0.64978300	L	C	-1	-4.30923700	-3.20322200	5.27490700	L
C	-1	6.02303500	8.60136700	-0.62347600	L	C	-1	-4.08515400	-1.86538600	5.93751100	L H 85
N	-1	5.39584500	7.83004200	-1.54864100	L	C	0	-4.62685000	-0.68255200	5.13813900	H
C	-1	4.78409100	6.77203800	-0.91169300	L	N	0	-3.98891400	-0.53229100	3.83545600	H
C	-1	5.04157500	6.89993200	0.47444900	L	C	0	-2.97111000	0.29120800	3.52944700	H
C	-1	4.49565200	5.95014000	1.35741000	L	N	0	-2.29978400	0.97272700	4.49661000	H
C	-1	3.74530100	4.91758100	0.82349900	L	N	0	-2.68703800	0.49624900	2.25105200	H
C	-1	3.53006100	4.79386200	-0.55230700	L	C	-1	-5.14202800	-4.76826200	7.07836900	L
C	-1	4.03095800	5.71856000	-1.44108700	L	O	-1	-5.26247400	-4.28650400	8.23460900	L
C	-1	6.61234000	10.87230700	3.13225600	L	C	0	0.53753400	-0.53790200	-2.98900700	H
N	0	0.07373300	6.53755100	2.70025300	H	O	0	0.75599400	-0.26106500	-4.34440500	H
C	0	-0.26718800	5.20410700	2.19408300	H	C	0	1.65832800	0.07150400	-2.09338100	H
C	0	-0.82069800	4.34287600	3.38243000	H	O	0	2.76997800	-0.79484000	-2.08491900	H
O	0	-0.70248000	2.96168100	3.12956400	H	O	0	-0.79304000	-0.03498500	-2.73634500	H
C	0	-2.28363100	4.61661700	3.72390500	H	C	0	-1.17055500	0.32573200	-1.42214600	H
C	0	-1.20998100	5.13139200	0.97970800	H	C	0	-0.12637600	1.19867400	-0.71910500	H
O	0	-1.38079500	4.07746400	0.36724700	H	O	0	-0.56544400	1.46618700	0.62126600	H
N	0	-1.86189200	6.29218200	0.65793100	H	C	0	1.23803300	0.52011900	-0.68482200	H
C	-1	-2.87088500	6.37835300	-0.46021900	L H 88	O	0	2.21704000	1.44946200	-0.23048200	H
C	-1	-3.98041300	7.36221500	-0.08478400	L	C	0	-2.47321100	1.08400000	-1.59796400	H
C	-1	-4.75581600	6.93397200	1.16795400	L	O	0	-3.53780900	0.17780800	-1.98508200	H
C	-1	-4.31946200	7.29031000	2.43616300	L	H	-1	2.63878100	-5.90241500	0.25783600	L
C	-1	-5.01459500	6.90265300	3.57879000	L	H	-1	3.17707700	-5.07394300	1.72647100	L
C	-1	-6.16206800	6.14078700	3.44583800	L	H	0	0.22443500	-4.95347000	0.84971000	H
O	-1	-6.86424200	5.75657300	4.58371300	L	H	0	1.09054400	-3.88799700	2.00144800	H
C	-1	-6.62017900	5.78692800	2.19818300	L	H	-1	1.61745400	-6.49283800	3.13734600	L
C	-1	-5.90464500	6.17629900	1.06361300	L	H	-1	3.41878700	-7.92287900	1.30667200	L
C	-1	-2.10008200	6.81453600	-1.70508500	L	H	-1	3.81310900	-7.20117300	2.73133800	L
O	-1	-2.13595600	7.99154300	-2.10531700	L	H	-1	1.69816400	-5.00759000	-3.00711400	L
N	-1	-1.41630800	5.84901600	-2.31905200	L	H	-1	2.61460000	-4.08190100	-4.20465900	L
C	-1	-0.34756400	6.11906700	-3.31522900	L H 102	H	-1	1.20981500	-4.69857300	-6.76212500	L
C	0	0.54519300	4.86939500	-3.42906500	H	H	-1	-0.36872700	-4.00660000	-2.82288200	L
C	0	-0.11671000	3.56703100	-4.01577400	H	H	-1	-0.89010400	-3.87808900	-7.74816100	L
O	0	-1.37229000	3.47139300	-4.07320300	H	H	-1	-2.45205700	-3.17055500	-3.78332200	L
O	0	0.71967000	2.67855000	-4.35057800	H	H	-1	-2.93423000	-3.04538400	-7.28151800	L
C	-1	-0.82911100	6.57217600	-4.68225200	L	H	-1	3.03002000	-5.96334700	-5.62633600	L
O	-1	0.01265700	6.69768100	-5.60920400	L	H	-1	1.89501600	-8.04250900	-5.25190200	L
N	-1	-8.89812900	5.73602300	-5.31925700	L	H	-1	0.90441200	-7.34958000	-4.15168100	L
C	-1	-8.71245700	5.36216300	-3.90582000	L	H	-1	5.61498300	-4.74097200	-0.29079400	L
C	-1	-7.29082600	5.65991300	-3.45812400	L	H	-1	7.33829500	-4.33631700	-0.30447700	L
C	-1	-6.27358900	4.70197500	-4.07115400	L	H	-1	8.41610000	-5.09610200	-2.80446300	L
C	-1	-4.86022800	4.97982700	-3.64372400	L	H	-1	4.47365400	-3.54638000	-1.99099800	L
O	-1	-4.52913200	6.08543400	-3.19546200	L	H	-1	8.25765400	-4.31009200	-5.12757000	L
N	-1	-3.99625400	3.97042500	-3.78049100	L	H	-1	4.31408900	-2.75431000	-4.33467100	L
C	-1	-9.73443100	6.06436300	-3.00648000	L	H	-1	7.09430100	-3.19927100	-6.51942400	L
O	-1	-10.17215800	5.48414400	-1.97919600	L	H	-1	7.95591100	-6.59591700	-1.15992900	L
N	-1	-11.28736200	0.64812500	2.15926400	L	H	-1	6.06610500	-6.85181600	-2.57516700	L
C	-1	-10.10253200	-0.12588200	2.49887800	L	H	-1	5.05834100	-7.08436800	-1.30892300	L
C	-1	-8.87142800	0.76397500	2.69201100	L	H	-1	3.42654900	-2.99053400	3.18486900	L
C	-1	-8.25234600	1.24347900	1.40244400	L	H	-1	3.35773200	-1.06745000	1.53904200	L
C	-1	-8.82669100	1.23324900	0.15342700	L	H	-1	5.00969300	-0.59509800	2.02038900	L
N	-1	-7.95836200	1.79104500	-0.76307800	L	H	-1	3.68497900	-0.49018400	3.17849900	L
C	-1	-6.81487900	2.18665600	-0.11864900	L	H	-1	4.14692100	-3.32064200	1.08623900	L
C	-1	-6.95938900	1.84921300	1.24507700	L	H	-1	6.37954400	-2.06107200	3.51103100	L
C	-1	-5.91900000	2.13571100	2.12685000	L	H	-1	5.05028500	-4.55657800	3.95258200	L
C	-1	-4.76449400	2.71543200	1.64189100	L	H	-1	6.62670500	-4.15853400	4.02561200	L
C	-1	-4.63039300	3.02444700	0.25867100	L	H	0	1.52407800	3.69468600	4.68944500	H
C	-1	-5.65472000	2.77442900	-0.62087500	L	H	0	3.27431200	4.02577200	4.72863700	H
C	-1	-10.43708200	-0.90528200	3.75527000	L	H	-1	2.71457000	2.86918700	6.76190700	L
O	-1	-10.80858700	-0.29740800	4.79259600	L	H	-1	4.28386900	1.44607500	4.82029200	L
N	-1	-7.25965800	-5.65498500	0.00425400	L	H	-1	4.57747500	1.76152800	6.40818800	L
C	-1	-7.09239000	-4.25047500	0.38530300	L	H	-1	1.68335800	-2.47363500	4.60133300	L
C	-1	-6.07676700	-3.56765200	-0.54218600	L H 134	H	-1	-0.29480200	-3.84860200	3.91440500	L
C	0	-6.07395500	-2.05053200	-0.46798500	H	H	-1	-1.39434100	-2.72093000	4.72376400	L
C	0	-5.19307200	-1.50465400	0.67895100	H	H	-1	-0.23527000	-3.67196700	5.67330800	L
O	0	-5.50717500	-1.78234000	1.85507200	H	H	-1	0.58243800	-2.12251000	2.40305400	L

H	-1	-0.53801300	-0.92662300	3.08649800	L	H	-1	-2.78816300	-8.38333200	1.40889700	L
H	-1	1.19701700	-0.56459100	2.97959100	L	H	-1	-4.61680300	-9.66413300	0.57474100	L
H	-1	-0.47090300	-0.46346200	5.59267800	L	H	-1	-5.29387900	-9.76042400	2.05315600	L
H	-1	2.33697000	-0.16229900	4.94363800	L	H	-1	-5.36787500	-3.29984100	4.95117400	L
H	0	7.05393400	-0.98456200	-2.70518300	H	H	-1	-3.72252200	-3.24349100	4.31570500	L
H	0	8.07966800	0.41569100	-2.43333900	H	H	-1	-4.52390400	-1.86873700	6.95785400	L
H	0	4.89858900	-0.75336500	-3.85471000	H	H	-1	-2.99604800	-1.69620300	6.09628300	L
H	0	7.58884600	2.59462800	-3.74913400	H	H	0	-5.70975700	-0.80837900	4.94929600	H
H	0	3.10600900	0.69538700	-4.65704800	H	H	0	-4.49631800	0.25632900	5.70903700	H
H	0	5.75749700	4.07324600	-4.52911300	H	H	0	-4.44870300	-1.03279300	3.04830100	H
H	0	2.43379800	3.01435000	-4.82947700	H	H	0	-3.26162600	0.02811700	1.52955100	H
H	-1	7.92507800	-1.29979900	-5.00888700	L	H	0	-1.79180400	0.88124400	1.92944800	H
H	-1	10.29328600	-1.50229200	-4.42853100	L	H	0	-2.03037200	0.46309800	5.33543200	H
H	-1	9.91777100	-1.06153500	-2.89635100	L	H	0	-1.60255600	1.64868000	4.15050500	H
H	-1	7.19918300	8.07462500	2.27779800	L	H	-1	-3.14262500	-3.91983000	6.86621200	L
H	-1	5.54777200	8.53744500	2.70900900	L	H	-1	-3.61860600	-5.40516300	4.51462900	L
H	-1	6.58802900	9.49772500	-0.89553800	L	H	-1	-2.19198900	-4.79979900	5.67026200	L
H	-1	5.57235900	7.86173700	-2.52036200	L	H	0	0.54470300	-1.62049600	-2.85505500	H
H	-1	4.66246400	6.03821900	2.43503500	L	H	0	0.64698500	0.71706700	-4.43429400	H
H	-1	3.30205200	4.16976500	1.49593500	L	H	0	1.98538900	0.98653900	-2.60088100	H
H	-1	3.86481200	5.59619500	-2.52165100	L	H	0	2.64916500	-1.52263400	-1.42637100	H
H	-1	2.93133400	3.94911700	-0.92252100	L	H	0	-1.33954000	-0.57049100	-0.80087800	H
H	-1	5.92060100	10.63780500	1.12628500	L	H	0	-0.62370000	2.14459300	-1.26386500	H
H	-1	8.69556400	9.84411100	1.63203600	L	H	0	-0.70867500	2.42815900	0.71128200	H
H	-1	8.20140200	11.30266500	1.09934900	L	H	0	1.18261200	-0.35334100	-0.01682300	H
H	0	-0.19340000	4.64576400	4.23475600	H	H	0	2.09682700	1.64663800	0.73042400	H
H	0	-2.54988300	4.09450700	4.64974400	H	H	0	-2.35003200	1.81395600	-2.40369000	H
H	0	-2.93506500	4.23361600	2.92455300	H	H	0	-2.75852300	1.59555600	-0.67109000	H
H	0	-2.49234400	5.68785000	3.86451300	H	H	0	-3.81807000	-0.31135600	-1.14198800	H
H	0	0.26802200	2.73741900	2.92119600	H	O	-1	7.65847800	11.03026400	3.81359300	L
H	0	0.66719400	4.71796900	1.89175300	H	H	-1	8.52646000	0.82405300	-6.06240400	L
H	0	0.54795700	7.10030400	1.99897800	H	H	-1	7.69063000	-7.07137300	1.24369800	L
H	0	-0.73641500	7.04494900	3.04986700	H	H	-1	1.02043900	-8.18550200	0.53159400	L
H	-1	-4.68248100	7.44551800	-0.93904400	L	H	-1	-2.63538900	-7.76806800	3.77658300	L
H	-1	-3.57608600	8.38393600	0.06850300	L	H	-1	-10.35937400	-2.00083300	3.75733700	L
H	-1	-3.39203700	7.87245400	2.54116700	L	H	-1	-10.07678700	7.07753600	-3.25941300	L
H	-1	-6.26671000	5.86864500	0.07288100	L	H	-1	5.64678200	11.23734400	3.50487400	L
H	-1	-4.64630100	7.19030700	4.57043300	L	H	-1	-1.89018100	6.79493300	-4.85503100	L
H	-1	-7.52747500	5.18195700	2.06910800	L	H	-1	5.58973500	-0.84623000	5.42384500	L
H	-1	-7.61415300	5.25441200	4.29069100	L	H	-1	4.26926700	-7.45942400	-4.03086300	L
H	-1	-3.32421400	5.34927900	-0.57405300	L	H	-1	-6.55709800	-6.16667900	-4.70249100	L
H	0	-1.62200800	7.14208400	1.15908300	H	H	-1	1.58724700	-1.96130600	7.44680400	L
H	0	1.44380600	5.09114000	-4.03918500	H	H	-1	-5.88318300	-5.47730800	6.68756900	L
H	0	0.95568300	4.59100200	-2.43399700	H	H	-1	-9.00559200	-3.51266200	-0.64437100	L
H	-1	0.24997800	6.97723300	-2.90944600	L	N	-1	10.00162100	2.13411500	2.53199500	L
H	-1	-1.90552400	4.97717000	-2.45779500	L	C	-1	8.63821700	1.62417000	2.25359600	L H 371
H	-1	-7.23108900	5.59130900	-2.35024200	L	C	0	8.21769200	1.70802700	0.77654800	H
H	-1	-7.00879800	6.70795900	-3.69568100	L	C	-1	8.55916000	0.13319600	2.68513500	L
H	-1	-6.56827600	3.65870300	-3.81839800	L	O	-1	7.54520300	-0.28742000	3.24088600	L
H	-1	-6.32673000	4.76585500	-5.17827400	L	N	-1	9.57813300	-0.64459500	2.33009200	L
H	-1	-4.26877100	3.20775300	-4.35470500	L	C	-1	9.57270000	-2.07799100	2.53589500	L H 376
H	-1	-2.98314900	4.06184300	-3.64395900	L	C	0	8.85603000	-2.85348800	1.41293600	H
H	-1	-8.88927100	4.25711600	-3.85377400	L	C	0	9.55251100	-2.67726100	-0.01545900	H
H	-1	-9.84961200	5.59065400	-5.58420400	L	O	0	10.06888600	-3.71995900	-0.47821700	H
H	-1	-8.65669100	6.69487800	-5.46321500	L	O	0	9.49135800	-1.51698800	-0.49815400	H
H	-1	-8.09613100	0.19226700	3.24298200	L	C	-1	10.97368100	-2.65082700	2.66452700	L
H	-1	-9.10572500	1.64665500	3.32212600	L	O	-1	11.97437200	-1.92423300	2.43161600	L
H	-1	-9.83366200	0.90244100	-0.11451400	L	H	0	9.03492700	1.34525200	0.12185000	H
H	-1	-8.00376400	1.61461900	-1.73473400	L	H	0	7.98878300	2.75448500	0.49528100	H
H	-1	-6.02892100	1.89234200	3.18932600	L	H	-1	7.88035400	2.18627400	2.85723700	L
H	-1	-3.94019500	2.99342500	2.31750200	L	H	-1	10.46407200	2.43227600	1.69808100	L
H	-1	-5.56215500	3.02625200	-1.68436200	L	H	-1	9.95086800	2.89680300	3.17172900	L
H	-1	-3.69955100	3.50163100	-0.09082900	L	H	0	8.82885000	-3.93403700	1.66597100	H
H	-1	-9.91490900	-0.83244200	1.65249300	L	H	0	7.80532900	-2.50113700	1.34178300	H
H	-1	-12.08750900	0.05041900	2.12494000	L	H	-1	9.03098800	-2.30623800	3.49134000	L
H	-1	-11.44496900	1.37538400	2.82708200	L	H	-1	10.25662900	-0.29898700	1.68146700	L
H	-1	-6.31286300	-3.81743300	-1.59765800	L	H	-1	11.08361100	-3.70729400	2.93723800	L
H	-1	-5.06364800	-3.97495300	-0.33594100	L	C	0	6.95984800	0.84801700	0.49758900	H
H	0	-5.70381800	-1.63574500	-1.42065400	H	C	0	5.86710100	1.54194900	-0.28529200	H
H	0	-7.09763900	-1.65060600	-0.31834400	H	O	0	5.88198800	2.69882700	-0.66203600	H
H	-1	-6.71263900	-4.23816400	1.43937600	L	H	0	6.42619000	0.52010000	1.41199900	H
H	-1	-6.60869400	-5.92139900	-0.70743500	L	H	0	7.24915200	-0.07714200	-0.01386200	H
H	-1	-8.18636000	-5.82590100	-0.33036400	L	O	0	4.85640600	0.68425900	-0.45151400	H
H	-1	-8.55522900	-2.83778700	-6.37889200	L	H	0	4.01320500	1.12440500	-0.70758900	H
H	-1	-8.01082200	-2.78958000	-4.69767400	L						
H	-1	-6.24057800	-3.73631900	-7.04336800	L						
H	-1	-5.70615200	-3.47567900	-5.38528000	L						
H	0	-6.79667400	-1.32792400	-7.33996900	H						
H	0	-5.09354300	-1.61113400	-6.99544200	H						
H	0	-7.11433800	-0.47922400	-5.15025000	H						
H	0	-3.73525600	-1.73353300	-5.19979700	H						
H	0	-3.34261000	-0.70146700	-3.82722100	H						
H	0	-6.30455200	1.06220700	-3.67520600	H						
H	0	-4.79277100	0.56411300	-2.78486100	H						
H	-1	-8.00914800	-5.32913200	-6.48027400	L						
H	-1	-10.17911500	-4.59305200	-5.89702000	L						
H	-1	-9.82091200	-4.54241200	-4.30527000	L						
H	-1	-5.11943800	-7.48433100	0.42376200	L						
H	-1	-5.46117900	-6.97723500	2.08463700	L						
H	-1	-2.98169200	-6.66156400	-0.72938900	L						
H	-1	-4.32806200	-4.60643100	2.97596500	L						
H	-1	-1.57142100	-4.67780600	-1.09289900	L						
H	-1	-3.02041200	-3.03158600	2.63579600	L						
H	-1	-0.94729400	-2.72140400	-0.26452600	L						
Glc_E777A											
ONIOM: extrapolated energy = -3124.119815 au											
N	-1	3.13819600	-7.58494600	2.27673300	L						
C	-1	1.95844700	-6.75571100	2.17003400	L						
C	-1	2.29258300	-5.51467200	1.29919800	L H 4						
C	0	1.19835700	-4.48314500	1.11456600	H						
C	0	1.53945800	-3.46208800	-0.02705900	H						
O	0	2.70656900	-2.97985900	-0.05269400	H						
O	0	0.59212200	-3.15573500	-0.81546800	H						
C	-1	0.83576400	-7.54475600	1.48430000	L						
O	-1	-0.34486200	-7.45933600	1.91137600	L						
N	-1	1.47275900	-7.24033400	-4.88645700	L						

