

**Table.** Cartesian coordinates of DFT/B3LYP-D3BJ optimized geometrical structures of  $L(HXX)^-$ ,  $[L(HX_aX_b)]^-$ ,  $[LX]^-$ ,  $[L(HX)]$ , and L compounds (X = Cl, Br, I; L = H<sub>3</sub>TriNOx).

$[L(HCl_2)]^-$ , 1Cl, $E_0=-2652.065925$ au				$[L(HCl_2)]^-$ , 2Cl, $E_0=-2652.057183$ au			
O	-3.54864200	-0.64773000	-0.81593700	N	0.00039400	-0.00020100	1.15940100
H	-3.01986900	-0.40245600	-1.61771900	C	-1.27933500	-0.65891000	1.64468800
O	-0.83062300	2.76788500	-2.46472100	H	-2.07824800	-0.12493700	1.15358800
H	-1.15166300	1.87950600	-2.75649400	H	-1.30345900	-0.46837400	2.71869500
O	3.64757400	-1.99876500	1.30552300	C	0.06995700	1.43733700	1.64472500
H	3.29539400	-1.53198200	2.10398300	H	0.93152800	1.86251100	1.15328700
N	-2.66763100	-1.50042600	-0.07066300	H	0.24737300	1.36275900	2.71866800
N	-0.93759400	2.71103100	-1.03852400	C	1.21086200	-0.77939900	1.64386600
N	3.16158900	-1.17462300	0.23670600	H	1.14803800	-1.73786800	1.15200000
N	0.56016600	-0.16796900	0.71274900	H	1.05819800	-0.89626300	2.71783900
H	1.55173300	-0.22701100	1.01964700	C	-1.30938400	-2.13361700	1.37245200
C	-0.12897300	-1.37720600	1.36859200	C	-1.00321200	-3.00582300	2.42335400
H	-0.23049300	-2.11380000	0.58460600	C	-1.56290800	-2.64920900	0.09202800
H	0.57621800	-1.72478400	2.11945800	C	-0.89958800	-4.37401100	2.20364800
C	-1.44594700	-1.03964400	2.00739800	H	-0.80836200	-2.58265300	3.40391500
C	-1.44495500	-0.64270400	3.35038600	C	-1.42018100	-4.02375000	-0.12825300
H	-0.50525000	-0.66768600	3.89276400	C	-1.08831000	-4.87695200	0.91745400
C	-2.59911600	-0.15882500	3.95252400	H	-0.64717000	-5.03687900	3.02314100
H	-2.57671500	0.16167600	4.98770800	H	-1.54686800	-4.40076900	-1.13228600
C	-3.76915100	-0.05112500	3.20217300	H	-0.97897200	-5.93912400	0.72595900
H	-4.66750900	0.36270900	3.64771900	C	2.50311300	-0.06804700	1.37218200
C	-3.79368500	-0.48107400	1.88154100	C	3.10622200	0.63091400	2.42412100
H	-4.69016400	-0.38980900	1.28608100	C	3.07626600	-0.02832400	0.09174200
C	-2.64741200	-1.01554900	1.28098900	C	4.24017300	1.40377500	2.20553100
C	-3.16154500	-2.92075000	-0.22816100	H	2.64248400	0.58688300	3.40471300
C	-3.08295900	-3.25951700	-1.72050400	C	4.19599100	0.78187500	-0.12743300
H	-2.06691700	-3.12375600	-2.08774400	C	4.76999400	1.49339600	0.91940400
H	-3.73919900	-2.61652700	-2.30452300	H	4.68881400	1.95190400	3.02587300
H	-3.37773500	-4.30170800	-1.87452700	H	4.58587900	0.86181300	-1.13135700
C	-2.23884600	-3.86864000	0.54672900	H	5.63591600	2.11845400	0.72884400
H	-1.22595200	-3.85381700	0.14104100	C	-1.19240400	2.20055500	1.37318000
H	-2.61962000	-4.88836900	0.44783500	C	-2.09999200	2.37167800	2.42479400
H	-2.20082300	-3.62813900	1.61071900	C	-1.51325900	2.67754000	0.09289700
C	-4.60975100	-3.08695800	0.26223300	C	-3.33676000	2.96620200	2.20602200
H	-4.96866200	-4.08960600	0.01397200	H	-1.83016700	1.99141700	3.40517900