C	-1	-1.88358100	-3.59790000	-5.78952800	L	C	-1	-7.52360300	5.45883700	-3.50730200	L
O	-1	-3.08239100	-3.16357900	-6.29465300	L	C	-1	-6.49207500	4.51199200	-4.11364800	L
C	-1	-1.72477500	-3.62335000	-4.41674700	L	C	-1	-5.08178700	4.82175700	-3.69817600	L
C	-1	-0.53092300	-4.06561100	-3.87891600	L	O	-1	-4.76892400	5.93917400	-3.26640400	L
C	-1	3.43821800	-6.83262900	-3.62024500	L	N	-1	-4.19987800	3.82690600	-3.82661300	L
O	-1	3.24999300	-6.66784200	-2.38696100	L	C	-1	-9.97177800	5.82363000	-3.04671800	L
N	-1	6.01647300	-7.10913800	-1.59112100	L	O	-1	-10.39281100	5.24899700	-2.00936600	L
C	-1	6.92051000	-6.31399300	-0.76775800	L	N	-1	-11.39415000	0.44820900	2.19864700	L
C	-1	6.54099400	-4.83800700	-0.82945800	L	C	-1	-10.19316300	-0.29902900	2.54145200	L
C	-1	6.40865800	-4.32748600	-2.24069600	L	C	-1	-8.97785800	0.61608700	2.71568700	L
C	-1	7.45064000	-4.53202200	-3.15171800	L	C	-1	-8.37509000	1.08994100	1.41634100	L
C	-1	7.34709700	-4.10750900	-4.45586900	L	C	-1	-8.95613200	1.05249000	0.17094600	L
C	-1	6.19337500	-3.48348400	-4.86159000	L	N	-1	-8.10353900	1.61419400	-0.75786300	L
O	-1	6.14031300	-3.06086400	-6.16322500	L	C	-1	-6.96406300	2.03953100	-0.12537900	L
C	-1	5.13984300	-3.26713800	-4.00089300	L	C	-1	-7.09459200	1.71752400	1.24347900	L
C	-1	5.24869300	-3.69136300	-2.68093700	L	C	-1	-6.05482000	2.03499500	2.11531500	L
C	-1	6.80831500	-6.75771000	0.68644100	L	C	-1	-4.91409300	2.62965800	1.61604500	L
O	-1	5.67527500	-6.90218200	1.21457000	L	C	-1	-4.79355200	2.92279400	0.22813100	L
N	-1	5.69581200	-3.75391100	4.31992700	L	C	-1	-5.81793500	2.64212100	-0.64205300	L
C	-1	5.39411200	-2.40729200	3.88670300	L	C	-1	-10.50603000	-1.06783800	3.80989800	L
C	-1	4.33611200	-2.42079500	2.80911700	L	O	-1	-10.88302300	-0.45332100	4.84131400	L
O	-1	4.82276000	-3.21034700	1.71488300	L	N	-1	-7.26138000	-5.80672400	0.10300900	L
C	-1	4.01767800	-1.01005800	2.32870700	L	C	-1	-7.11828200	-4.39442300	0.46461000	L
C	-1	4.92531200	-1.55546000	5.07914300	L	C	-1	-6.12082600	-3.70512600	-0.47768300	L
O	-1	3.86894500	-1.85851000	5.69218300	L	C	-1	-8.47595400	-3.66868900	0.37267700	L
N	-1	3.79998500	1.54267800	5.70219200	L	O	-1	-8.91946100	-3.03552700	1.36564200	L
C	-1	2.56386000	2.36248600	5.76415100	L	N	-1	-9.64649200	-5.24175200	-5.07358200	L
C	0	2.37873600	3.32383000	4.58711000	H	C	-1	-8.24166500	-5.03463600	-5.42354100	L
C	0	2.57428200	2.60594500	3.22563000	H	C	-1	-7.93176200	-3.55592400	-5.58997700	L
O	0	3.71713500	2.19232200	2.97473300	H	C	-1	-6.50953900	-3.32640800	-6.08593900	L
O	0	1.53691900	2.49012100	2.47007000	H	C	0	-6.23392900	-1.89307100	-6.53025300	H
C	-1	1.33384700	1.43018400	5.89356000	L	N	0	-6.33950600	-0.90241800	-5.45583400	H
O	-1	0.27876300	1.89799300	6.35098900	L	C	0	-5.40795500	-0.67141100	-4.49785600	H
N	-1	1.49629500	0.16181000	5.52128200	L	N	0	-4.18893400	-1.19166600	-4.53788700	H
C	-1	0.47579300	-0.88615800	5.67791200	L	N	0	-5.76443300	0.12113900	-3.47147600	H
C	-1	0.61529800	-1.96019300	4.56573400	L	C	-1	-7.35017700	-5.64238200	-4.32221800	L
C	-1	-0.38967900	-3.07759800	4.75721000	L	O	-1	-7.51655700	-5.30599200	-3.12108000	L
C	-1	0.39908200	-1.32401600	3.19238600	L	N	-1	-4.35243100	-9.72739400	1.69185700	L
C	-1	0.56769400	-1.59047200	7.04178100	L	C	-1	-3.72693600	-8.44770000	2.02992800	L
O	-1	-0.48153300	-1.86643800	7.67938200	L	C	-1	-4.59953300	-7.29578000	1.48867100	L
N	-1	9.45520800	-1.31928500	-3.80856100	L	C	-1	-3.79486000	-6.04061400	1.22337800	L
C	-1	8.35620100	-0.54945100	-4.35649200	L	C	-1	-2.98692600	-5.91948900	0.08089900	L
C	0	7.38963800	-0.06168800	-3.27381700	H	C	-1	-2.21078200	-4.80616800	-0.12751200	L
C	0	6.24364800	0.81125500	-3.78361500	H	C	-1	-2.22614500	-3.78930800	0.79364200	L
C	0	4.98750600	0.27073300	-4.08654200	H	O	-1	-1.45885700	-2.68370600	0.60047500	L
C	0	3.90115000	1.07044700	-4.44734800	H	C	-1	-3.00805800	-3.88534200	1.93241200	L
C	0	4.04157900	2.46309900	-4.49892900	H	C	-1	-3.79895700	-5.00370200	2.12045600	L
O	0	3.02038100	3.31018400	-4.80854400	H	C	-1	-3.47966300	-8.30788000	3.53605600	L
C	0	5.29769100	3.02409100	-4.22214900	H	O	-1	-4.31121500	-8.77610100	4.35633600	L
C	0	6.36970800	2.20914800	-3.86638100	H	N	-1	-3.28101700	-5.46145300	5.53788300	L
C	-1	8.83943400	0.65428700	-5.17746400	L	C	-1	-3.93426000	-4.38626200	6.26807600	L
O	-1	9.76119900	1.38812600	-4.73541500	L	C	-1	-4.32785100	-3.23090800	5.32368700	L
N	-1	7.68147600	10.47266900	0.93322900	L	C	-1	-4.12512800	-1.88048300	5.96736100	L
C	-1	6.38733900	10.27358600	1.60129400	L	O	0	-4.74082300	-0.73321300	5.17421800	H
C	-1	6.06572500	8.78976800	1.76119700	L	N	0	-4.14743100	-0.56422300	3.84329500	H
C	-1	5.56481100	8.19019800	0.49154800	L	C	0	-3.12996400	0.26448800	3.49369700	H
C	-1	5.74857900	8.68507100	-0.78942000	L	N	0	-2.50589400	1.03420400	4.38115100	H
N	-1	5.13075200	7.89002300	-1.70070000	L	N	0	-2.80806500	0.31733500	2.19927300	H
C	-1	4.54247500	6.82932400	-1.04635600	L	C	-1	-5.12110300	-4.78719700	7.15237100	L
C	-1	4.80528500	6.98031800	0.33645900	L	O	-1	-5.24405900	-4.29251300	8.30287500	L
C	-1	4.28218100	6.03228400	1.23498400	L	C	0	0.50333600	-0.62089300	-2.82230900	H
C	-1	3.54830000	4.97894800	0.71906400	L	O	0	0.69462700	-0.29557400	-4.16308400	H
C	-1	3.32768800	4.83306800	-0.65371400	L	C	0	1.55637300	0.06116500	-1.89358200	H
C	-1	3.80622700	5.75508700	-1.55746700	L	O	0	2.70848100	-0.75145400	-1.80500000	H
C	-1	6.31633500	11.01608000	2.93267900	L	O	0	-0.88065000	-0.25928200	-2.55901700	H
N	0	-0.18509600	6.54861200	2.64405300	H	C	0	-1.28878600	0.18761200	-1.29255200	H
C	0	-0.52381100	5.20798900	2.17079700	H	C	0	-0.31157000	1.15117500	-0.61533300	H
C	0	-1.07606200	4.37908400	3.37999300	H	O	0	-0.80796500	1.46908600	0.69400300	H
O	0	-0.95640700	2.98409900	3.15540700	H	C	0	1.06112100	0.05098600	-0.50786100	H
C	0	-2.53743200	4.65731300	3.71760100	H	O	0	1.99706000	1.45220300	-0.00862700	H
C	0	-1.46326300	5.09518400	0.95493900	H	C	0	-2.62518000	0.85502100	-1.52627800	H
O	0	-1.64579100	4.00944200	0.39511600	H	O	0	-3.60728300	-0.14821600	-1.94015500	H
N	0	-2.08591700	6.24401100	0.57183200	H	H	-1	2.64122200	-5.86631700	0.30191200	L
C	-1	-3.10114700	6.29909700	-0.54498700	L	H	-1	3.17214600	-5.00860500	1.75637600	L
C	-1	-4.22676400	7.26699500	-0.17601000	L	H	0	0.22058000	-4.95038400	0.87993700	H
C	-1	-4.98698800	6.84098900	1.08675300	L	H	0	1.05717900	-3.87350700	2.04239400	H
C	-1	-4.55027700	7.22214100	2.34760400	L	H	-1	1.64726700	-6.43752200	3.19484600	L
C	-1	-5.23162400	6.83674900	3.49926500	L	H	-1	3.46475000	-7.85784700	1.37258900	L
C	-1	-6.36537100	6.05194600	3.38303600	L	H	-1	3.85348000	-7.11013600	2.78533200	L
O	-1	-7.05384800	5.66980200	4.52994200	L	H	-1	1.66575000	-5.03244100	-2.96894000	L
C	-1	-6.82376600	5.67313900	2.14283300	L	H	-1	2.55798500	-4.10576300	-4.18387000	L
C	-1	-6.12201000	6.06073000	0.99908500	L	H	-1	1.15067300	-4.78227800	-6.72476200	L
C	-1	-2.34562800	6.73305600	-1.79996000	L	H	-1	-0.41844900	-4.06777100	-2.78577400	L
O	-1	-2.40575300	7.90379400	-2.21538200	L	H	-1	-0.96971900	-4.01417500	-7.70918000	L
N	-1	-1.64735900	5.77241400	-2.40518700	L	H	-1	-2.52239400	-3.28347700	-3.74489800	L
C	-1	-0.58946700	6.04911500	-3.41101000	L	H	-1	-3.02641700	-3.21359700	-7.24155500	L
C	0	0.33936100	4.82971100	-3.49573600	H	H	-1	3.00055500	-5.99778500	-5.58314200	L
C	0	-0.35587300	3.45109100	-3.71553000	H	H	-1	1.90675800	-8.09259600	-5.17482600	L
O	0	-1.56804700	3.31820400	-3.35646900	H	H	-1	0.90954500	-7.40375000	-4.07801600	L
O	0	0.39918700	2.54339700	-4.16447700	H	H	-1	5.59205500	-4.65698600	-0.27931000	L
C	-1	-1.08704300	6.47505300	-4.78107200	L	H	-1	7.30739200	-4.22051200	-0.30838300	L
O	-1	-0.25297900	6.60394600	-5.71449700	L	H	-1	8.38519700	-4.99308900	-2.80444500	L
N	-1	-9.14245200	5.48036100	-5.35983900	L	H	-1	4.41908500	-3.50646600	-1.98835500	L
C	-1	-8.94190200	5.12875600	-3.94272900	L	H	-1	8.19906000	-4.24096700	-5.13669900	L