H	-5.25443800	-2.35731300	-0.22898700	C	-2.77515400	3.24129500	-0.12643500
H	-4.68703800	-2.95901600	1.34400700	C	-3.67900100	3.38095200	0.92005400
C	0.01324200	1.16015500	1.17844300	H	-4.03633100	3.07928900	3.02608100
H	0.07186300	1.14129100	2.26243500	H	-3.03918900	3.53927600	-1.13030500
H	-1.01738900	1.19254200	0.85295900	H	-4.65361200	3.81752100	0.72933000
C	0.80156300	2.31427900	0.62687700	N	-1.90379200	-1.74500200	-0.97077600
C	2.02793200	2.64385300	1.21191600	N	-0.56063700	2.52023300	-0.97072200
H	2.35247300	2.08263500	2.08273000	N	2.46293300	-0.77382400	-0.97204500
C	2.82756600	3.63962600	0.66323800	O	-1.33127100	-2.28553700	-2.17066800
H	3.78345400	3.87520000	1.11638100	H	-0.88174900	-1.51819600	-2.59859800
C	2.40830100	4.30174200	-0.48981700	O	2.64412600	-0.00559800	-2.17077900
H	3.04109200	5.05644500	-0.94480800	H	1.75510800	-0.00122000	-2.59924300
C	1.17632600	4.00392700	-1.06043200	O	-1.31614300	2.29436100	-2.16994600
H	0.84906500	4.49376300	-1.96623500	H	-0.87606900	1.52203800	-2.59867500
C	0.34430600	3.03475000	-0.48925000	C	-3.38890000	-1.57065000	-1.23231500
C	-2.08607500	3.58931000	-0.61612000	C	3.05449500	-2.14667000	-1.23616800
C	-1.93098500	5.02124900	-1.15558900	C	0.33243700	3.71929500	-1.23340700
H	-1.78382600	4.99645800	-2.23547400	H	0.00006900	-0.00005200	0.13147100
H	-1.08248100	5.53148500	-0.69304700	Cl	0.00192500	-0.00120900	4.82475700
H	-2.83309800	5.59983000	-0.93776000	C	-4.03842600	-2.89408100	-1.66842800
C	-3.35704200	2.94229200	-1.17767800	H	-4.04727500	-3.62297700	-0.85446100
H	-3.45768600	1.91981800	-0.81096200	H	-5.07320300	-2.71169200	-1.97076600
H	-3.32503600	2.90610400	-2.26594800	H	-3.49766100	-3.31492300	-2.51586200
H	-4.23415600	3.51956300	-0.86939200	C	-4.09955700	-1.04469500	0.02038800
C	-2.17777400	3.62632400	0.91502400	H	-3.93909500	-1.68416700	0.89036400

H	-1.26417100	4.00969500	1.37350900	H	-3.79404300	-0.02466000	0.25794100
H	-2.39715100	2.64173400	1.33041300	H	-5.17367900	-1.02086400	-0.17944900
H	-2.99818000	4.29092600	1.19748000	C	-3.51680000	-0.52257500	-2.34299600
C	0.57960800	-0.27411200	-0.79073400	H	-4.57412700	-0.30094400	-2.51607100
H	1.09107600	0.60990200	-1.16019300	H	-3.00611300	0.39867900	-2.05959500
H	-0.44788200	-0.23583400	-1.14403300	H	-3.07852400	-0.87846600	-3.27439400
C	1.24219200	-1.55101800	-1.23895800	C	-0.48915500	4.94265400	-1.67150700
C	0.58401000	-2.32705000	-2.19880300	H	-1.11626800	5.31602500	-0.85834600
H	-0.31635700	-1.92614200	-2.65134400	H	0.18610900	5.74723400	-1.97500600
C	1.07223300	-3.57784100	-2.55689400	H	-1.12375400	4.68333500	-2.51869500
H	0.54543500	-4.16807300	-3.29800000	C	1.14263300	4.07355100	0.01916900
C	2.21157600	-4.08060000	-1.93071900	H	0.50827200	4.25487800	0.88878900
H	2.57449000	-5.07441000	-2.17011000	H	1.87358800	3.29953800	0.25759400