H	-1	4.23158700	-2.74857400	-4.34122900	L	H	-1	-8.64517000	-3.09883900	-6.30886700	L
H	-1	7.00735000	-3.17052300	-6.53618000	L	H	-1	-8.09234800	-3.01826200	-4.63163900	L
H	-1	7.96236600	-6.47933000	-1.13770800	L	H	-1	-6.31787500	-3.96280300	-6.97502300	L
H	-1	6.06977700	-6.78909400	-2.53838800	L	H	-1	-5.77913600	-3.67034000	-5.32365300	L
H	-1	5.07365100	-7.02361000	-1.26332900	L	H	0	-6.94594800	-1.58308200	-7.31428300	H
H	-1	3.39076900	-2.90179900	3.18582600	L	H	0	-5.23170800	-1.80504300	-6.98519500	H
H	-1	3.27676900	-1.00227100	1.51533700	L	H	0	-7.28437900	-0.69826500	-5.15639600	H
H	-1	4.92227600	-0.49289800	1.98077300	L	H	0	-3.88399100	-1.90767300	-5.21021000	H
H	-1	3.60234200	-0.39737100	3.14513600	L	H	0	-3.50819700	-0.88478200	-3.82997100	H
H	-1	4.10535800	-3.24618400	1.08761100	L	H	0	-6.47410800	0.82711100	-3.61528400	H
H	-1	6.32764200	-1.91324800	3.48248500	L	H	0	-5.06679000	0.25111100	-2.71771200	H
H	-1	5.04779200	-4.42702700	3.96451100	L	H	-1	-8.05315700	-5.58070100	-6.38074200	L
H	-1	6.61687500	-3.99875000	4.02309000	L	H	-1	-10.23321200	-4.87752500	-5.79451400	L
H	0	1.38956200	3.81290100	4.65438100	H	H	-1	-9.86710600	-4.79916800	-4.20568800	L
H	0	3.14401400	4.12148100	4.64295700	H	H	-1	-5.08499700	-7.59016800	0.53395900	L
H	-1	2.58935600	2.99044700	6.68976900	L	H	-1	-5.42685200	-7.06760000	2.19000700	L
H	-1	4.17409700	1.57125900	4.75784900	L	H	-1	-2.96951200	-6.74304200	-0.64237400	L
H	-1	4.47064300	1.91310500	6.33972500	L	H	-1	-4.33330600	-4.66451400	3.04350600	L
H	-1	1.64617800	-2.39877400	4.60555800	L	H	-1	-1.59865500	-4.73833700	-1.04012600	L
H	-1	-0.30973300	-3.81932400	3.94831300	L	H	-1	-3.05727100	-3.07021700	2.67505900	L
H	-1	-1.42562200	-2.70172500	4.74922400	L	H	-1	-1.00660600	-2.75986900	-0.24116200	L
H	-1	-0.24366200	-3.61835800	5.70436900	L	H	-1	-2.73182900	-8.43246900	1.51715200	L
H	-1	0.52658200	-2.09733200	2.40933800	L	H	-1	-4.54083600	-9.75803900	0.71058500	L
H	-1	-0.61219700	-0.91359200	3.08357300	L	H	-1	-5.20769800	-9.84736200	2.19407100	L
H	-1	1.11513100	-0.52074300	2.96177800	L	H	-1	-5.38629500	-3.35150800	5.00744900	L
H	-1	-0.53972100	-0.41614700	5.58302400	L	H	-1	-3.74587100	-3.27292400	4.36168100	L
H	-1	2.25834700	-0.07133600	4.91367500	L	H	-1	-4.55801100	-1.87850700	6.99020700	L
H	0	6.98121400	-0.94882700	-2.75973500	H	H	-1	-3.03850200	-1.68895000	6.11752300	L
H	0	7.95774000	0.48654100	-2.50149400	H	H	0	-5.82540800	-0.89177600	5.02993500	H
H	0	4.82917700	-0.80698900	-4.01176100	H	H	0	-4.63815700	0.22390300	5.71330800	H
H	0	7.32665800	2.67185900	-3.62219200	H	H	0	-4.31988700	-1.31362000	3.18391100	H
H	0	2.93861100	0.60734700	-4.64370000	H	H	0	-3.46717000	-0.02176400	1.51386600	H
H	0	5.39987000	4.10699700	-4.25204200	H	H	0	-1.95817200	0.77393200	1.81057300	H
H	0	2.13499800	2.89518600	-4.65275300	H	H	0	-2.47008200	0.77131400	5.35752000	H
H	-1	7.81090100	-1.23608700	-5.05558100	L	H	-1	-1.84864700	1.76901400	4.03827300	H
H	-1	10.18569700	-1.38672800	-4.48648200	L	H	-1	-3.13914100	-3.90454200	6.91740800	L
H	-1	9.81059400	-0.93281200	-2.95804800	L	H	-1	-3.60042300	-5.42946400	4.58834200	L
H	-1	6.95061200	8.21875900	2.11158700	L	H	-1	-2.17892600	-4.78239200	5.72756800	L
H	-1	5.29327400	8.65639600	2.54634000	L	H	0	0.59786200	-1.70338200	-2.71068100	H
H	-1	6.29517200	9.58812300	-1.07652000	L	H	0	0.49086400	0.66984100	-4.23791600	H
H	-1	5.30119500	7.91214400	-2.67376800	L	H	0	1.86924100	0.97891700	-2.40285300	H
H	-1	4.45335200	6.13770400	2.31036700	L	H	0	2.52961500	-1.55953800	-1.25385600	H
H	-1	3.12289200	4.23196800	1.40383700	L	H	0	-1.41885500	-0.67182900	-0.59865400	H
H	-1	3.63634700	5.61536600	-2.63533900	L	H	0	-0.24295600	2.06946600	-1.20575000	H
H	-1	2.74281900	3.97248300	-1.00930500	L	H	0	-0.98682500	2.43594000	0.73993100	H
H	-1	5.61787400	10.74221600	0.93403800	L	H	0	0.99201400	-0.36812700	0.16015600	H
H	-1	8.40998900	10.00712000	1.43392000	L	H	0	1.79475200	1.71500100	0.93428700	H
H	-1	7.88565200	11.44904000	0.88503900	L	H	0	-2.53040300	1.57364900	-2.34518200	H
H	0	-0.44603800	4.69083700	4.22466800	H	H	0	-2.98960900	1.32213500	-0.62351500	H
H	0	-2.79881800	4.18533400	4.67152900	H	H	0	-3.47748600	-0.92964500	-1.37603600	H
H	0	-3.19175200	4.23841200	2.93795300	H	O	-1	7.36313500	11.20250000	3.60575400	L
H	0	-2.75236500	5.73114400	3.80967000	H	H	-1	8.36653500	0.88447900	-6.14037800	L
H	0	0.01472300	2.75748400	2.96473300	H	H	-1	7.71949800	-6.92780800	1.27346100	L
H	0	0.41094700	4.71582300	1.88006300	H	H	-1	1.06743000	-8.17533800	0.61506600	L
H	0	0.30992100	7.09529000	1.94532100	H	H	-1	-2.57732700	-7.78319700	3.87562700	L
H	0	-0.98730600	7.07424300	2.98298400	H	H	-1	-10.40783200	-2.16162800	3.82588600	L
H	-1	-4.93504200	7.32589500	-1.02716800	L	H	-1	-10.33443800	6.82681400	-3.31091600	L
H	-1	-3.84076700	8.29801000	-0.03851100	L	H	-1	5.34622000	11.36796200	3.30611700	L
H	-1	-3.63333100	7.82280100	2.43953300	L	H	-1	-2.15304800	6.67570200	-4.90547000	L
H	-1	-6.48380200	5.73330500	0.01460900	L	H	-1	5.52597600	-0.68813400	5.38378100	L
H	-1	-4.86322500	7.14430800	4.48487700	L	H	-1	4.27649100	-7.44927700	-3.97545100	L
H	-1	-7.72029500	5.04971500	2.02701600	L	H	-1	-6.57575500	-6.36745900	-4.60064600	L
H	-1	-7.79586400	5.14992500	4.24792600	L	H	-1	1.55644500	-1.85072800	7.44457400	L
H	-1	-3.53577700	5.26033800	-0.64265400	L	H	-1	-5.85104200	-5.51503700	6.77525100	L
H	0	-1.84992400	7.11029500	1.04780300	H	H	-1	-9.05069100	-3.70606800	-0.56344800	L
H	0	1.10739200	4.97420000	-4.27941400	H	N	-1	9.86505100	2.33540800	2.42731900	L
H	0	0.92400000	4.72419000	-2.55490200	H	C	-1	8.50992700	1.79644600	2.16361600	L
H	-1	-0.00580000	6.92357000	-3.02009700	L	C	0	8.17480900	1.92530500	0.66723600	H
H	-1	-2.12094800	4.88983700	-2.52961500	L	C	0	6.81883800	1.39620700	0.30427900	H
H	-1	-7.45638700	5.40601900	-2.39898300	L	N	0	6.66381700	0.10271000	-0.16251400	H
H	-1	-7.26256500	6.50872100	-3.76023500	L	C	0	5.38148500	-0.09378600	-0.46032500	H
H	-1	-6.76577500	3.46684500	-3.84550500	L	N	0	4.70409800	1.02830900	-0.19390000	H
H	-1	-6.55260500	4.56021900	-5.22118100	L	C	0	5.57560300	1.97016400	0.29588300	H
H	-1	-4.46127700	3.05177600	-4.38931300	L	C	-1	8.46116200	0.31013000	2.61513400	L
H	-1	-3.18787500	3.93896300	-3.69748500	L	O	-1	7.45838600	-0.12191500	3.18227600	L
H	-1	-9.09772000	4.02139200	-3.87515400	L	N	-1	9.49250600	-0.45317000	2.26437200	L
H	-1	-10.09251900	5.31379800	-5.61728600	L	C	-1	9.51504300	-1.88357000	2.48899500	L
H	-1	-8.91980300	6.44156000	-5.51777700	L	C	0	8.77372200	-2.67407100	1.39181700	H
H	-1	-8.18892700	0.06626100	3.26956800	L	C	0	9.28984100	-2.32772400	-0.05277000	H
H	-1	-9.22509100	1.50250700	3.33552600	L	O	0	10.11709700	-3.09202700	-0.55437700	H
H	-1	-9.95822500	0.69946300	-0.08673600	L	O	0	8.81130200	-1.25180300	-0.57258300	H
H	-1	-8.15107600	1.42411500	-1.72683800	L	C	-1	10.92719100	-2.42845500	2.61693500	L
H	-1	-6.15421400	1.80369700	3.18151900	L	O	-1	11.91279400	-1.68648700	2.36866100	L
H	-1	-4.09137100	2.93187600	2.28312200	L	H	0	8.92167700	1.37915100	0.05736200	H
H	-1	-5.73605700	2.88153500	-1.70927600	L	H	0	8.22330900	2.99133400	0.36873400	H
H	-1	-3.87377100	3.41257200	-0.13304000	L	H	0	5.22626900	2.94257700	0.61779000	H
H	-1	-9.99710100	-1.01310600	1.70332800	L	H	0	3.66976700	1.12189700	-0.23104600	H
H	-1	-12.18315500	-0.16470300	2.17685000	L	H	0	4.93501700	-0.99752900	-0.84159400	H
H	-1	-11.56158800	1.18117700	2.85777500	L	H	-1	7.74504900	2.35230300	2.76424400	L
H	-1	-6.35811400	-3.97320200	-1.52838900	L	H	-1	10.31718300	2.63103100	1.58686800	L
H	-1	-5.09912200	-4.09071600	-0.27204200	L	H	-1	9.80363900	3.10538100	3.05727200	L
H	-1	-6.73292800	-4.36109500	1.51619100	L	H	0	8.92082300	-3.75869200	1.55604800	H
H	-1	-6.60954400	-6.07035500	-0.60891900	L	H	0	7.68409800	-2.46898500	1.46443600	H
H	-1	-8.18658300	-5.99928600	-0.22391200	L	H	-1	8.98305500	-2.10921200	3.45050400	L

H -1 10.16077400 -0.10359200 1.60731000 L
H -1 11.05839100 -3.47899000 2.90283800 L
H 0 7.50959500 -0.58877100 -0.28396900 H
H 0 -6.11523100 -2.61743000 -0.36786000 L

Glc_E777Q

ONIOM: extrapolated energy = -3333.331872 au

N -1 3.12649000 -7.60418800 2.25346200 L
C -1 1.95789300 -6.75946400 2.14556700 L
C -1 2.31006700 -5.52152400 1.27744600 L H 4
C 0 1.22878000 -4.47694900 1.11064600 H
C 0 1.57445400 -3.48147100 -0.04490800 H
O 0 2.73668300 -2.97355200 -0.04859000 H
O 0 0.64604900 -3.22129400 -0.86306000 H
C -1 0.82649800 -7.53271000 1.45616200 L
O -1 -0.35383500 -7.43256700 1.88084400 L
N -1 1.48119300 -7.22657700 -4.91271800 L
C -1 2.49330100 -6.22409600 -4.64719100 L
C -1 1.86613100 -4.93169000 -4.08534600 L
C -1 0.55652700 -4.47971500 -4.71095000 L
C -1 0.38468200 -4.43378200 -6.08567600 L
C -1 -0.80791500 -3.98355100 -6.64367300 L
C -1 -1.82538700 -3.53924200 -5.81713000 L
O -1 -3.01733400 -3.08851700 -6.32412700 L
C -1 -1.66989700 -3.56892500 -4.44405600 L
C -1 -0.48307700 -4.02758000 -3.90437800 L
C -1 3.44905800 -6.84654800 -3.64164400 L
O -1 3.26033200 -6.68126600 -2.40850400 L
N -1 6.01909100 -7.15987400 -1.60744500 L
C -1 6.93163900 -6.37789200 -0.78087200 L
C -1 6.57154400 -4.89698400 -0.84101500 L
C -1 6.44893200 -4.38255500 -2.25171300 L
C -1 7.49012600 -4.59923200 -3.16082600 L
C -1 7.39495100 -4.17134700 -4.46451300 L
C -1 6.25034800 -3.53168300 -4.87170400 L
O -1 6.20561900 -3.10635400 -6.17276900 L
C -1 5.19786800 -3.30296600 -4.01292000 L
C -1 5.29831800 -3.73065800 -2.69341700 L
C -1 6.81052000 -6.82240100 0.67237000 L
O -1 5.67455200 -6.95291000 1.19783600 L
N -1 5.72943300 -3.81007700 4.30828000 L
C -1 5.44626300 -2.45895500 3.87657300 L
C -1 4.39051300 -2.45694800 2.79670000 L
O -1 4.86914100 -3.25107700 1.70229900 L
C -1 4.09154600 -1.04142500 2.31787600 L
C -1 4.98603600 -1.60296000 5.06937200 L
O -1 3.92448100 -1.89316800 5.67965900 L
N -1 3.89987500 1.50861600 5.69498600 L
C -1 2.67441200 2.34437100 5.75559600 L H 43
C 0 2.51464600 3.32048300 4.58817800 H
C 0 2.74058100 2.62544000 3.22050100 H
O 0 3.87996500 2.18360000 2.99791700 H
O 0 1.72708600 2.56056700 2.42959800 H
C -1 1.43206600 1.42800300 5.88088800 L
O -1 0.38218800 1.90881500 6.33679900 L
N -1 1.57876100 0.15820400 5.50691700 L
C -1 0.54434100 -0.87660500 5.65967700 L
C -1 0.67223000 -1.95061300 4.54607800 L
C -1 -0.34764900 -3.05511100 4.73360600 L
C -1 0.46730200 -1.30950400 3.17329400 L
C -1 0.62409500 -1.58420800 7.02260800 L
O -1 -0.43002000 -1.84746700 7.65751500 L
N -1 9.53784900 -1.41188900 -3.80821400 L
C -1 8.45016500 -0.62692400 -4.35725900 L H 58
C 0 7.48212400 -0.13664700 -3.27738000 H
C 0 6.34224900 0.74376800 -3.78906800 H
C 0 5.06761600 0.22256500 -4.04712700 H
C 0 3.99309400 1.03857600 -4.40867700 H
C 0 4.16537700 2.42490800 -4.50872600 H
O 0 3.15540300 3.28173700 -4.82594400 H
C 0 5.43930400 2.96430900 -4.27698000 H
C 0 6.49841800 2.13511300 -3.91825500 H
C -1 8.95083200 0.57170500 -5.17526100 L
O -1 9.88113300 1.29275600 -4.73006200 L
N -1 7.90782600 10.39470800 0.94869000 L
C -1 6.60976000 10.21147400 1.61365900 L
C -1 6.26847200 8.73172800 1.77049000 L
C -1 5.76252900 8.14074900 0.49880900 L
C -1 5.95550700 8.63520200 -0.78096500 L
N -1 5.32933600 7.84972100 -1.69484200 L
C -1 4.72585800 6.79575600 -1.04346400 L
C -1 4.98762300 6.94112800 0.34015100 L
C -1 4.45025400 5.99858300 1.23603000 L
C -1 3.70381300 4.95572800 0.71684800 L
C -1 3.48428500 4.81490200 -0.65663400 L
C -1 3.97676800 5.73202500 -1.55787600 L
C -1 6.54556600 10.95273100 2.94607900 L
N 0 -0.02879400 6.62157900 2.64642300 H
C 0 -0.36422400 5.27808200 2.17815300 H
C 0 -0.91129300 4.45344200 3.39741200 H
O 0 -0.76543500 3.05670200 3.21166700 H
C 0 -2.38060400 4.70840500 3.71868800 H
C 0 -1.29778800 5.16906400 0.95623000 H

O 0 -1.47877700 4.08729300 0.38703600 H
N 0 -1.91277000 6.31641800 0.56231900 H
C -1 -2.92509600 6.36451200 -0.55932700 L H 88
C -1 -4.03878700 7.34643700 -0.19121400 L
C -1 -4.80723500 6.92839300 1.06923400 L
C -1 -4.36831900 7.30182500 2.33162800 L
C -1 -5.05712500 6.92354000 3.48120600 L
C -1 -6.20075900 6.15378000 3.36128800 L
O -1 -6.89664200 5.77884300 4.50610100 L
C -1 -6.66137100 5.78294300 2.11949900 L
C -1 -5.95214600 6.16314800 0.97788100 L
C -1 -2.16126600 6.79056000 -1.81197900 L
O -1 -2.20521700 7.96263600 -2.22565100 L
N -1 -1.47428300 5.82183700 -2.41725600 L
C -1 -0.41068100 6.08630800 -3.42040200 L H 102
C 0 0.52035200 4.87274000 -3.49797700 H
C 0 -0.17559500 3.50205500 -3.68125200 H
O 0 -1.40858200 3.38327000 -3.42041700 H
O 0 0.60027900 2.55610300 -4.01169800 H
C -1 -0.89970900 6.52086300 -4.79079800 L
O -1 -0.06201600 6.64033300 -5.72222700 L
N -1 -8.96613500 5.63226900 -5.38842500 L
C -1 -8.77325500 5.27584200 -3.97145400 L
C -1 -7.35171700 5.58670200 -3.53246000 L
C -1 -6.33131800 4.62743700 -4.13811400 L
C -1 -4.91801100 4.91811900 -3.71912300 L
O -1 -4.59153500 6.03067600 -3.28488800 L
N -1 -4.04886300 3.91205000 -3.84738600 L
C -1 -9.79591600 5.98268000 -3.07653800 L
O -1 -10.22665300 5.41195400 -2.04101500 L
N -1 -11.29963100 0.61800800 2.15713000 L
C -1 -10.10923800 -0.14537600 2.50130800 L
C -1 -8.88247900 0.75352900 2.67961600 L
C -1 -8.27077100 1.22152700 1.38232700 L
C -1 -8.84955600 1.19362500 0.13563100 L
N -1 -7.98770100 1.74562100 -0.79044600 L
C -1 -6.84414500 2.15505700 -0.15484000 L
C -1 -6.98182500 1.83262200 1.21321700 L
C -1 -5.93988800 2.13512200 2.08778800 L
C -1 -4.79042200 2.71564200 1.59191400 L
C -1 -4.66306700 3.00936500 0.20473900 L
C -1 -5.68913900 2.74345600 -0.66808800 L
C -1 -10.43485000 -0.91203700 3.76784500 L
O -1 -10.80602700 -0.29428200 4.79943500 L
N -1 -7.24427800 -5.68700100 0.06031400 L
C -1 -7.08355300 -4.27726000 0.42448700 L
C -1 -6.07515700 -3.59955400 -0.51455700 L H 134
C 0 -6.08896000 -2.07725100 -0.41887400 H
C 0 -5.17178600 -1.62150000 0.71361500 H
O -1 -5.48302300 -1.74049200 1.90193800 H
C -1 -8.43144000 -3.53373000 0.33081100 L
O -1 -8.86879900 -2.89640200 1.32383800 L
N -1 -9.61061100 -5.08279300 -5.12046300 L
C -1 -8.20244800 -4.89347300 -5.46707700 L
C -1 -7.87292300 -3.41866900 -5.63047300 L
C -1 -6.44675900 -3.20694800 -6.12302100 L H 143
C 0 -6.18315800 -1.77341200 -6.57031800 H
N 0 -6.16025500 -0.81155900 -5.46424500 H
C 0 -5.07221300 -0.32283200 -4.83751400 H
N 0 -3.83366000 -0.66276000 -5.19304700 H
N 0 -5.21998600 0.59137400 -3.86837700 H
C -1 -7.32134800 -5.51453500 -4.36482300 L
O -1 -7.48592500 -5.17789800 -3.16350600 L
N -1 -4.39016300 -9.64779400 1.64909600 L
C -1 -3.74876200 -8.37690500 1.99056100 L
C -1 -4.60508500 -7.21284500 1.44928500 L
C -1 -3.78353600 -5.96786800 1.18773200 L
C -1 -2.97162000 -5.85549300 0.04718300 L
C -1 -2.18057100 -4.75206700 -0.15777700 L
C -1 -2.18466300 -3.73654600 0.76497400 L
O -1 -1.40260100 -2.64074700 0.57522700 L
C -1 -2.97022300 -3.82416700 1.90191000 L
C -1 -3.77604800 -4.93240800 2.08646400 L
C -1 -3.50294600 -8.24269800 3.49743800 L
O -1 -4.34230800 -8.70132400 4.31518100 L
N -1 -3.27151900 -5.40226700 5.50425300 L
C -1 -3.91225800 -4.31979800 6.23476900 L
C -1 -4.28871700 -3.15792100 5.29140600 L
C -1 -4.06974600 -1.81125100 5.93766000 L H 166
C 0 -4.65582500 -0.61501500 5.20147700 H
N 0 -4.01586700 -0.35192800 3.91303500 H
C 0 -2.97323800 0.45316100 3.66730900 H
N 0 -2.23664000 1.02685000 4.62513800 H
N 0 -2.67712800 0.70688100 2.37812500 H
C -1 -5.10614200 -4.70660700 7.11587400 L
O -1 -5.22512500 -4.21217700 8.26690500 L
C 0 0.41927900 -0.67703300 -2.63857900 H
O 0 0.09764900 -0.09772800 -3.86742900 H
C 0 1.59834600 -0.00060700 -1.85594800 H
O 0 2.73393700 -0.83497400 -1.82698100 H
O 0 -0.78724200 -0.81382600 -1.83005900 H
C 0 -1.21937900 0.24132800 -0.97968100 H
C 0 -1.4235200 1.20374100 -0.50632100 H
O 0 -0.52983500 1.65035900 0.79202900 H

C	0	1.20538900	0.50191600	-0.45179100	H	-1	-1.95907400	4.94571900	-2.54411300	L	
O	0	2.18134300	1.43964900	-0.02498300	H	-1	-7.28759400	5.53126400	-2.42408600	L	
C	0	-2.38874400	0.93512800	-1.67570300	H	-1	-7.07646000	6.63348900	-3.78314700	L	
O	0	-3.15404900	-0.13064300	-2.31981700	H	-1	-6.61920700	3.58552900	-3.87223600	L	
H	-1	2.65625100	-5.87610600	0.28034200	H	-1	-6.38881700	4.67819600	-5.24569500	L	
H	-1	3.19516900	-5.02769000	1.73731500	L	-1	-4.31914900	3.14127000	-4.41174700	L	
H	0	0.24012800	-4.92883200	0.89425400	H	-1	-3.03580000	4.01070700	-3.71565500	L	
H	0	1.11666100	-3.86023300	2.03751500	H	-1	-8.94365000	4.17050000	-3.90599100	L	
H	-1	1.64867200	-6.43885800	3.17021900	L	-1	-9.91773400	5.47852200	-5.64817500	L	
H	-1	3.45141200	-7.87989900	1.34958300	L	-1	-8.73062600	6.59072800	-5.54434200	L	
H	-1	3.84680400	-7.13955400	2.76435400	L	-1	-8.10198800	0.19258400	3.23430300	L	
H	-1	1.69881800	-5.02441800	-2.99125000	L	-1	-9.11946900	1.64212100	3.30034600	L	
H	-1	2.60569200	-4.10754400	-4.20277500	L	-1	-9.85560900	0.85411000	-0.12476500	L	
H	-1	1.19517600	-4.76163100	-6.74776100	L	-1	-8.03561700	1.55770700	-1.75982400	L	
H	-1	-0.37301900	-4.03291800	-2.81100100	L	-1	-6.04459800	1.90346000	3.15340400	L	
H	-1	-0.91288100	-3.96437500	-7.73548500	L	-1	-3.96528100	3.00604200	2.26124900	L	
H	-1	-2.46446700	-3.21973500	-3.77337200	L	-1	-5.60183700	2.98346400	-1.73474700	L	
H	-1	-2.95996800	-3.13777100	-7.27098500	L	-1	-3.73619700	3.48767100	-0.15367300	L	
H	-1	3.02657100	-6.00297000	-5.60413100	L	-1	-9.92069400	-0.86062700	1.66246100	L	
H	-1	1.90466100	-8.08397300	-5.20152400	L	-1	-12.09651500	0.01547800	2.13265800	L	
H	-1	0.91414800	-7.38390500	-4.10574900	L	-1	-11.45892000	1.35205700	2.81707300	L	
H	-1	5.62385800	-4.70446600	-0.29261300	L	-1	-6.31364300	-3.86285000	-1.56619900	L	
H	-1	7.34480100	-4.29036400	-0.31730800	L	-1	-5.05901300	-3.99876200	-0.30734700	L	
H	-1	8.41783500	-5.07300000	-2.81229200	L	0	-5.74472500	-1.63612700	-1.37145500	H	
H	-1	4.46968300	-3.53604100	-2.00230300	L	0	-7.10225200	-1.68288900	-0.21806500	L	
H	-1	8.24657100	-4.31483600	-5.14372900	L	-1	-6.70007300	-4.25062200	1.47694500	L	
H	-1	4.29719100	-2.77206100	-4.35436900	L	-1	-6.59439800	-5.95799100	-0.65063800	L	
H	-1	7.07195700	-3.22672800	-6.54404100	L	-1	-8.17120500	-5.86960000	-0.26889700	L	
H	-1	7.97204800	-6.55622500	-1.14885300	L	-1	-8.57875200	-2.95118200	-6.35015700	L	
H	-1	6.07861500	-6.83905900	-2.55408200	L	-1	-8.02855600	-2.88047000	-4.67162100	L	
H	-1	5.07675800	-7.06256900	-1.28153800	L	-1	-6.26148700	-3.84438500	-7.01271000	L	
H	-1	3.43816200	-2.92617500	3.17061100	L	-1	-5.72255500	-3.56158100	-5.35972100	L	
H	-1	3.35256300	-1.02268900	1.50293400	L	0	-6.95950300	-1.43809200	-7.28175000	H	
H	-1	5.00356400	-0.53556300	1.97271300	L	0	-5.22515900	-1.69268100	-7.10973000	H	
H	-1	3.68247200	-0.42465900	3.13439600	L	0	-7.03804600	-0.66683700	-4.98338600	H	
H	-1	4.15279900	-3.27652400	1.07330900	L	0	-3.60809600	-1.034852700	-5.65717900	H	
H	-1	6.38703100	-1.97649600	3.47515100	L	0	-3.05765000	-0.21837000	-4.70439700	H	
H	-1	5.07346000	-4.47411900	3.95039600	L	0	-6.13738100	0.93722800	-3.62153900	H	
H	-1	6.64786500	-4.06644400	4.01302500	L	0	-4.46937600	0.56519800	-3.15246700	H	
H	0	1.52475800	3.80920000	4.64063800	H	-1	-8.01900800	-5.44044100	-6.42474800	L	
H	0	3.27852100	4.11739800	4.67337400	H	-1	-10.19096900	-4.70980600	-5.84206500	L	
H	-1	2.70609500	2.97049100	6.68228500	L	-1	-9.82731000	-4.63873800	-4.25233400	L	
H	-1	4.27636500	1.53379400	4.75148800	L	-1	-5.09228100	-7.49936800	0.49306300	L	
H	-1	4.57392300	1.86924900	6.33454300	L	-1	-5.43087300	-6.97499600	2.14921200	L	
H	-1	1.69721300	-2.40267000	4.58740700	L	-1	-2.96338500	-6.67806100	-0.67737200	L	
H	-1	-0.27563600	-3.79654100	3.92369300	L	-1	-4.30792300	-4.58773200	3.00891000	L	
H	-1	-1.37858100	-2.66574200	4.72400300	L	-1	-1.56563800	-4.69078800	-1.06896600	L	
H	-1	-0.21074800	-3.59922400	5.68020700	L	-1	-3.01040700	-3.00964100	2.64575800	L	
H	-1	0.58639800	-2.08318200	2.38928000	L	-1	-0.94956500	-2.72147900	-0.26555800	L	
H	-1	-0.53829900	-0.88574900	3.06297200	L	-1	-2.75243400	-8.37384900	1.47994400	L	
H	-1	1.19426600	-0.51527900	2.94551000	L	-1	-4.57682800	-9.67443000	0.66737400	L	
H	-1	-0.46474800	-0.39323600	5.56336900	L	-1	-5.24800700	-9.75738500	2.14928300	L	
H	-1	2.33902100	-0.08390700	4.90057200	L	-1	-5.34794200	-3.26419700	4.97269400	L	
H	0	7.06726900	-1.02252100	-2.76661500	H	-1	-3.70523900	-3.20600700	4.33057400	L	
H	0	8.04921000	0.40766800	-2.50168300	L	-1	-4.50481900	-1.80527200	6.95958200	L	
H	0	4.88707400	-0.84834700	-3.93764700	H	-1	-2.98107100	-1.63416900	6.09047100	L	
H	0	7.47100000	2.58171900	-3.70879200	H	0	-5.72802100	-0.77257200	4.98965200	H	
H	0	3.01333000	0.60103800	-4.58187700	H	0	-4.57494500	0.29574100	5.82353300	H	
H	0	5.56612000	4.04262700	-4.34466400	H	0	-4.41048900	-0.87633000	3.12043600	H	
H	0	2.27328000	2.88839900	-4.61027600	H	0	-3.43750400	0.75588800	1.70904900	H	
H	-1	7.89746700	-1.30527800	-5.05862100	L	0	-1.80665100	1.17374700	2.08749800	H	
H	-1	10.26885900	-1.48779000	-4.48467500	L	0	-2.05035100	0.54748900	5.50268800	H	
H	-1	9.89640200	-1.03143000	-2.95632000	L	0	-1.56848100	1.75612400	4.32335300	H	
H	-1	7.14507600	8.14867100	2.12185800	L	-1	-3.11233200	-3.84951800	6.88657700	L	
H	-1	5.49265100	8.60720800	2.55376100	L	-1	-3.58842500	-5.36461600	4.55408200	L	
H	-1	6.51445400	9.53149600	-1.06544300	L	-1	-2.16107700	-4.73794300	5.69738900	L	
H	-1	5.50215700	7.87115100	-2.66750700	L	0	0.68317700	-1.71992000	-2.80690200	H	
H	-1	4.62045800	6.10006500	2.31194600	L	0	0.21991300	0.89062100	-3.85809900	L	
H	-1	3.26721800	4.21328200	1.39950800	L	0	1.89655300	0.88851100	-2.42179200	H	
H	-1	3.80741200	5.59623000	-2.63633500	L	0	2.58474500	-1.62675700	-1.23602500	H	
H	-1	2.88901400	3.96258200	-1.01485500	L	0	-1.56641900	-0.26560400	-0.07135300	H	
H	-1	5.84791900	10.69115600	0.94550900	L	0	-0.05560100	2.06583900	-1.17630500	H	
H	-1	8.62911800	9.91890400	1.45019300	L	0	-0.71892700	2.61406600	0.75647000	H	
H	-1	8.12482400	11.36840700	0.90250500	L	0	1.15029500	-0.35367700	0.24079100	H	
H	0	-0.29338100	4.79881800	4.23865200	H	0	1.99423900	1.75540200	0.90787900	H	
H	0	-2.64050100	4.23585100	4.67236000	H	0	-2.05547800	1.65226000	-2.43282500	H	
H	0	-3.01974000	4.27099300	2.93654400	H	0	-3.05151300	1.44377800	-0.96370100	H	
H	0	-2.61627100	5.77902400	3.80116900	H	0	-2.41249500	-0.75831900	-2.54873500	H	
H	0	0.19476700	2.84141600	2.97447300	H	0	-1.759325000	11.12441500	3.62169500	L	
H	0	0.57245200	4.78772200	1.88882400	H	-1	8.48306100	0.80956500	-6.13881700	L	
H	0	0.45148500	7.17355600	1.94163000	H	-1	7.71813400	-7.00529800	1.26106600	L	
H	0	-0.83031400	7.13942600	2.99898400	H	-1	1.05179900	-8.16488900	0.58641500	L	
H	-1	-4.74439600	7.41591200	-1.04378900	L	-1	-2.59457900	-7.73037000	3.83978300	L	
H	-1	-3.63967400	8.37210700	-0.05122900	L	-1	-10.35096300	-2.00703900	3.78228700	L	
H	-1	-3.44381600	7.89032300	2.42648600	L	-1	-10.14488700	6.99092600	-3.33990200	L	
H	-1	-6.31604700	5.84202500	-0.00789200	L	-1	5.57931800	11.31665100	3.31800200	L	
H	-1	-4.68687900	7.22471000	4.46809800	L	-1	-1.96263600	6.73566300	-4.96223800	L	
H	-1	-7.56570400	5.17145300	2.00076000	L	-1	5.59730100	-0.74402700	5.37668800	L	
H	-1	-7.64476400	5.26913700	4.22166100	L	-1	4.27998400	-7.47352000	-3.99604200	L	
H	-1	-3.37302600	5.33167000	-0.65959600	L	-1	-6.55585000	-6.24921400	-4.64275500	L	
H	0	-1.69587700	7.18150900	1.05004300	H	-1	1.60849300	-1.85797800	7.42710100	L	
H	0	1.27744400	5.00178100	-4.29565200	H	-1	-5.84469600	-5.42426500	6.73602300	L	
H	0	1.12197700	4.78110100	-2.56662500	H	-1	-9.00458900	-3.56213000	-0.60660200	L	
H	-1	0.18347600	6.95244700	-3.02677500	L	N	-1	9.98183400	2.22730300	2.43439000	L

C	-1	8.62036300	1.70648200	2.16691800	L H 370	C	-1	-8.50224800	-0.40461900	4.08271600	L H 58
C	0	8.29776600	1.83861800	0.66783300	H	C	0	-7.47916400	0.05499100	3.03830900	H
C	0	6.94686200	1.30771800	0.29267100	H	C	0	-6.39225100	0.98406800	3.57640100	H
N	0	6.79095400	0.00980800	-0.16146600	H	C	0	-5.13235300	0.49716800	3.94828700	H
C	0	5.50949600	-0.18318400	-0.46595200	H	C	0	-4.09460600	1.33975200	4.34915700	H
N	0	4.83631000	0.94546000	-0.21942300	H	C	0	-4.28637800	2.72921100	4.37321700	H
C	0	5.70711900	1.88801700	0.26784200	H	O	0	-3.32122200	3.61576400	4.71640300	H
C	-1	8.55124500	0.22022100	2.61594400	L	C	0	-5.55039500	3.23593100	4.02184800	H
O	-1	7.54169100	-0.19959800	3.18024100	L	C	0	-6.57293300	2.37771300	3.62527500	H
N	-1	9.57330000	-0.55591700	2.26616700	L	C	-1	-9.02525900	0.82764200	4.83403900	L
C	-1	9.57668600	-1.98683800	2.48854300	L H 380	O	-1	-9.92025200	1.54619800	4.31805400	L
C	0	8.82796600	-2.76834200	1.39003300	H	N	-1	-7.51781700	10.42401100	-1.54713400	L
C	0	9.36184100	-2.44304600	-0.05172900	H	C	-1	-6.19051300	10.20052600	-2.13794100	L
O	0	10.17399100	-3.22777800	-0.54529900	H	C	-1	-5.86479600	8.71174700	-2.22831800	L
O	0	8.91148800	-1.35885100	-0.58225500	H	C	-1	-5.43371800	8.15683000	-0.91353800	L
C	-1	10.98133000	-2.55030600	2.61863300	L	C	-1	-5.68404100	8.69661400	0.33766900	L
O	-1	11.97706300	-1.82087000	2.37366300	L	N	-1	-5.11767400	7.93363800	1.30789500	L
H	0	9.05163400	1.29691900	0.06215000	H	C	-1	-4.49825000	6.85010800	0.72343300	L
H	0	8.34595600	2.90562900	0.37322300	H	C	-1	-4.68673600	6.95255900	-0.67586000	L
H	0	5.35944500	2.86409300	0.58021000	H	C	-1	-4.11910500	5.97308300	-1.51143000	L
H	0	3.80224200	1.04997200	-0.25868500	H	C	-1	-3.41650900	4.93797400	-0.92051500	L
H	0	5.06022300	-1.09237800	-0.83287500	H	C	-1	-3.26960600	4.84031700	0.46634000	L
H	-1	7.86151000	2.27132900	2.76679800	H	C	-1	-3.79308800	5.79394100	1.31040800	L
H	-1	10.43960000	2.51832700	1.59538600	L	C	-1	-6.04682100	10.89565600	-3.48889300	L
H	-1	9.92910800	2.99701700	3.06544500	L	N	0	0.40645900	6.47333100	-2.68729000	H
H	0	8.95176200	-3.85458100	1.56179900	H	C	0	0.69397400	5.14046900	-2.14105000	H
H	0	7.74211500	-2.54145400	1.45377800	H	C	0	1.30051800	4.25472100	-3.28277400	H
H	-1	9.03972600	-2.20704100	3.44854500	L	O	0	1.14785600	2.87863600	-3.02117900	H
H	-1	10.24749000	-0.21405200	1.61110200	L	C	0	2.78621300	4.49550600	-3.53731100	H
H	-1	11.09819600	-3.60291300	2.90313000	L	C	0	1.55417700	5.07170200	-0.86557200	H
H	0	7.64108400	-0.68848400	-0.28254300	H	O	0	1.65347200	4.03002200	-0.22043300	H
H	0	-3.22426800	-1.06204800	0.95661700	H	N	0	2.20118500	6.22427100	-0.51547600	H
H	0	-3.75049000	-1.03299500	-0.68546600	H	C	-1	3.15978200	6.29655200	0.64870700	L H 88
N	0	-3.99826600	-1.09770700	0.30090300	H	C	-1	4.30600300	7.24997600	0.30644600	L