C	2.89364600	-3.30403500	-1.00227900	H	1.69988200	4.99195100	-0.18146600
C	3.76943300	-3.68342900	-0.49626900	C	1.30473700	3.30505800	-2.34316400
C	2.44465300	-2.01876600	-0.68562300	H	2.02515100	4.10998700	-2.51671400
C	4.33075400	-0.42232900	-0.35264100	H	1.84744500	2.40270200	-2.05848700
C	3.80647800	0.52643700	-1.43557600	H	0.77794500	3.10224800	-3.27462600
H	3.13218400	1.27172300	-1.01455400	C	2.20931400	-2.78046300	-2.34632800
H	3.29391400	-0.01170300	-2.23497300	H	2.54551200	-3.80696500	-2.52030900
H	4.65111200	1.05886400	-1.87976900	H	1.15646800	-2.79866900	-2.06180900
C	5.38725500	-1.36751400	-0.94591300	H	2.29751000	-2.22251300	-3.27753400
H	5.01578400	-1.88514700	-1.83231700	C	4.52463900	-2.04670800	-1.67455000
H	5.68857900	-2.10622400	-0.20157500	H	5.16175100	-1.69086400	-0.86131900
H	6.26982200	-0.79047900	-1.23552900	H	4.88369300	-3.03357700	-1.97886300
C	4.95706900	0.39208500	0.78483000	H	4.61706700	-1.36687300	-2.52129000
H	5.43038400	-0.26251700	1.51520700	C	2.95621300	-3.02645800	0.01570800
H	4.19897700	0.97509200	1.30373600	H	3.43106600	-2.56873200	0.88550100
H	5.71070100	1.07028600	0.37467300	H	1.92036100	-3.27200300	0.25438500
C	2.32468300	-0.26020400	3.45563500	H	3.47229000	-3.96842300	-0.18582300
Cl	-1.94367500	0.03083100	-3.32156300	Cl	-0.00121200	0.00030000	-3.66653500
<b>[L(HCl<sub>2</sub>)]<sup>-</sup>, 3Cl, E<sub>0</sub>=-2652.048970 au</b>				<b>[L(HCl<sub>2</sub>)]<sup>-</sup>, 4Cl, E<sub>0</sub>=-2652.048682 au</b>			
N	-0.70031100	0.22844900	1.31032700	O	-1.13844200	1.09927500	-0.97269700
C	-0.03814300	-0.77994700	2.22796500	O	2.74739400	-0.78375500	-2.55264200
H	-0.39149400	-1.74989700	1.90324300	O	-3.28144000	-0.57158500	-1.11306700
H	-0.42332000	-0.56073200	3.22607700	N	-1.11779500	2.50337100	-0.71888400
C	-2.19666500	0.01486500	1.25704400	N	2.75820800	-0.08654800	-1.30401500
H	-2.58168600	0.80245200	0.62524000	N	-2.78057200	-1.48667300	-0.11035300
H	-2.54545700	0.16684800	2.28182600	N	0.04794100	-0.43983600	1.82927400
C	-0.37653500	1.64308500	1.76109900	C	-1.10311500	0.56748200	1.78057200
H	0.70314500	1.68912600	1.81768900	C	-0.59131600	1.98640500	1.72468500
H	-0.81710400	1.73305400	2.75690800	C	-0.02764100	2.48195400	2.90996800
C	1.45481300	-0.66932400	2.14412700	C	0.60561400	3.71554600	2.96519200
C	2.15717600	-0.07992800	3.19977900	C	0.71526400	4.47268700	1.80235500
C	2.14613900	-1.08389700	0.99491100	C	0.16065500	4.00184900	0.62113000
C	3.52906600	0.12525800	3.10855800	C	-0.53865200	2.78673600	0.55914900
H	1.60722200	0.23439700	4.08008200	C	-2.48560400	3.08187800	-0.97509400
C	3.51780500	-0.83623500	0.89125100	C	-3.52538600	2.59145100	0.04734100
C	4.20180400	-0.23790500	1.94388000	C	-2.40199700	4.61363800	-0.91186500
H	4.06426300	0.58534300	3.93144200	C	-2.88481200	2.68573800	-2.40362600
H	4.03925000	-1.08348000	-0.02625500	C	1.20357000	0.00254200	0.98171000