Glc_R786A

ONIOM: extrapolated energy = -3107.380446 au

N	-1	-2.95754900	-7.67326700	-2.01224200	L	O	-1	6.62764100	5.90876600	-3.08883200	L
C	-1	-1.78294400	-6.84172100	-1.87204200	L	O	-1	7.37512700	5.48596100	-4.18333200	L
C	-1	-2.15962000	-5.70549000	-1.06432900	L H 4	C	-1	7.01841400	5.57347200	-1.81345000	L
C	0	-1.08831900	-4.52202600	-0.84811800	H	C	-1	6.25785100	6.00162100	-0.72300100	L
C	0	-1.51991100	-3.46956900	0.24151500	H	C	-1	2.33973700	6.77499300	1.84566000	L
O	0	-2.71187500	-3.04122700	0.21028800	H	O	-1	2.38079800	7.95957700	2.22235400	L
O	0	-0.61645300	-3.09464900	1.03874600	H	N	-1	1.60771700	5.83678600	2.44619300	L
C	-1	-0.70042500	-7.60703100	-1.10023000	L	C	-1	0.49854500	6.14955500	3.38396700	L H 102
O	-1	0.50146900	-7.53762100	-1.46656900	L	C	0	-0.43744400	4.93600000	3.46953100	H
N	-1	-1.67455300	-7.07812700	5.21295500	L	C	0	0.14779300	3.66344400	4.18371800	H
C	-1	-2.65601900	-6.07115800	4.86285300	L	O	0	1.38407800	3.58055800	4.37413000	H
C	-1	-1.98089300	-4.80719000	4.29196200	L	O	0	-0.73880100	2.79955800	4.47534400	H
C	-1	-0.69804200	-4.35270900	4.96906200	L	C	-1	0.92369800	6.62304100	4.76274200	L
C	-1	-0.59590800	-4.26302900	6.34856900	L	O	-1	0.04151100	6.78535600	5.64533200	L
C	-1	0.57352700	-3.81093400	6.95221400	L	N	-1	8.93424600	5.64298600	5.80418100	L
C	-1	1.63867800	-3.40881600	6.16507500	L	C	-1	8.80841800	5.24189200	4.39161600	L
O	-1	2.81007600	-2.95793400	6.71776600	L	C	-1	7.41616900	5.55756300	3.86996900	L
C	-1	1.55304500	-3.48242900	4.78752600	L	C	-1	6.35133700	4.63345300	4.45338400	L
C	-1	0.38831700	-3.94240100	4.20274000	L	C	-1	4.96597100	4.92951800	3.95279000	L
C	-1	-3.56879200	-6.71368200	3.83035400	L	O	-1	4.67948900	6.03129600	3.46602200	L
O	-1	-3.31480100	-6.59254100	2.60382000	L	N	-1	4.07581400	3.94051000	4.06905000	L
N	-1	-6.03619900	-7.05938900	1.67777600	L	C	-1	9.88633800	5.90399600	3.52788200	L
C	-1	-6.89304500	-6.29299600	0.78004500	L	O	-1	10.36042000	5.29288600	2.53522800	L
C	-1	-6.51342500	-4.81605200	0.81002700	L	N	-1	11.57138600	0.34621600	-1.44241400	L
C	-1	-6.45498000	-4.25629500	2.20752300	L	C	-1	10.38834900	-0.41167500	-1.82224700	L
C	-1	-7.54448200	-4.42782700	3.06838400	L	C	-1	9.18647000	0.49770000	-2.09295800	L
C	-1	-7.50932200	-3.95776900	4.36049500	L	C	-1	8.51670700	1.01745500	-0.84498300	L
C	-1	-6.37715800	-3.32076300	4.80492500	L	C	-1	9.03058500	1.02339200	0.43013100	L
O	-1	-6.39227800	-2.85264700	6.09190300	L	N	-1	8.13129500	1.61810100	1.29193700	L
C	-1	-5.27876700	-3.13566500	3.99448600	L	C	-1	7.02820700	2.02181700	0.58513800	L
C	-1	-5.31838400	-3.60598800	2.68630900	L	C	-1	7.23050100	1.65174000	-0.76268200	L
C	-1	-6.70484400	-6.78769600	-0.64964800	L	C	-1	6.23942000	1.93915600	-1.69925200	L
O	-1	-5.54570600	-6.95155400	-1.11129800	L	C	-1	5.07533800	2.55191500	-1.28261000	L
N	-1	-5.39267300	-3.91448600	-4.32191700	L	C	-1	4.88192800	2.89380200	0.08577200	L
C	-1	-5.11086200	-2.55369500	-3.92077000	L	C	-1	5.85782700	2.64311600	1.01858200	L
C	-1	-4.11171600	-2.53010300	-2.78856500	L	C	-1	10.76619300	-1.22488700	-3.04447000	L
O	-1	-4.65794200	-3.28029200	-1.69479600	L	O	-1	11.19914500	-0.64734100	-4.07527900	L
C	-1	-3.81553300	-1.10358900	-2.34168900	L	N	-1	7.31638400	-5.82784700	0.64841300	L
C	-1	-4.57703900	-1.74471800	-5.11571500	L	C	-1	7.19647700	-4.42903300	0.23036300	L
O	-1	-3.49037000	-2.06998400	-5.66062100	L	C	-1	6.15215000	-3.70621900	1.09343500	L H 134
N	-1	-3.41193200	1.32869300	-5.78630600	L	C	0	6.17724200	-2.19193300	0.96979300	H
C	-1	-2.17208400	2.14483400	-5.81108100	L H 43	C	0	5.37163300	-1.68295900	-0.24828900	H
C	0	-2.04987300	3.15339300	-4.66700500	H	O	0	5.76986300	-1.98759800	-1.40191300	H
C	0	-2.37642100	2.50591000	-3.29256600	H	O	0	4.36174100	-0.97741600	0.03916300	H
O	0	-3.55010700	2.11644500	-3.13598400	H	C	-1	8.54926200	-3.70158300	0.36893300	L
O	0	-1.41616600	2.42833800	-2.44985800	H	O	-1	9.04663800	-3.10410200	-0.62061500	L
C	-1	-0.93941300	1.20759200	-5.84201800	L	N	-1	9.42428100	-5.08295400	5.92164300	L
O	-1	0.13974700	1.65818400	-6.25875000	L	C	-1	8.00338500	-4.86254600	6.18881500	L
N	-1	-1.12480400	-0.04677000	-5.43463200	L	C	-1	7.68900100	-3.37864900	6.28651300	L
C	-1	-0.10020700	-1.10040300	-5.49982400	L	C	-1	7.17012300	-5.50796600	5.06359200	L
C	-1	-0.30152500	-2.13452900	-4.35964500	L	O	-1	7.40104700	-5.21418000	3.86195400	L
C	-1	0.70923900	-3.25877000	-4.45800200	L	N	-1	4.48564300	-9.79970500	-0.95450000	L
C	-1	-0.15696900	-1.45059200	-2.99990600	L	C	-1	3.88242000	-8.53220700	-1.37010200	L
C	-1	-0.12130900	-1.85219900	-6.84109200	L	C	-1	4.72805400	-7.36264300	-0.82390900	L
O	-1	0.95960800	-2.15125600	-7.41184000	L	C	-1	3.91375000	-6.09828500	-0.64605400	L
N	-1	-9.57259800	-1.19239000	3.50439800	L	C	-1	3.04651900	-5.93639900	0.44682700	L
						C	-1	2.26335200	-4.81582400	0.57441300	L

C	-1	2.33039300	-3.83201800	-0.37973500	L	H	-1	-3.68115000	5.69209800	2.40003900	L
O	-1	1.55685800	-2.71970100	-0.26662000	L	H	-1	-2.70677400	3.99231500	0.88254800	L
C	-1	3.17150900	-3.96867900	-1.47118100	L	H	-1	-5.45638400	10.69173800	-1.44751800	L
C	-1	3.96831300	-5.09358600	-1.57747900	L	H	-1	-8.21990300	9.94170600	-2.06925900	L
C	-1	3.71597800	-8.44527500	-2.89123700	L	H	-1	-7.72167000	11.40163300	-1.54418100	L
O	-1	4.58873400	-8.94272500	-3.64913700	L	H	0	0.73001700	4.55481700	-4.17649000	H
N	-1	3.63165600	-5.67089400	-4.99946400	L	H	0	3.09877600	3.95750700	-4.43891000	H
C	-1	4.32567000	-4.62257800	-5.73112000	L	H	0	3.37866800	4.10600600	-2.69620200	H
C	-1	4.67154600	-3.43501900	-4.80824400	L	H	0	3.02613700	5.56056500	-3.67523500	H
C	-1	4.50693200	-2.10791900	-5.50879300	L	H	0	0.17792800	2.67097100	-2.84906900	H
C	0	5.08827500	-0.93606200	-4.71520700	H	H	0	-0.26511800	4.67744400	-1.88479000	H
N	0	4.42715300	-0.72165900	-3.44051900	H	H	0	-0.04534400	7.06853600	-1.99718500	H
C	0	3.41202200	0.12645400	-3.20038700	H	H	0	1.24722600	6.94068600	-3.02227000	H
N	0	2.86259800	0.86294300	-4.20152200	H	H	-1	4.96816000	7.33823500	1.19152200	L
N	0	3.00577400	0.28411400	-1.95225100	H	H	-1	3.93060800	8.27582100	0.11249200	L
C	-1	5.55679600	-5.05531400	-6.53634600	L	H	-1	3.85400400	7.71387400	-2.35487600	L
O	-1	5.74208600	-4.60151700	-7.69532200	L	H	-1	6.56589700	5.70875500	0.29022600	L
C	0	-0.59669900	-0.40258400	3.10221900	H	H	-1	5.18913600	6.96286300	-4.30675400	L
O	0	-0.99648200	-0.09993100	4.41399000	H	H	-1	7.90585300	4.95380300	-1.62825100	L
C	0	-1.60843300	0.16271700	2.06403900	H	H	-1	8.09970700	4.97574400	-3.84413400	L
O	0	-2.73877500	-0.69184100	1.93793700	H	H	-1	3.58583800	5.26152800	0.80577200	L
O	0	0.70765800	0.15261400	2.98920100	H	H	0	2.05435700	7.06130000	-1.07085500	H
C	0	1.28914100	0.34419500	1.70875600	H	H	0	-1.37888000	5.21442700	3.98438500	H
C	0	0.34710500	1.19767400	0.84452200	H	H	0	-0.76067000	4.61626800	2.45468800	H
O	0	0.86847900	1.42064100	-0.47495000	H	H	-1	-0.06115000	7.01015900	2.93201800	L
C	0	-1.00763200	0.51574200	0.70086000	H	H	-1	2.07167100	4.95876900	2.62656000	L
O	0	-1.93291000	1.40175000	0.05378400	H	H	-1	7.40785700	5.46583300	2.76218100	L
C	0	2.63593300	1.02707400	1.96781300	H	H	-1	7.14484100	6.61590300	4.07164200	L
O	0	3.63761400	0.14321500	2.44875700	H	H	-1	6.63613000	3.57930300	4.23704000	L
H	-1	-2.56174600	-5.88660400	-0.07529300	L	H	-1	6.35300100	4.72057400	5.56019200	L
H	-1	-3.01227600	-5.08018500	-1.58516800	L	H	-1	4.30487700	3.18542200	4.67157300	L
H	0	-0.12136900	-4.96483900	-0.53418100	H	H	-1	3.07246200	4.04874200	3.88208800	L
H	0	-0.88798300	-3.93959200	-1.78272600	H	H	-1	8.96466400	4.13271400	4.37133900	L
H	-1	-1.41685200	-6.56003300	-2.88936500	L	H	-1	9.86882800	5.48483600	6.11754000	L
H	-1	-3.33245500	-7.91392700	-1.11774900	L	H	-1	8.70606800	6.60932100	5.91620800	L
H	-1	-3.64350300	-7.21608400	-2.57455700	L	H	-1	8.42665600	-0.07065400	-2.66842400	L
H	-1	-1.75941000	-4.93892300	3.21157800	L	H	-1	9.46867700	1.36156500	-2.72947900	L
H	-1	-2.71253400	-3.96936600	4.34400200	L	H	-1	10.01661100	0.67886200	0.75303800	L
H	-1	-1.44416400	-4.55716300	6.97840200	L	H	-1	8.12672100	1.46219800	2.26814100	L
H	-1	0.33413800	-3.98293600	3.10591000	L	H	-1	6.39476700	1.67040600	-2.74987600	L
H	-1	0.62290300	-3.75656600	8.04676700	L	H	-1	4.29006900	2.83112200	-2.00274500	L
H	-1	2.38617000	-3.16703600	4.14758800	L	H	-1	5.71993900	2.91999900	2.07087000	L
H	-1	2.70368300	-2.97455900	7.66151400	L	H	-1	3.94554500	3.39670900	0.38004200	L
H	-1	-3.23393200	-5.81063100	5.78326100	L	H	-1	10.14608800	-1.09566400	-0.97120900	L
H	-1	-2.12554100	-7.91937300	5.50753700	L	H	-1	12.35648200	-0.26617000	-1.35713700	L
H	-1	-1.06957500	-7.27033200	4.44188500	L	H	-1	11.77559400	1.05540500	-2.11700800	L
H	-1	-5.53608900	-4.65524900	0.30517600	L	H	-1	6.33250500	-3.93734800	2.16404400	L
H	-1	-7.24937700	-4.21667200	0.22753200	L	H	-1	5.14180900	-4.09800400	0.84733900	L
H	-1	-8.46046800	-4.90009200	2.68823500	L	H	0	5.74610900	-1.73550600	1.87588400	H
H	-1	-4.45261600	-3.44622700	2.03281400	L	H	0	7.21496700	-1.81164100	0.87433200	H
H	-1	-8.39664300	-4.06651800	4.99925800	L	H	-1	6.86769000	-4.43242500	-0.84076600	L
H	-1	-4.38852200	-2.60616300	4.36429300	L	H	-1	6.62690600	-6.06575100	1.33343500	L
H	-1	-7.27821300	-2.94843100	6.42178000	L	H	-1	8.22237300	-6.00951600	1.03069200	L
H	-1	-7.95354000	-6.44439300	1.09956700	L	H	-1	8.36437700	-2.89711400	7.02588700	L
H	-1	-6.13896000	-6.70616900	2.60904500	L	H	-1	7.90176200	-2.87516800	5.31981000	L
H	-1	-5.07705300	-6.98619000	1.39785400	L	H	-1	7.76278000	-5.37444400	7.15319400	L
H	-1	-3.14895600	-3.02481100	-3.09728900	L	H	-1	9.97279200	-4.69404800	6.65956700	L
H	-1	-3.11891600	-1.06777000	-1.49079600	L	H	-1	9.69192000	-4.67135700	5.05173000	L
H	-1	-4.73597800	-0.57379400	-2.06078200	L	H	-1	5.16126700	-7.62363700	0.16504200	L
H	-1	-3.35573300	-0.52033600	-3.15584200	L	H	-1	5.59210900	-7.15993300	-1.48777200	L
H	-1	-3.97508900	-3.29457800	-1.02926400	L	H	-1	2.98847000	-6.73397800	1.19660400	L
H	-1	-6.06325400	-2.04499900	-3.58442300	L	H	-1	4.55190100	-4.78750700	-2.48210000	L
H	-1	-4.76626700	-4.57518900	-3.90909500	L	H	-1	1.60373400	-4.71544000	1.45019300	L
H	-1	-6.32886900	-4.14800300	-4.06613700	L	H	-1	3.26232000	-3.18022900	-2.23830300	L
H	0	-1.04124000	3.60483300	-4.67372300	H	H	-1	1.06028500	-2.76584600	0.55189400	L
H	0	-2.78140300	3.97149500	-4.81950700	H	H	-1	2.86149300	-8.49815900	-0.91189200	L
H	-1	-2.14664200	2.73986000	-6.75821700	L	H	-1	4.62150700	-9.79595100	0.03588200	L
H	-1	-3.83566300	1.39077600	-4.86480700	L	H	-1	5.36608900	-9.93794400	-1.40594000	L
H	-1	-4.04674300	1.67698300	-6.47125100	L	H	-1	5.71134600	-3.54524900	-4.43205500	L
H	-1	-1.32999000	-2.57342800	-4.43888900	L	H	-1	4.03911100	-3.44270100	-3.87771100	L
H	-1	0.58441000	-3.97151100	-3.62897700	L	H	-1	4.99361500	-2.14227700	-6.50657700	L
H	-1	1.74428600	-2.88366500	-4.40806000	L	H	-1	3.43034900	-1.92093300	-5.72323500	L
H	-1	0.61236800	-3.83240800	-5.39203000	L	H	0	6.15573300	-1.12376400	-4.49098300	H
H	-1	-0.32799400	-2.19577500	-2.19810100	L	H	0	5.04745300	-0.00630400	-5.31653200	H
H	-1	0.84817800	-1.03739000	-2.85186900	L	H	0	4.83735400	-1.23206200	-2.62034500	H
H	-1	-0.88213200	-0.63913800	-2.83608700	L	H	0	3.51383300	-0.21149900	-1.18675000	H
H	-1	0.91006900	-0.62814500	-5.36755000	L	H	0	2.13414500	0.75158400	-1.68758800	H
H	-1	-1.91871300	-0.25779200	-4.86065800	L	H	0	2.83335700	0.47853200	-5.13507900	H
H	0	-7.01413600	-0.84577600	2.60133400	H	H	0	2.12819000	1.53023600	-3.93832700	H
H	0	-8.01224500	0.54449200	2.20337200	H	H	-1	3.56749700	-4.16337800	-6.43837600	L
H	0	-4.92632400	-0.57174700	3.89020400	H	H	-1	3.90019000	-5.60576500	-4.03597000	L
H	0	-7.53287100	2.80172800	3.32350900	H	H	-1	2.54302500	-4.99806100	-5.27127900	L
H	0	-3.12742900	0.91055400	4.59337300	H	H	0	-0.56504700	-1.49497600	2.99975000	H
H	0	-5.69301600	4.31536900	4.02753500	H	H	0	-0.75806200	0.85143200	4.53910100	H
H	0	-2.40025500	3.22005100	4.65967100	H	H	0	-1.98493400	1.10261500	2.48232500	H
H	-1	-7.99672900	-1.06665900	4.83351700	L	H	0	-2.48602700	-1.52234000	1.46351600	H
H	-1	-10.33828700	-1.23536200	4.14440800	L	H	0	1.45712900	-0.62227400	1.20438400	H
H	-1	-9.88121500	-0.83580400	2.62312800	L	H	0	0.20222200	2.16540200	1.34058100	H
H	-1	-6.73131000	8.12946000	-2.60507400	L	H	0	1.11506300	2.36345900	-0.54198600	H
H	-1	-5.05203600	8.55022200	-2.96605000	L	H	0	-0.87581600	-0.39871800	0.10304300	H
H	-1	-6.24272700	9.60963900	0.56338600	L	H	0	-1.63827700	1.63698700	-0.86476900	H
H	-1	-5.33957200	7.99011900	2.26913000	L	H	0	2.47295500	1.79586200	2.73111900	H
H	-1	-4.23255500	6.04073300	-2.59743900	L	H	0	2.96449500	1.52442800	1.03881000	H
H	-1	-2.95726800	4.16702800	-1.55502600	L	H	0	3.91693500	-0.37531300	1.66220500	H

O	-1	-7.05584100	11.05910100	-4.22288100	L	C	0	-1.77865600	2.36259600	-5.27509600	H
H	-1	-8.60363400	1.09120100	5.81209600	L	C	0	-2.11436300	1.99566500	-3.80499200	H
H	-1	-7.58396400	-6.97762600	-1.27802200	L	O	0	-3.31457000	1.81095900	-3.54020900	H
H	-1	-0.97967100	-8.20645400	-0.22297100	L	O	0	-1.12479100	1.90820200	-2.98919900	H
H	-1	2.83437900	-7.93215600	-3.29657900	L	C	-1	-1.01024900	0.10295600	-6.11310700	L
H	-1	10.66607600	-2.31848500	-3.02726700	L	O	-1	0.10720000	0.30864300	-6.61339400	L
H	-1	10.23709900	6.91557000	3.77564700	L	N	-1	-1.36275700	-1.02236800	-5.49412200	L
H	-1	-5.05728500	11.23341600	-3.82226300	L	C	-1	-0.50730000	-2.21456400	-5.38898900	L
H	-1	1.97970800	6.82868400	4.98159600	L	C	-1	-0.81597200	-2.99970300	-4.08582700	L
H	-1	-5.15834100	-0.88817700	-5.48215600	L	C	-1	0.01420100	-4.26416500	-4.00107200	L
H	-1	-4.42640900	-7.31678900	4.16184100	L	C	-1	-0.52207500	-2.12664900	-2.86560000	L
H	-1	6.38006200	-6.22218700	5.32566400	L	C	-1	-0.68846000	-3.16927600	-6.58077300	L
H	-1	-1.08792500	-2.12568900	-7.28658100	L	O	-1	0.31481500	-3.71998600	-7.10396300	L
H	-1	6.26370600	-5.77000800	-6.09558200	L	N	-1	-9.54944900	0.64221600	3.60484400	L
H	-1	9.07329400	-3.70645100	1.33506800	L	C	-1	-8.35420100	1.34503300	4.02689200	L H 58
N	-1	-9.64046600	2.24093900	-2.86887500	L	C	0	-7.31992400	1.45319600	2.90222900	H
C	-1	-8.30273200	1.71052500	-2.51463500	L H 328	C	0	-6.08785700	2.28573500	3.24877000	H
C	0	-8.03235600	1.88049500	-1.00786300	L	C	0	-4.91295600	1.69136500	3.72517500	H
C	0	-6.69246100	1.36216500	-0.56502700	H	C	0	-3.75111200	2.42851000	3.95939700	H
N	0	-6.56300900	0.09420100	-0.02072200	H	C	0	-3.72691800	3.80466400	3.69808900	H
C	0	-5.29274000	-0.09100700	0.34464500	H	O	0	-2.62278900	4.58119800	3.86938500	H
N	0	-4.60124000	1.01137100	0.04663600	H	C	0	-4.89876600	4.42271200	3.23463700	H
C	0	-5.44501300	1.92671500	-0.53237800	H	C	0	-6.04924600	3.67073100	3.01059100	H
C	-1	-8.23396300	0.20920100	-2.91047300	L	C	-1	-8.66214500	2.75079900	4.56120200	L
O	-1	-7.20359600	-0.24332200	-3.40790200	L	O	-1	-9.46032500	3.49926000	3.93968000	L
N	-1	-9.28454000	-0.54047200	-2.58855800	L	N	-1	-5.99842200	10.79745200	-3.39103100	L
C	-1	-9.29888000	-1.97786000	-2.76372200	L H 366	C	-1	-4.74124400	10.27973400	-3.94978600	L
C	0	-8.63490700	-2.72895700	-1.59139800	L	C	-1	-4.64148800	8.76508300	-3.78668600	L
C	0	-9.26321000	-2.32078400	-0.20418700	H	C	-1	-4.24815200	8.38050000	-2.40112000	L
O	0	-10.15072200	-3.05482500	0.24566300	H	C	-1	-4.36978700	9.15457900	-1.25851200	L
O	0	-8.80844200	-1.23710600	0.30718600	H	N	-1	-3.88610100	8.48892600	-0.17814400	L
C	-1	-10.70368300	-2.52580900	-2.94747000	L	C	-1	-3.45480600	7.24152500	-0.57474800	L
O	-1	-11.69912000	-1.77478900	-2.77822600	L	C	-1	-3.67800000	7.13447500	-1.96858100	L
H	0	-8.80700900	1.35151800	-0.41742800	H	C	-1	-3.29192600	5.95403000	-2.62983100	L
H	0	-8.09307400	2.95489900	-0.74218300	H	C	-1	-2.72766700	4.93890500	-1.87789600	L
H	0	-5.07248800	2.87376400	-0.89904200	H	C	-1	-2.54533300	5.05481800	-0.49666400	L
H	0	-3.55565200	1.10343700	0.13008500	H	C	-1	-2.89125300	6.20483700	0.17689500	L
H	0	-4.86017700	-0.97337600	0.78941100	H	C	-1	-4.54718600	10.70792300	-5.40165400	L
H	-1	-7.50550400	2.24429500	-3.09282000	L	N	0	1.20237300	5.54864500	-3.91629900	H
H	-1	-10.13587200	2.56630700	-2.06458500	L	C	0	1.32800900	4.29752500	-3.16538500	H
H	-1	-9.54358800	2.98822000	-3.52129800	L	C	0	1.76744200	3.16775900	-4.16026500	H
H	0	-8.76958200	-3.81993200	-1.72724700	H	O	0	1.42545200	1.87858900	-3.69005200	H
H	0	-7.54399000	-2.52222400	-1.59327600	H	C	0	3.26236600	3.15015100	-4.46447000	H
H	-1	-8.71712800	-2.23763500	-3.68702800	L	C	0	2.21542700	4.31768500	-1.90648000	H
H	-1	-9.98586900	-0.16746500	-1.98068200	L	O	0	2.18839000	3.39245900	-1.09087700	H
H	-1	-10.82228400	-3.58564900	-3.20291200	L	N	0	3.02818100	5.40267200	-1.76341000	H
H	0	-7.39523600	-0.57593000	0.09106400	H	C	-1	4.03056200	5.53202800	-0.64083400	L H 88
H	0	6.65063300	-3.17670000	6.56588200	L	C	-1	5.29097300	6.22991400	-1.15494000	L

G1c_R786H

ONIOM: extrapolated energy = -3373.553118 au

N	-1	-4.16830500	-7.59862700	-0.79126500	L	C	-1	7.89864600	3.29249800	-5.30958100	L
C	-1	-2.87984200	-6.94261600	-0.80950200	L	C	-1	7.64689900	3.83025000	-2.98607400	L
C	-1	-3.03532500	-5.51158200	-0.22800600	L H 4	C	-1	6.99854300	4.54568400	-1.97679800	L
C	0	-1.80972000	-4.62054600	-0.20679000	H	C	-1	3.33476100	6.32336000	0.46539300	L
C	0	-2.02414200	-3.33543300	0.67442500	H	O	-1	3.56345400	7.53440300	0.63241100	L
O	0	-3.12366900	-2.71856400	0.56710600	H	N	-1	2.49558800	5.62112300	1.22656400	L
O	0	-1.04539500	-2.97771800	1.39339600	H	C	-1	1.48001900	6.25118900	2.10925200	L H 312
C	-1	-1.89367800	-7.72194300	0.06991400	L	C	0	0.40175300	5.20471000	2.42627700	H
O	-1	-0.70907500	-7.89764200	-0.31662800	L	C	0	0.81615800	4.05100600	3.39673500	H
N	-1	-2.54443300	-5.99768600	6.20900400	L	O	0	2.04046000	3.89001400	3.69577900	H
C	-1	-3.37953400	-4.92731100	5.70231000	L	O	0	-0.14188900	3.33983500	3.81056800	H
C	-1	-2.54761100	-3.89416700	4.91500900	L	C	-1	2.02104500	6.88002600	3.38119400	L
C	-1	-1.18764700	-3.53151700	5.48921000	L	O	-1	1.20568000	7.31994100	4.23279200	L
C	-1	-1.02229900	-3.22758700	6.83152200	L	N	-1	9.83359700	4.88951400	4.48385700	L
C	-1	0.22248300	-2.86246900	7.33507400	L	C	-1	9.59782600	4.28025900	3.16277000	L
C	-1	1.30520600	-2.76417300	6.47840700	L	C	-1	8.24870700	4.71049400	2.61059600	L
O	-1	2.54986700	-2.40912300	6.93195000	L	C	-1	7.08200400	4.06942300	3.35628600	L
C	-1	1.15860600	-3.05463000	5.13507500	L	C	-1	5.73758800	4.48305800	2.82813900	L
C	-1	-0.08198300	-3.42495400	4.65140000	L	O	-1	5.59830000	5.51773600	2.16258000	L
C	-1	-4.41453200	-5.58885300	4.80610200	L	N	-1	4.71665400	3.67376400	3.12280300	L
O	-1	-4.19120300	-5.71553400	3.57417400	L	C	-1	10.72854500	4.61698700	2.18582700	L
N	-1	-6.98414600	-5.91462500	2.77333100	L	O	-1	11.07046800	3.78308800	1.30760600	L
C	-1	-7.75176000	-5.18953800	1.76711000	L	N	-1	11.39264600	-1.88748700	-1.77434100	L
C	-1	-7.15831400	-3.80320200	1.53848300	L	C	-1	10.09777900	-2.51078000	-2.00471800	L
C	-1	-6.96638400	-3.03174100	2.81822900	L	C	-1	9.03341400	-1.48879700	-2.41391400	L
C	-1	-8.03654800	-2.88933900	3.70816700	L	C	-1	8.49412300	-0.67136300	-1.26624800	L
C	-1	-7.88473200	-2.21945800	4.89978600	L	C	-1	9.05027100	-0.52881000	-0.01708900	L
C	-1	-6.65552000	-1.69536400	5.21515000	L	N	-1	8.28078700	0.33138800	0.73992200	L
O	-1	-6.55387900	-1.02063700	6.40262100	L	C	-1	7.22355500	0.77253200	-0.01307500	L
C	-1	-5.57270500	-1.81741800	4.37244700	L	C	-1	7.31907600	0.15477600	-1.27946900	L
C	-1	-5.72956200	-2.48958300	3.16510000	L	C	-1	6.34693000	0.42705600	-2.24009900	L
C	-1	-7.69152700	-5.94032700	0.44164600	L	C	-1	5.30184300	1.26999500	-1.92167200	L
O	-1	-6.58701200	-6.35281800	0.00179400	L	C	-1	5.21172200	1.86240700	-0.63028000	L
N	-1	-6.10851000	-3.95754400	-3.68452900	L	C	-1	6.17412100	1.62756800	0.32050700	L
C	-1	-5.61503900	-2.60714100	-3.52645800	L	C	-1	10.30634600	-3.56560700	-3.07324500	L
C	-1	-4.58194200	-2.54478500	-2.42665700	L	O	-1	10.78092000	-3.24184200	-4.19285500	L
O	-1	-5.19152200	-3.00901000	-1.21406100	L	N	-1	6.35690400	-6.90670300	1.39495500	L
C	-1	-4.06290600	-1.12484500	-2.23499900	L	C	-1	6.42847800	-5.59630700	0.74412700	L
C	-1	-5.01283300	-2.10079600	-4.84867900	L	C	-1	5.53452800	-4.58919600	1.48203500	L H 327
O	-1	-4.00676600	-2.67355900	-5.34197500	L	C	0	5.77212100	-3.12973200	1.12563200	H
N	-1	-3.43431800	0.60407400	-6.05075500	L	C	0	5.03250000	-2.74637200	-0.15196100	H
C	-1	-2.08975600	1.20747200	-6.22960200	L H 43	O	0	5.30339300	-3.22681400	-1.24102000	H