H	5.26483000	-0.04959200	1.84459400	C	2.38787100	-0.91820600	0.94670900
C	-0.92668900	2.65400200	0.79988000	C	2.77824900	-1.70430600	2.03413800
C	-2.12350300	3.31278700	1.10045200	C	3.78832900	-2.64986700	1.88772500
C	-0.29137400	2.89291200	-0.42733300	C	4.41249000	-2.81670000	0.65132100
C	-2.71517400	4.16182600	0.17216800	C	4.07887800	-1.98828000	-0.41420900
H	-2.59315800	3.12407500	2.05997600	C	3.10078400	-1.00226500	-0.26238000
C	-0.91773800	3.70810100	-1.37457600	C	3.63524400	1.12801000	-1.43470200
C	-2.12160400	4.33656900	-1.07719900	C	5.06041100	0.75256200	-1.87525700
H	-3.64681500	4.66142500	0.41105300	C	2.98310200	2.03997200	-2.47978400
H	-0.46327200	3.82666200	-2.34734300	C	3.68310200	1.87070000	-0.09398200
H	-2.59673300	4.96482300	-1.82248800	C	-0.45148600	-1.86229800	1.62707400
C	-2.55754300	-1.34818300	0.74499400	C	-0.51128100	-2.35837700	0.20377300
C	-3.06025700	-2.28252200	1.65746400	C	0.58531200	-3.06579300	-0.30196500
C	-2.36490300	-1.72370500	-0.59426600	C	0.64524800	-3.45416200	-1.63355900
C	-3.34616800	-3.58405400	1.26390300	C	-0.40804100	-3.14423500	-2.48536800

H	-3.19300500	-1.97307900	2.68870700	C	-1.53762800	-2.51173800	-1.98627500
C	-2.62895400	-3.04298200	-0.97517600	C	-1.61543200	-2.14794500	-0.64099700
C	-3.11482100	-3.96474000	-0.05628100	C	-3.94182700	-2.35618700	0.25621600
H	-3.72225400	-4.29949900	1.98576900	C	-3.47997900	-3.41664400	1.26194000
H	-2.41974600	-3.33951700	-1.99217300	C	-4.56479300	-3.05353300	-0.96676000
H	-3.30730000	-4.98405800	-0.37239500	C	-4.97770700	-1.44203700	0.92455000
N	1.38696900	-1.74331700	-0.04088400	H	0.34208700	-0.44346600	2.85843300
N	-1.83199300	-0.75688400	-1.52744100	H	-1.73607000	0.29164200	0.95391500
O	0.97555600	2.25446400	-0.65925300	H	-1.63550400	0.40136800	2.71806700
O	1.55726300	-1.05750500	-1.29438900	H	-0.05418600	1.84955400	3.79215800
H	2.48506600	-1.19937000	-1.70406200	H	1.03759100	4.06023000	3.89719200
O	0.93059800	1.64478700	-1.96008000	H	1.25085600	5.41565800	1.80523100
H	1.17614100	0.72134600	-1.76135300	H	0.27642200	4.55885700	-0.29792500
O	-0.94938200	-1.45686100	-2.42111200	H	-3.24126100	2.88403500	1.06134800
H	-0.05168700	-1.25463100	-2.08518200	H	-3.64404100	1.50959100	0.01025500
C	1.61521300	-3.24084100	-0.14609100	H	-4.49946600	3.03831700	-0.17190400
C	2.18155500	3.15611300	-0.59714600	H	-2.15831200	4.97313200	0.08821500
C	-2.84843800	-0.07553800	-2.41555700	H	-3.37462700	5.02658500	-1.19052600
C	3.41228700	2.26314800	-0.77123500	H	-1.65524600	4.98965100	-1.61408200
H	4.32056300	2.86349300	-0.66922900	H	-2.08385100	2.93466200	-3.10179700
H	3.42369500	1.48882000	-0.00785400	H	-3.79103200	3.22744200	-2.68806900
H	3.43116000	1.77573200	-1.74516500	H	-3.08521400	1.62091100	-2.50282000
C	2.17112400	4.23922300	-1.68862300	H	1.49124500	0.96947400	1.38307800
H	1.39378000	4.98639500	-1.51670300	H	0.84330400	0.15927000	-0.03097800
H	3.13490900	4.75481800	-1.69583700	H	2.27423000	-1.59563200	2.98958900
H	2.02233500	3.78106500	-2.66734100	H	4.07020200	-3.26768800	2.73270200
C	2.21933200	3.80860400	0.78990100	H	5.17416400	-3.57864600	0.52372100
H	1.33055700	4.41214200	0.98520500	H	4.55229400	-2.10143000	-1.37948800
H	2.31632200	3.05674400	1.57534900	H	5.01813700	0.14463800	-2.77978400
H	3.09116100	4.46463500	0.84839400	H	5.58496900	0.19470100	-1.09581000
C	-2.06975300	0.85005100	-3.35732000	H	5.63563500	1.65788700	-2.08922900
H	-2.76946400	1.50903700	-3.87968300	H	3.55152600	2.97195200	-2.55947200
H	-1.35864200	1.45337500	-2.79691500	H	1.95435800	2.26798100	-2.19842900
H	-1.51251600	0.27339100	-4.09400500	H	2.95273500	1.55940800	-3.45624000
C	-3.79616100	0.76381600	-1.55449900	H	2.69609100	2.24077800	0.18578200
H	-4.30165800	0.16342000	-0.79528400	H	4.34284900	2.73611500	-0.19646900
H	-3.27003200	1.58990300	-1.07643400	H	4.07320200	1.24600500	0.71173900
H	-4.56522800	1.19464600	-2.20023200	H	-1.41726800	-1.88118200	2.11829100
C	-3.66217700	-1.08625300	-3.24145900	H	0.22251800	-2.48608500	2.20913400
H	-4.28556500	-0.54632700	-3.95923300	H	1.42006200	-3.27974200	0.35077300
H	-2.99518400	-1.74601600	-3.79744300	H	1.53297500	-3.94754400	-2.00861600
H	-4.31830000	-1.69087600	-2.61186800	H	-0.34628300	-3.37137300	-3.54235400
C	3.08864100	-3.67702100	-0.05839600	H	-2.34558000	-2.23353300	-2.64547400
H	3.52471300	-3.44568200	0.91492200	H	-3.14175900	-2.96561400	2.19609000
H	3.13505600	-4.76149400	-0.19439900	H	-2.67624900	-4.03399800	0.85786600
H	3.69023000	-3.21245000	-0.84119500	H	-4.32399900	-4.06981100	1.49627600
C	1.03852800	-3.74187100	-1.47307600	H	-3.87175100	-3.77483400	-1.40368600
H	1.08041200	-4.83427300	-1.47421300	H	-4.83166900	-2.32082500	-1.72789800
H	0.00482900	-3.43183800	-1.59876900	H	-5.46823800	-3.59011400	-0.66344800
H	1.62271200	-3.37754300	-2.31825600	H	-5.81905900	-2.03450800	1.29470900
C	0.82710200	-3.86671200	1.01385600	H	-5.35055600	-0.70258100	0.21699900
H	1.17734200	-3.49848700	1.98108900	H	-4.52292300	-0.91531500	1.76669400
H	-0.24008400	-3.66157000	0.91564800	H	-0.66775000	0.95734400	-1.85291800
H	0.96922900	-4.95035500	1.00367200	H	1.85223400	-0.56355000	-2.90637400
H	-0.33022200	0.08572400	0.36250000	H	-2.57877400	0.11369800	-1.12605300
Cl	4.16303200	-1.27048300	-2.59840200	Cl	0.01056800	0.30073400	-3.57851900
Cl	-2.15434400	0.72420800	4.60424500	Cl	0.49130600	-0.62700100	4.77430300
<b>[L(HCl<sub>2</sub>)], 5Cl, E<sub>0</sub>=-2652.051244 au</b>				<b>[L(HCl<sub>2</sub>)], 6Cl, E<sub>0</sub>=-2652.046543 au</b>			
N	0.32730600	-0.33613000	1.25113700	N	-0.40476400	-0.23017500	0.15238800
C	-1.04109500	-0.89453400	1.62283100	C	-1.01983000	-0.01275500	-1.20639800
H	-1.73068600	-0.09451200	1.39984800	H	-0.28885400	-0.36201600	-1.92917600