O	0	4.05729300	-1.85683600	-0.02792400	H	H	-1	-7.92397300	0.749999400	4.87446500	L
C	-1	7.87770300	-5.06890800	0.74014100	L	H	-1	-10.28884300	0.82375100	4.25143400	L
O	-1	8.42041900	-4.72852400	-0.34299000	L	H	-1	-9.83479700	0.88800100	2.67899300	L
N	-1	2.91554500	-10.61731400	0.53095800	L	H	-1	-5.59756300	8.26551100	-4.04783000	L
C	-1	2.49017900	-9.36135700	-0.08935600	L	H	-1	-3.88925300	8.36079700	-4.49493200	L
C	-1	3.51823200	-8.25806800	0.23800600	L	H	-1	-4.77942800	10.16637400	-1.18668400	L
C	-1	2.90579600	-6.87344900	0.20523400	L	H	-1	-4.06144700	8.73915600	0.76155900	L
C	-1	2.11295600	-6.40084500	1.26388300	L	H	-1	-3.43443700	5.85442700	-3.70993800	L
C	-1	1.50829500	-5.16944500	1.20594600	L	H	-1	-2.41061500	4.01178900	-2.37568800	L
C	-1	1.68375200	-4.38173500	0.09621900	L	H	-1	-2.75512800	6.27197100	1.26646300	L
O	-1	1.08686200	-3.16227000	0.02533600	L	H	-1	-2.09820600	4.21369800	0.05261800	L
C	-1	2.45453900	-4.82557800	-0.96505300	L	H	-1	-3.91776500	10.76335800	-3.36249500	L
C	-1	3.07283300	-6.05967900	-0.88555800	L	H	-1	-6.78267100	10.34596600	-3.81443600	L
C	-1	2.28196900	-9.50734800	-1.60079600	L	H	-1	-6.05610500	11.78106200	-3.55379800	L
O	-1	3.04337900	-10.25131900	-2.27186400	L	H	0	1.21479900	3.40551100	-5.08157200	H
N	-1	2.52817100	-7.14666700	-4.15334100	L	H	0	3.46793800	2.45764000	-5.28797500	H
C	-1	3.34109700	-6.35348100	-5.06216100	L	H	0	3.82169600	2.80065200	-3.58367000	H
C	-1	3.89179500	-5.09376000	-4.36112000	L	H	0	3.64761700	4.13870200	-4.75382000	H
C	-1	3.89815500	-3.89398000	-5.27737700	L	H	0	0.43639900	1.84916000	-3.48202600	H
C	0	4.68350900	-2.69957300	-4.74797100	H	H	0	0.32563000	4.01745300	-2.82298800	H
N	0	4.07881100	-2.09413100	-3.57028600	H	H	0	0.83552700	6.30441400	-3.34415800	H
C	0	3.19684200	-1.07966600	-3.53519000	H	H	0	2.07707300	5.84549200	-4.34389100	H
N	0	2.75269900	-0.47878000	-4.65335300	H	H	-1	5.99130700	6.36463800	-0.30583500	L
N	0	2.81750600	-0.62582200	-2.34506700	H	H	-1	5.06350900	7.25331000	-1.51799900	L
C	-1	4.46448900	-7.09655100	-5.79506900	L	H	-1	4.81359100	6.30252500	-3.85104500	L
O	-1	4.67131700	-6.87744500	-7.01683200	L	H	-1	7.29759400	4.38424600	-0.93190600	L
C	0	-0.60891200	-0.08957600	2.88827800	H	H	-1	5.95043600	5.04085200	-5.65996300	L
O	0	-0.86542900	0.46832700	4.14630900	H	H	-1	8.43986800	3.12362200	-2.70730100	L
C	0	-1.54377500	0.48900700	1.79231600	H	H	-1	8.55244400	2.74300800	-4.89605800	L
O	0	-2.79560900	-0.16876400	1.81622100	H	H	-1	4.30538200	4.48582700	-0.31311500	L
O	0	0.78471900	0.19511500	2.66229100	H	H	0	2.97952200	6.14745800	-2.45267600	H
C	0	1.32904200	0.12877100	1.35880700	H	H	0	-0.48968700	5.69291700	2.86696800	H
C	0	0.50969000	1.01042800	0.40635400	H	H	0	0.02068800	4.72859400	1.49721000	H
O	0	1.04438300	0.96360800	-0.91704100	H	H	-1	1.03652100	7.09810100	1.52256700	L
C	0	-0.94330100	0.54307500	0.37898800	H	H	-1	2.83180700	4.72604700	1.54981300	L
O	0	-1.73045800	1.46883100	-0.36683200	H	H	-1	8.18588200	4.43608200	1.53522200	L
C	0	2.77132400	0.61079500	1.48466400	H	H	-1	8.14357000	5.81635300	2.63047900	L
O	0	3.67111000	-0.37758400	2.02979300	H	H	-1	7.20052100	2.96314200	3.32107800	L
H	-1	-3.44254400	-5.59231900	0.80516500	L	H	-1	7.13754400	4.34018500	4.43156400	L
H	-1	-3.82538000	-4.99262100	-0.81558000	L	H	-1	4.85445000	3.00498300	3.84348100	L
H	0	-0.91405600	-5.15092000	0.17447000	L	H	-1	3.73388100	3.89949600	2.93152900	L
H	0	-1.55655100	-4.25148800	-1.23252100	H	H	-1	9.58847200	3.17278400	3.33162600	L
H	-1	-2.51434200	-6.89467000	-1.86421900	L	H	-1	10.74576200	4.64687700	4.80902000	L
H	-1	-4.54104600	-7.62593500	0.13550800	L	H	-1	9.75426000	5.88415200	4.43075100	L
H	-1	-4.80000300	-7.14416200	-1.41589800	L	H	-1	8.17747600	-2.02434700	-2.87441400	L
H	-1	-2.38816000	-4.23767500	3.87087600	L	H	-1	9.41571200	-0.79702800	-3.19261000	L
H	-1	-3.14570800	-2.95868800	4.83065800	L	H	-1	9.98624300	-0.95916900	0.34892200	L
H	-1	-1.88060300	-3.27993600	7.51219500	L	H	-1	8.28959000	0.34439900	1.72838300	L
H	-1	-0.18220800	-3.64072000	3.57854600	L	H	-1	6.42197400	-0.03491700	-3.23061200	L
H	-1	0.31991400	-2.63288700	8.40336100	L	H	-1	4.53995700	1.53956700	-2.67004200	L
H	-1	2.00470300	-2.98097900	4.44096700	L	H	-1	6.11759200	2.09510400	1.31106400	L
H	-1	2.47728400	-2.25049100	7.86567000	L	H	-1	4.37101200	2.54333700	-0.41612200	L
H	-1	-3.87830200	-4.43136700	6.57080200	L	H	-1	9.78937100	-2.99729200	-1.04608000	L
H	-1	-3.10292900	-6.69941600	6.64891500	L	H	-1	12.08181600	-2.58835400	-1.59408000	L
H	-1	-2.00332500	-6.40605300	5.47556700	L	H	-1	11.67369500	-1.34099800	-2.56306800	L
H	-1	-6.18738100	-3.87922300	1.00236100	L	H	-1	5.71854400	-4.66152400	2.57430300	L
H	-1	-7.81927900	-3.20605800	0.87010500	L	H	-1	4.46912500	-4.85947100	1.31850600	L
H	-1	-9.02547800	-3.27483000	3.42533900	L	H	0	5.45083600	-2.47920600	1.95593300	H
H	-1	-4.87458000	-2.57475300	2.48401200	L	H	0	6.84507100	-2.92246400	0.94952700	H
H	-1	-8.75406800	-2.08381700	5.55784200	L	H	-1	6.06323100	-5.73005700	-0.30664700	L
H	-1	-4.60118800	-1.37401900	4.63554700	L	H	-1	5.66585700	-6.91900000	2.11851200	L
H	-1	-7.43140600	-0.92452700	6.75416300	L	H	-1	7.23990900	-7.15633500	1.79237700	L
H	-1	-8.81038800	-5.12295200	2.12000700	L	H	-1	3.94478700	-8.41146500	1.25207500	L
H	-1	-6.99922500	-5.39839400	3.63115600	L	H	-1	4.37745100	-8.30288700	-0.46065700	L
H	-1	-6.03571800	-6.03540100	2.47404000	L	H	-1	1.96617400	-7.04288500	2.14018600	L
H	-1	-3.71449100	-3.22414800	-2.65676400	L	H	-1	3.66108400	-6.00189900	-1.83593800	L
H	-1	-3.33748700	-1.05215800	-1.41094700	L	H	-1	0.90357000	-4.82464900	2.05893300	L
H	-1	-4.88440600	-0.42238100	-2.03880800	L	H	-1	2.63171900	-4.20030100	-1.85724800	L
H	-1	-3.55291100	-0.76314200	-3.14248100	L	H	-1	0.61963000	-2.99448500	0.84522900	L
H	-1	-4.49395400	-3.01422100	-0.56383500	L	H	-1	1.50306800	-9.09678600	0.36783400	L
H	-1	-6.46916000	-1.91107500	-3.27166400	L	H	-1	3.08715600	-10.46762800	1.50434100	L
H	-1	-5.57113800	-4.62639700	-3.17149800	L	H	-1	3.74873400	-10.96099900	0.09994900	L
H	-1	-7.05871400	-4.00046300	-3.38173100	L	H	-1	4.91734000	-5.29505800	-3.98350300	L
H	0	-0.72255500	2.66845600	-5.38856400	H	H	-1	3.30008900	-4.84913100	-3.43593700	L
H	0	-2.40556400	3.23588000	-5.54063000	H	H	-1	4.33711600	-4.16883000	-6.25992200	L
H	-1	-2.01230400	1.62394100	-7.26513100	L	H	-1	2.85354000	-3.58514700	-5.50844300	H
H	-1	-3.80981700	0.88359200	-5.14884900	L	H	0	5.70591400	-3.00408100	-4.45882400	H
H	-1	-4.03602300	0.92411300	-6.77805700	L	H	0	4.79604600	-1.92789300	-5.53302900	H
H	-1	-1.90000600	-3.28508000	-4.07669500	L	H	0	4.35065400	-2.50989000	-2.67359600	H
H	-1	-0.18317600	-4.80014000	-3.06052100	L	H	0	3.21003200	-1.04127400	-1.50389300	H
H	-1	1.09427600	-4.04685200	-4.02818100	L	H	0	2.03552500	0.01507000	-2.19230000	H
H	-1	-0.20054500	-4.96538900	-4.82145200	L	H	0	2.73509000	-0.97859800	-5.53015300	H
H	-1	-0.77089300	-2.69182000	-1.94575800	L	H	0	2.13191200	0.33394900	-4.53229200	H
H	-1	0.53768700	-1.85120700	-2.80228400	L	H	-1	2.63293000	-5.91051000	-5.82908800	L
H	-1	-1.11349600	-1.19903700	-2.83538500	L	H	-1	2.83894300	-6.96177500	-3.21851000	L
H	-1	0.56562700	-1.88502300	-5.35140900	L	H	-1	1.54093400	-6.37240400	-4.52426900	L
H	-1	-2.15719900	-1.01136800	-4.88337800	L	H	0	-0.76129700	-1.17076500	2.95731100	H
H	0	-7.01154800	0.42992100	2.62564100	H	H	0	-0.58674800	1.41119600	4.08997500	H
H	0	-7.80697100	1.86549000	2.00093100	H	H	0	-1.74257000	1.53112300	2.07072000	H
H	0	-4.88065100	0.61411700	3.89156600	H	H	0	-2.71319100	-1.09657800	1.46956000	H
H	0	-6.93826100	4.16800500	2.62013200	H	H	0	1.31689800	-0.90665200	0.98032400	H
H	0	-2.85904400	1.91599100	4.30470100	H	H	0	0.53630300	2.04402400	0.77347800	H
H	0	-4.87231900	5.48919800	3.01969600	H	H	0	1.36325800	1.86111600	-1.14965000	H
H	0	-1.79655500	4.03436100	3.91874900	H	H	0	-0.97919300	-0.45822900	-0.07832000	H

H	0	-1.46694600	1.49398100	-1.32883900	H	O	-1	-3.21661000	-6.67661500	2.42179200	L
H	0	2.79835900	1.51597400	2.10179500	H	N	-1	-5.96183200	-7.17453200	1.58672000	L
H	0	3.16288000	0.85518600	0.49103900	H	C	-1	-6.86680800	-6.40294700	0.74224400	L
H	0	3.94254500	-1.44473600	0.89283000	H	C	-1	-6.51475800	-4.91988500	0.79670200	L
O	-1	-5.54776600	10.89622700	-6.14121900	L	C	-1	-6.41389600	-4.39488600	2.20522600	L
H	-1	-8.17034200	3.10828600	5.47452600	L	C	-1	-7.46632600	-4.61027700	3.10161700	L
H	-1	-8.61173000	-6.09811900	-0.13464100	L	C	-1	-7.39101800	-4.17271300	4.40338800	L
H	-1	-2.22524100	-8.11607900	1.04027100	L	C	-1	-6.25519300	-3.52452400	4.82153200	L
H	-1	1.47093800	-8.94241800	-2.07817600	L	O	-1	-6.23027800	-3.08978400	6.12001400	L
H	-1	10.04727300	-4.61284500	-2.86721400	L	C	-1	-5.19222200	-3.29668200	3.97553200	L
H	-1	11.23314400	5.59099900	2.25203400	L	C	-1	-5.27259100	-3.73419200	2.65787300	L
H	-1	-3.53181600	10.83127000	-5.79940800	L	C	-1	-6.72372500	-6.85712200	-0.70600300	L
H	-1	3.10320100	6.95750900	3.54935600	L	O	-1	-5.58007500	-6.98572000	-1.21502300	L
H	-1	-5.47511300	-1.24019500	-5.35019400	L	N	-1	-5.60778800	-3.86528500	-4.34829500	L
H	-1	-5.33858100	-5.99093300	5.24609400	L	C	-1	-5.33709300	-2.50975600	-3.92243700	L
H	-1	-1.70064100	-3.36447700	-6.96154700	L	C	-1	-4.29619200	-2.49487900	-2.82834300	L
H	-1	5.07453500	-7.82546800	-5.24615600	L	O	-1	-4.78578400	-3.28360500	-1.73497200	L
H	-1	8.43082800	-4.99038100	1.68667900	L	C	-1	-4.01065700	-1.07454300	-2.35562000	L
N	-1	-9.34845600	2.92496500	-3.26244200	L	C	-1	-4.86480200	-1.65995500	-5.11494800	L
C	-1	-8.09099400	2.26563400	-2.83764600	L H 345	O	-1	-3.79362700	-1.94921500	-5.70865000	L
C	0	-7.75322700	2.65414900	-1.38712900	H	N	-1	-3.78532400	1.45245300	-5.74793500	L
C	0	-6.49359100	2.02277200	-0.87092200	H	C	-1	-2.56322200	2.29382200	-5.79784700	H 43
N	0	-6.53652100	0.85013600	-0.13621200	H	C	0	-2.40135300	3.24963600	-4.61128000	H
C	0	-5.29878800	0.53493900	0.24202400	H	C	0	-2.63270000	2.53341200	-3.24746800	H
N	0	-4.46027500	1.46252300	-0.23086600	H	O	0	-3.78799100	2.12163800	-3.03926200	H
C	0	-5.17766100	2.39469000	-0.93939500	H	O	0	-1.62479200	2.42921100	-2.45799500	H
C	-1	-8.25840900	0.72623600	-2.97034700	L	C	-1	-1.31485100	1.38274800	-5.89967100	L
O	-1	-7.32493400	0.04600800	-3.39436100	L	O	-1	-0.26119800	1.86551500	-6.34468400	L
N	-1	-9.39507800	0.20894700	-2.51238700	L	N	-1	-1.46046700	0.11491700	-5.51867300	L
C	-1	-9.62706300	-1.21850500	-2.43774700	L H 355	C	-1	-0.41904800	-0.91581300	-5.64995300	L
C	0	-9.03101300	-1.85432500	-1.16520700	H	C	-1	-0.55689700	-1.98253500	-4.53055300	L
C	0	-9.52232000	-1.13313700	0.14391700	H	C	-1	0.47079300	-3.08326800	-4.69629700	L
O	0	-10.47513600	-1.63745400	0.74287400	H	C	-1	-0.37382400	-1.39072100	-3.15972200	L
O	0	-8.89388900	-0.05252600	0.44975500	H	C	-1	-0.47677200	-1.63342900	-7.00875200	L
C	-1	-11.10297800	-1.57078200	-2.50851800	L	O	-1	0.58716900	-1.89595100	-7.62736600	L
O	-1	-11.97023100	-0.66026600	-2.45947800	L	N	-1	-9.53813500	-1.42861200	3.69830800	L
H	0	-8.57837800	2.35969700	-0.70843000	H	C	-1	-8.46186200	-0.63440200	4.25648000	H 58
H	0	-7.64516700	3.75479400	-1.31575900	H	C	0	-7.48902500	-0.13403800	3.18454800	H
H	0	-4.68332500	3.21124500	-1.44881700	H	C	0	-6.38993500	0.79083600	3.70208700	H
H	0	-3.41981800	1.41034600	-0.17734500	H	C	0	-5.11810100	0.30506900	4.03088900	H
H	0	-4.99295400	-0.32365200	0.81757500	H	C	0	-4.07367900	1.14951200	4.40970500	H
H	-1	-7.24599500	2.56781900	-3.50804100	L	C	0	-4.27053700	2.53735400	4.45168400	H
H	-1	-9.76045000	3.45206900	-2.52042100	L	O	0	-3.29623700	3.42311500	4.77533700	H
H	-1	-9.16707300	3.52851300	-4.03464700	L	C	0	-5.54514500	3.04219700	4.14419200	H
H	0	-9.33442000	-2.91737700	-1.10639100	H	C	0	-6.57524800	2.18265400	3.77190600	H
H	0	-7.92223100	-1.82473600	-1.22414600	H	C	-1	-8.97945600	0.56748700	5.05901000	L
H	-1	-9.12447400	-1.71476700	-3.30927000	L	O	-1	-9.90708400	1.28075700	4.59605800	L
H	-1	-10.01091200	0.78055200	-1.96967900	L	N	-1	-7.90072100	10.35195700	-1.12019200	L
H	-1	-11.38548000	-2.62819800	-2.57664300	L	C	-1	-6.59283300	10.17045200	-1.76611600	L
H	0	-7.46893300	0.33545300	0.09331500	H	C	-1	-6.24226000	8.69134100	-1.90771700	L
N	0	6.99199600	2.85615600	6.76865900	L	C	-1	-5.75084400	8.11188700	-0.62508300	L
C	0	5.78334000	3.21069100	7.54656800	L H 383	C	-1	-5.96365500	8.61442100	0.64838400	L
C	0	5.54305400	2.27050000	8.71978200	L	N	-1	-5.34619900	7.83853600	1.57628100	L
O	0	6.30525100	1.40838900	9.08643700	L	C	-1	-4.72878600	6.78299000	0.94071700	L
H	0	6.00494500	4.21101800	7.99955000	L	C	-1	-4.97235900	6.91727000	-0.44733500	L
H	0	7.04708500	3.44953800	5.95890700	L	C	-1	-4.41825300	5.97108200	-1.32906600	L
H	0	6.92480700	1.90062600	6.46687200	L	C	-1	-3.67391100	4.93563300	-0.79234200	L
H	0	4.59415000	2.43070000	9.26068400	L	C	-1	-3.47244900	4.80562100	0.58497300	L
C	0	4.50162700	3.34442800	6.71160200	H	C	-1	-3.98162500	5.72664600	1.47285500	L
H	0	3.66896500	3.65633800	7.37399700	H	C	-1	-6.51407300	10.90257000	-3.10280000	L
H	0	4.61241200	4.17696100	5.98290500	L	N	0	0.00863100	6.53204400	-2.62253600	H
C	0	4.09022400	2.08119500	5.99273400	H	C	0	0.36370800	5.20514400	-2.11496200	H
N	0	2.78764900	1.92484100	5.54375800	H	C	0	0.95360600	4.36035700	-3.29672100	H
C	0	4.72623800	0.90491600	5.65506100	H	O	0	0.85721100	2.97563500	-3.05233000	H
C	0	2.71321800	0.70611100	4.95093200	H	C	0	2.41453300	4.66669100	-3.61303300	H
N	0	3.86196100	0.04954400	4.99744200	H	C	0	1.27948300	5.14888600	-0.87972400	H
H	0	5.75139900	0.61700000	5.88545800	H	O	0	1.42168200	4.10878600	-0.23445600	H
H	0	1.80620000	0.35520200	4.47808100	H	N	0	1.93068600	6.30611300	-0.56234700	H
H	0	3.63454300	-0.40568800	3.01279800	H	C	-1	2.93001900	6.38620100	0.56382300	L H 88
H	0	2.20506200	2.70290600	5.18821800	H	C	-1	4.04389400	7.37100900	0.20385800	L
Glc_R786K											
ONIOM: extrapolated energy = -3243.304787 au											
N	-1	-3.01472300	-7.63182800	-2.23121100	L	O	-1	6.25987400	6.16396800	-3.31029600	L
C	-1	-1.85182300	-6.78058600	-2.11346600	L	O	-1	6.97311600	5.78439000	-4.44283100	L
C	-1	-2.22180300	-5.53829700	-1.25908500	L H 4	C	-1	6.70530200	5.80421200	-2.05973900	L
C	0	-1.15946900	-4.47874500	-1.05013400	H	C	-1	5.97873700	6.18896900	-0.93061900	L
C	0	-1.55986300	-3.46792900	0.08690700	H	C	-1	2.14715800	6.81733200	1.80285900	L
O	0	-2.75239400	-3.04877500	0.11092200	H	O	-1	2.17977900	7.99250600	2.20871400	L
O	0	-0.63008100	-3.10858900	0.87055200	H	N	-1	1.45669600	5.84952200	2.40564100	L
C	-1	-0.72619300	-7.54332400	-1.40323000	L	C	-1	0.37823500	6.11582300	3.39232700	H 102
O	-1	0.45932200	-7.44034500	-1.81252000	L	O	0	-0.51792400	4.87116400	3.48633700	H
N	-1	-1.46916200	-7.19537800	4.95380700	L	C	0	0.12547900	3.55546300	4.05664400	H
C	-1	-2.48240900	-6.19982500	4.66738400	L	O	0	1.37371200	3.44808800	4.15486200	H
C	-1	-1.85391500	-4.90833700	4.10490400	L	O	0	-0.73116200	2.65844000	4.33749600	H
C	-1	-0.55517600	-4.44546600	4.74502000	L	C	-1	0.84642300	6.56247400	4.76609500	L
C	-1	-0.40231900	-4.38895900	6.12159400	L	O	-1	-0.00446700	6.68438400	5.68516600	L
C	-1	0.78035900	-3.92889300	6.69253200	L	N	-1	8.90816600	5.71807900	5.47972600	L
C	-1	1.80683600	-3.48540500	5.87675400	L	C	-1	8.73636000	5.35068300	4.06284500	L
O	-1	2.98956600	-3.02521700	6.39668400	L	C	-1	7.31944900	5.65138800	3.60234400	L
C	-1	1.67023500	-3.52558100	4.50193800	L	C	-1	6.29555400	4.69139100	4.20089800	L
C	-1	0.49311200	-3.99392100	3.94945800	L	C	-1	4.88669800	4.97210100	3.76065400	L
C	-1	-3.42133100	-6.83410000	3.65339900	L	O	-1	4.56077600	6.07992900	3.31408500	L
						N	-1	4.02077100	3.96269000	3.88430500	L