H	-0.98907800	-1.07628900	2.69906400	H	-1.11909700	1.05222300	-1.37489100
C	0.59553200	0.91950400	2.07171500	C	-1.08678400	0.50049200	1.32199300
H	1.56237100	1.28553000	1.74035300	H	-0.28961000	1.03189600	1.82596200
H	0.63341300	0.58100500	3.10929000	H	-1.46095400	-0.27514900	1.99139000
C	1.41724600	-1.35792600	1.47641600	C	1.06026200	0.07631500	0.09177200

H	1.11577400	-2.23229000	0.91896800	H	1.13706300	1.15855700	0.14695500
H	1.38952500	-1.57960500	2.54612200	H	1.42316700	-0.19053500	-0.89975100
C	-1.40037100	-2.13636300	0.86217800	C	-2.33865600	-0.71712600	-1.36541100
C	-1.00872400	-3.38471900	1.36258800	C	-3.36913300	-0.01738500	-1.99964500
C	-2.11439000	-2.07201000	-0.34604200	C	-2.57975300	-2.02480000	-0.91066800
C	-1.22890200	-4.54670200	0.63344900	C	-4.62396100	-0.58264700	-2.17121500
H	-0.51638600	-3.42275100	2.32853900	H	-3.18211000	1.00114900	-2.31858800
C	-2.28784500	-3.24049400	-1.09785400	C	-3.85944000	-2.57182000	-1.04475600
C	-1.83983400	-4.46418000	-0.61747300	C	-4.87107200	-1.86183800	-1.67655500
H	-0.90959400	-5.50407200	1.02867100	H	-5.41282600	-0.01489500	-2.65055100
H	-2.76677500	-3.16352000	-2.06306800	H	-4.04543400	-3.54158600	-0.60830100
H	-1.98451700	-5.35892600	-1.21334500	H	-5.85691500	-2.30365700	-1.77114500
C	2.77261400	-0.87997000	1.04515400	C	1.90640600	-0.62153900	1.11514500
C	3.70914400	-0.53494100	2.02457900	C	1.39025000	-1.28897700	2.22216700
C	3.11372700	-0.75973300	-0.31136900	C	3.30594100	-0.62457600	0.87878300
C	4.96288600	-0.04935300	1.67095300	C	2.22805900	-1.96328300	3.10972000
H	3.42599500	-0.63426200	3.06705200	H	0.32567100	-1.33743600	2.41879500
C	4.36481100	-0.24267400	-0.65945200	C	4.13135600	-1.27969400	1.79794100
C	5.28296000	0.10734000	0.32338000	C	3.59805600	-1.95223800	2.89614300
H	5.67572800	0.22393500	2.44036900	H	1.78967600	-2.48590400	3.95086400
H	4.58593600	-0.08279600	-1.70467500	H	5.20071300	-1.26902300	1.66478700
H	6.24846600	0.50941800	0.03587400	H	4.26624800	-2.45798900	3.58504400
C	-0.46794100	1.95066900	1.84402100	C	-2.21100300	1.41365700	0.93511200
C	-1.48968600	2.12833100	2.77938700	C	-3.51690400	1.00933400	1.22763800
C	-0.46903400	2.70144400	0.65672400	C	-1.99257300	2.62845500	0.26720900
C	-2.52394200	3.02390400	2.52711000	C	-4.60328300	1.77365500	0.82150200
H	-1.46899000	1.54475800	3.69347600	H	-3.66187600	0.07131300	1.75216200
C	-1.53654000	3.56153000	0.38838300	C	-3.09121300	3.36818300	-0.17919600
C	-2.55419000	3.72502200	1.32344200	C	-4.38679800	2.94336500	0.09643800
H	-3.31557200	3.15504100	3.25594800	H	-5.61101600	1.43974800	1.03875300
H	-1.59326500	4.06250600	-0.56607300	H	-2.91461800	4.25627300	-0.76855800
H	-3.38195300	4.38847900	1.10004000	H	-5.22873800	3.52832100	-0.25846400
N	-2.64993800	-0.81396100	-0.77148500	N	-1.53488900	-2.75091800	-0.21500100
N	0.64446900	2.49133500	-0.21855400	N	-0.63716100	3.02299000	-0.01805300