C	-1	9.76768800	6.05622600	3.17689600	L	H	-1	-5.01562500	-7.07487100	1.27297400	L
O	-1	10.21527100	5.48032600	2.15143100	L	H	-1	-3.33656200	-2.96202100	-3.18590500	L
N	-1	11.36866100	0.66216600	-1.99738200	L	H	-1	-3.28295600	-1.04638300	-1.53085600	L
C	-1	10.18679200	-0.10951800	-2.35226000	L	H	-1	-4.92974100	-0.57077300	-2.02651700	L
C	-1	8.95823000	0.78201900	-2.55365400	L	H	-1	-3.59348300	-0.46155300	-3.17088400	L
C	-1	8.32662200	1.25615000	-1.26818100	L	H	-1	-4.07810500	-3.30106400	-1.09598300	L
C	-1	8.88848000	1.23993600	-0.01356100	L	H	-1	-6.28557900	-2.02913200	-3.53730500	L
N	-1	8.01140600	1.79419700	0.89674100	L	H	-1	-4.95354000	-4.52352200	-3.97678700	L
C	-1	6.87465100	2.19345800	0.24272900	L	H	-1	-6.52890600	-4.12410000	-4.06373600	L
C	-1	7.03253900	1.86203700	-1.12099000	L	H	0	-1.40852800	3.73105800	-4.65398700	H
C	-1	6.00117000	2.15317800	-2.01179200	L	H	0	-3.16051400	4.05139700	-4.67881600	H
C	-1	4.84224800	2.73149600	-1.53576300	L	H	-1	-2.58530500	2.91320200	-6.72932300	L
C	-1	4.69455900	3.03439200	-0.15257800	L	H	-1	-4.17476800	1.48244700	-4.80985400	L
C	-1	5.70991000	2.77974800	0.73600200	L	H	-1	-4.45233300	1.80521300	-6.39916500	L
C	-1	10.53336500	-0.88350000	-3.60874100	L	H	-1	-1.57901500	-2.43994100	-4.58259100	L
O	-1	10.91557100	-0.27122900	-4.63957400	L	H	-1	0.39134100	-3.81929600	-3.88216300	L
N	-1	7.31574300	-5.64784900	0.08905700	L	H	-1	1.49959700	-2.68874200	-4.67545200	L
C	-1	7.15315700	-4.24153200	-0.28733000	L	H	-1	0.34945700	-3.63473700	-5.64076100	L
C	-1	6.12876100	-3.56219700	0.63304700	L	H	-1	-0.49984500	-2.09941200	-2.37189500	L
C	0	6.14484300	-2.04435300	0.58227800	H	H	-1	0.62810900	-0.90122300	-3.03876100	L
C	0	5.22632900	-1.48024800	-0.52145300	H	H	-1	-1.10767500	-0.53851300	-2.94752700	L
O	0	5.51799000	-1.73954300	-1.70713100	H	H	-1	0.58627500	-0.42678500	-5.54338100	L
O	0	4.24456600	-0.77956400	-0.11447200	H	H	-1	-2.22774100	-0.12665800	-4.92101200	L
C	-1	8.49601600	-3.49069400	-0.18064000	L	H	0	-7.03557100	-1.01439100	2.69961400	H
O	-1	8.94377800	-2.85825100	-1.17215200	L	H	0	-8.05723200	0.37436900	2.38677200	H
N	-1	9.60824100	-4.99529000	5.29709500	L	H	0	-4.91204600	-0.76303800	3.95896000	H
C	-1	8.19457800	-4.81049600	5.62316100	L	H	0	-7.54530100	2.60391600	3.50567600	H
C	-1	7.85570100	-3.33622100	5.77152200	L	H	0	-3.09938200	0.72490700	4.62886900	H
C	-1	6.42191800	-3.12808900	6.24310000	L	H	0	-5.69165900	4.11989400	4.16483100	H
C	0	6.01551500	-1.66349200	6.37972500	H	H	0	-2.38353300	3.04082700	4.65620800	H
N	0	4.19264400	-1.15993300	4.53505500	H	H	-1	-7.91549700	-1.30503500	4.97011800	L
C	-1	7.33161900	-5.44369500	4.51348800	L	H	-1	-10.27792700	-1.50334100	4.36528700	L
O	-1	7.51092600	-5.11475700	3.31214700	L	H	-1	-9.88688100	-1.05596900	2.83891900	L
N	-1	4.50282000	-9.63386600	-1.51007100	L	H	-1	-7.11114900	8.10147900	-2.26680400	L
C	-1	3.85997400	-8.36861700	-1.86929900	L	H	-1	-5.45523200	8.56512400	-2.67945300	L
C	-1	4.70317500	-7.19653100	-1.32475300	L	H	-1	-6.53077300	9.50992800	0.91882300	L
C	-1	3.87210200	-5.95381600	-1.08329800	L	H	-1	-5.53237200	7.86599200	2.54632700	L
C	-1	3.04417100	-5.83739500	0.04526800	L	H	-1	-4.57425900	6.06410400	-2.40789400	L
C	-1	2.24505300	-4.73647600	0.23156300	L	H	-1	-3.22444600	4.19054900	-1.46367900	L
C	-1	2.25680000	-3.72750200	-0.69827700	L	H	-1	-3.82633700	5.59932500	2.55446200	L
O	-1	1.46691500	-2.63427600	-0.52701700	L	H	-1	-2.87799100	3.95881300	0.95733400	L
C	-1	3.05820800	-3.81927500	-1.82376700	L	H	-1	-5.84251200	10.65861500	-1.09110800	L
C	-1	3.87184500	-4.92479100	-1.98942200	L	H	-1	-8.61278900	9.86905100	-1.62804900	L
C	-1	3.63408200	-8.24629500	-3.38030000	L	H	-1	-8.12305200	11.32487200	-1.08391900	L
O	-1	4.48673500	-8.70653300	-4.18325400	L	H	0	0.33416100	4.65596400	-4.15761800	H
N	-1	3.41626000	-5.42131400	-5.41031500	L	H	0	2.70813000	4.15753900	-4.53608900	H
C	-1	4.06164300	-4.34088300	-6.13976200	L	H	0	3.06111100	4.29461400	-2.80604200	H
C	-1	4.41953700	-3.17050700	-5.19967500	L	H	0	2.60371800	5.74086200	-3.74557600	H
C	-1	4.20292000	-1.82957100	-5.85846700	L	H	0	-0.10926100	2.73287200	-2.87538400	H
C	0	4.78707500	-0.66362700	-5.06176500	H	H	0	-0.56331600	4.69838500	-1.82604700	H
N	0	4.17556500	-0.48899500	-3.75342800	H	H	0	-0.44357800	7.10484800	-1.91732600	H
C	0	3.15109200	0.32594400	-3.44837200	H	H	0	0.80356400	7.03410700	-3.00809800	H
N	0	2.53266900	1.06864700	-4.39116500	H	H	-1	4.73746000	7.45001300	1.06543500	L
N	0	2.79211500	0.43323900	-2.17629200	H	H	-1	3.64175000	8.39367800	0.05113400	L
C	-1	5.26929400	-4.72800000	-7.00175900	L	H	-1	3.48204200	7.89341100	-2.42551100	L
O	-1	5.40156100	-4.24114500	-8.15456600	L	H	-1	6.33071500	5.87663400	0.06228100	L
C	0	-0.52799400	-0.56340200	3.07413500	H	H	-1	4.75604800	7.21953100	-4.44521800	L
O	0	-0.84357900	-0.23778000	4.39887900	H	H	-1	7.61088900	5.19806100	-1.92434500	L
C	0	-1.55628100	0.05347300	2.07565900	H	H	-1	7.71975500	5.28041900	-4.14460700	L
O	0	-2.68919600	-0.78968000	1.96142200	H	H	-1	3.38165300	5.35636200	0.67747800	L
O	0	0.83584500	-0.12626300	2.91415800	H	H	0	1.73972700	7.14084300	-1.10601300	H
C	0	1.34044100	0.25466100	1.64203100	H	H	0	-1.41772900	5.09182200	4.09227900	H
C	0	0.35313800	1.16205500	0.87956200	H	H	0	-0.92252100	4.60528200	2.48673500	H
O	0	0.87412200	1.48208800	-0.41099000	H	H	-1	-0.21468500	6.97619600	2.98445600	L
C	0	-0.99111500	0.45477100	0.71146700	H	H	-1	1.94396200	4.97673700	2.54533800	L
O	0	-1.94680000	1.33153000	0.10590200	H	H	-1	7.27071700	5.58779200	2.49362500	L
C	0	2.66066400	0.96397800	1.93861500	H	H	-1	7.03572000	6.69854700	3.84178200	L
O	0	3.73582800	0.04727500	2.27746200	H	H	-1	6.59209600	3.64906700	3.94640900	L
H	-1	-2.57983000	-5.88751900	-0.26426900	L	H	-1	6.33769400	4.75027100	5.30876800	L
H	-1	-3.10294100	-5.05211200	-1.73446200	L	H	-1	4.28707900	3.19724800	4.45773500	L
H	0	-0.17431900	-4.91465700	-0.79140100	H	H	-1	3.00914000	4.05536700	3.73802800	L
H	0	-1.00719900	-3.86210600	-1.97014700	H	H	-1	8.91299500	4.24576400	4.00760100	L
H	-1	-1.53021500	-6.46571100	-3.13608100	L	H	-1	9.85686800	5.57088700	5.75348700	L
H	-1	-3.35060000	-7.90274200	-1.32989000	L	H	-1	8.66590200	6.67643900	5.62557500	L
H	-1	-3.73025000	-7.17439200	-2.75516000	L	H	-1	8.18810800	0.21330500	-3.11488600	L
H	-1	-1.67125000	-5.00797500	3.01387600	L	H	-1	9.19934700	1.66735900	-3.17743400	L
H	-1	-2.59900100	-4.08705200	4.20637300	L	H	-1	9.89252400	0.90725700	0.26291400	L
H	-1	-1.22016600	-4.71612400	6.77491700	L	H	-1	8.04700900	1.61338700	1.86799800	L
H	-1	0.39803300	-4.00751500	2.85474600	L	H	-1	6.12152600	1.91450400	-3.07420200	L
H	-1	0.87033000	-3.90147200	7.78550600	L	H	-1	4.02490300	3.01306200	-2.21830700	L
H	-1	2.47217200	-3.17721300	3.83964800	L	H	-1	5.60690500	3.02686400	1.79963400	L
H	-1	2.91952100	-3.06804800	7.34300300	L	H	-1	3.76055600	3.51061900	0.18978000	L
H	-1	-3.02974700	-5.97457600	5.61537600	L	H	-1	9.99030000	-0.81974000	-1.51096700	L
H	-1	-1.89236300	-8.05279600	5.24294200	L	H	-1	12.16805200	0.06377800	-1.95777000	L
H	-1	-0.89040700	-7.35560300	4.15577000	L	H	-1	11.53337000	1.39230700	-2.66032300	L
H	-1	-5.56062800	-4.72656200	0.25988000	L	H	-1	6.35417600	-3.81686100	1.68968800	L
H	-1	-7.28373700	-4.32082100	0.25820500	L	H	-1	5.11749800	-3.96789100	0.41488800	L
H	-1	-8.38688600	-5.09108700	2.74388800	L	H	0	5.81920000	-1.62829100	1.55198300	H
H	-1	-4.43554600	-3.54036500	1.97670600	L	H	0	7.16255300	-1.65110200	0.39618400	H
H	-1	-8.25111700	-4.31560700	5.07196400	L	H	-1	6.78394100	-4.22424100	-1.34506900	L
H	-1	-4.29887400	-2.75892100	4.32540000	L	H	-1	6.65755000	-5.91701600	0.79301900	L
H	-1	-7.10100400	-3.21181600	6.48031700	L	H	-1	8.23895500	-5.82088200	0.43212300	L
H	-1	-7.91126000	-6.58382000	1.09730400	L	H	-1	8.54937200	-2.86016500	6.49738200	L
H	-1	-6.03581700	-6.84732600	2.53014300	L	H	-1	8.02178200	-2.80405700	4.81105600	L

H	-1	6.22766400	-3.76011800	7.13472100	L	H	-1	-0.96026300	-8.17044000	-0.53213500	L
H	-1	5.70994900	-3.49168900	5.47256600	L	H	-1	2.72799300	-7.74090500	-3.73862100	L
H	0	6.85080500	-1.06622900	6.78615500	H	H	-1	10.45499800	-1.97897800	-3.61650200	L
H	0	5.18583800	-1.55619100	7.10286300	H	H	-1	10.10813500	7.06802600	3.43777500	L
H	0	3.92107900	-2.13883300	4.34440900	H	H	-1	-5.54462100	11.26862900	-3.46413400	L
H	0	3.49665600	-0.79073600	5.19367300	H	H	-1	1.90585600	6.78374100	4.95044000	L
H	-1	8.00075300	-5.35157400	6.58213000	L	H	-1	-5.47598200	-0.80625500	-5.43667900	L
H	-1	10.17688500	-4.61433700	6.02384200	L	H	-1	-4.25395900	-7.46265500	4.00093100	L
H	-1	9.83460100	-4.55632100	4.42884500	L	H	-1	6.56597600	-6.18017100	4.78622200	L
H	-1	5.17866900	-7.47386400	-0.35997000	L	H	-1	-1.45422200	-1.91492400	-7.42463300	L
H	-1	5.53726800	-6.95955400	-2.01506300	L	H	-1	6.00607300	-5.43928800	-6.60678000	L
H	-1	3.03004900	-6.65484600	0.77550200	L	H	-1	9.05645900	-3.50962200	0.76466200	L
H	-1	4.41457100	-4.58402200	-2.90698500	L	N	-1	-9.91460400	2.16407800	-2.57559300	L
H	-1	1.61746100	-4.67179700	1.13384100	L	C	-1	-8.55439900	1.65190700	-2.28591300	H
H	-1	3.10457800	-3.00984500	-2.57279800	L	C	0	-8.20769600	1.78868900	-0.79121700	H
H	-1	1.00285000	-2.71129500	0.30807900	L	C	0	-6.83654800	1.28454600	-0.41786300	H
H	-1	2.85677100	-8.36688100	-1.37231700	L	N	0	-6.66513600	0.00404100	0.08434200	H
H	-1	4.67620600	-9.65263000	-0.52573600	L	C	0	-5.38206800	-0.15932500	0.40551400	H
H	-1	5.36792800	-9.74274500	-1.99774800	L	N	0	-4.71836000	0.96794400	0.12238100	H
H	-1	5.47483900	-3.26928400	-4.86584700	L	C	0	-5.60165600	1.88076400	-0.40442300	H
H	-1	3.82326900	-3.21468300	-4.24656000	L	C	-1	-8.47194600	0.16286800	-2.72332900	L
H	-1	4.65180200	-1.82862900	-6.87439500	L	O	-1	-7.45276500	-0.25593000	-3.27082800	L
H	-1	3.11554700	-1.65894200	-6.02732600	L	N	-1	-9.49490200	-0.61582700	-2.38195400	L
H	0	5.86745000	-0.82392800	-4.89025300	H	C	-1	-9.48829700	-2.04827900	-2.59412900	H
H	0	4.69987000	0.27752700	-5.63742700	H	C	0	-8.75023800	-2.81091600	-1.47561900	H
H	0	4.60367200	-1.01175100	-2.96099700	H	C	0	-9.28181800	-2.43043800	-0.04703700	H
H	0	3.33230800	-0.04366700	-1.43664300	H	O	0	-10.15068400	-3.15455900	0.44442400	H
H	0	1.94097200	0.90404600	-1.86902300	H	O	0	-8.77564700	-1.36700600	0.47325900	H
H	0	2.53424100	0.76471500	-5.35176900	H	C	-1	-10.88829300	-2.61960700	-2.73928300	L
H	0	1.80744800	1.72644300	-4.07918500	H	O	-1	-11.89080200	-1.89339400	-2.51310000	L
H	-1	3.26840400	-3.87919200	-6.80573100	L	H	0	-8.94053400	1.23226400	-0.17558500	H
H	-1	3.71999300	-5.37537200	-4.45621400	L	H	0	-8.27401100	2.85330400	-0.49518600	H
H	-1	2.30534400	-4.76388000	-5.62327800	L	H	0	-5.26548800	2.84852600	-0.75005500	H
H	0	-0.57279300	-1.65405200	2.96905400	H	H	0	-3.68414700	1.07097800	0.19633900	H
H	0	-0.68652500	0.73286800	4.47571500	H	H	0	-4.91766500	-1.04579100	0.80787200	H
H	0	-1.91142700	0.98197600	2.53599100	H	H	-1	-7.79018300	2.21624500	-2.87943300	L
H	0	-2.47430400	-1.58624300	1.42012500	H	H	-1	-10.38517800	2.45876000	-1.74499300	L
H	0	1.53475600	-0.63120400	1.01470800	H	H	-1	-9.85701400	2.92955700	-3.21135400	L
H	0	0.19887500	2.08280900	1.45418500	H	H	0	-8.89333400	-3.89889800	-1.61317700	H
H	0	0.97183600	2.45189300	-0.48028900	H	H	0	-7.66240400	-2.60280900	-1.54347900	H
H	0	-0.83844300	-0.44186700	0.09235600	H	H	-1	-8.93724400	-2.27262000	-3.54514200	L
H	0	-1.70462300	1.57345800	-0.82094000	H	H	-1	-10.17960900	-0.27267800	-1.73857600	L
H	0	2.50637300	1.64257700	2.78306300	H	H	-1	-10.99615700	-3.67476600	-3.01782200	L
H	0	2.97432700	1.54169100	1.06066000	H	H	0	-7.51099600	-0.70439200	0.20541300	H
H	0	4.00093100	-0.37026400	1.38887200	H	C	0	5.61525100	-0.98141100	5.02828900	H
O	-1	-7.55326600	11.06428100	-3.79381400	L	H	0	6.25620500	-1.31506600	4.20727000	H
H	-1	-8.52602600	0.81447400	6.02711600	L	H	0	5.73237500	0.09961300	5.11756700	H
H	-1	-7.62232800	-7.04867200	-1.30567100	L	H	0	4.02306600	-0.66063700	3.65863400	H