N	2.11556800	-1.07828200	-1.29918800	N	3.75897500	-0.01236500	-0.31731900
O	-2.56474200	-0.78024300	-2.20265800	O	-2.14687600	-3.56448100	0.78516700
H	-2.27434300	0.13732800	-2.41395300	H	-2.06118100	-3.05357100	1.64091700
O	2.18113000	-0.07438600	-2.32631600	O	3.52341500	1.40057900	-0.25815500
H	1.47813800	0.54507300	-2.03739600	H	2.98967700	1.60063700	-1.06905100
O	0.31716700	1.47327400	-1.17228000	O	-0.61554400	3.48781200	-1.37879300
H	-0.45435600	1.77068400	-1.75180900	H	0.13799400	2.99551500	-1.79396800
C	-4.09908800	-0.57903600	-0.38606400	C	-0.69067800	-3.69409500	-1.04502800
C	2.22206900	-2.40260900	-1.99932600	C	5.07793100	-0.28410100	-0.94239800
C	1.41431000	3.62874600	-0.78603000	C	-0.05707900	4.10062200	0.85992900
H	0.31689900	-0.07306800	0.25232400	H	-0.55590900	-1.25368800	0.31710300
C	-4.27647000	-0.72099800	1.13103000	CI	1.69414600	1.95600500	-2.69187400
H	-3.71988400	0.04219700	1.67634500	C	-0.04014000	-2.94697200	-2.21180300
H	-5.33461200	-0.58297300	1.36682300	H	-0.77794600	-2.46603200	-2.85624700
H	-3.98023100	-1.70570300	1.49586300	H	0.67895800	-2.20300600	-1.86744600
C	-4.42920800	0.86181200	-0.78831900	H	0.51154400	-3.66747700	-2.81961800
H	-3.72900800	1.55531800	-0.32083900	C	-1.53866600	-4.85275600	-1.59237100
H	-4.35934300	1.00310600	-1.86544000	H	-2.28209900	-4.49402500	-2.30803800
H	-5.44459900	1.10990700	-0.46439400	H	-0.89107300	-5.56798900	-2.10632000
C	-5.04158100	-1.55980700	-1.10273400	H	-2.05002600	-5.36417700	-0.77787700
H	-6.08001600	-1.27763300	-0.90873900	C	0.40518700	-4.22405000	-0.11272800
H	-4.86594600	-1.52711200	-2.17773600	H	1.06471500	-4.89954400	-0.66443200
H	-4.89863700	-2.58362300	-0.74914000	H	1.00635700	-3.40280400	0.28354400
C	0.72895800	4.38835900	-1.93523000	H	-0.03438600	-4.75921900	0.72687700
H	-0.10889000	4.99271500	-1.58598000	C	1.42016200	4.23971000	0.47187600
H	1.45079100	5.06528100	-2.40226600	H	1.95508000	3.29900300	0.61361700
H	0.35279700	3.70514000	-2.69670300	H	1.52360500	4.53042700	-0.57298300
C	1.70775900	4.57812700	0.38567800	H	1.89361100	5.00295300	1.09627400
H	0.79856900	5.03983300	0.77321800	C	-0.77678900	5.44709800	0.67498200
H	2.19754800	4.04241200	1.20239400	H	-1.80066800	5.40884900	1.05319900
H	2.37507200	5.37284900	0.04376300	H	-0.24394400	6.22760700	1.22486600
C	2.74627600	3.04972900	-1.28862900	H	-0.79649300	5.71683500	-0.38122700

H	3.41283300	3.86553500	-1.58218000	C	-0.15377600	3.66346200	2.32608400
H	3.22730800	2.46297900	-0.50457300	H	-1.18297600	3.46003300	2.62769500
H	2.60330300	2.40242000	-2.15181100	H	0.45349900	2.77803600	2.51921200
C	0.99406400	-2.51084500	-2.91191600	H	0.22984800	4.46740900	2.95896300
H	0.94365300	-3.51315600	-3.34708200	C	5.01919400	0.32974900	-2.35395300
H	0.07989400	-2.32983300	-2.34589500	H	4.95732500	1.41610700	-2.31150600
H	1.04400100	-1.77848000	-3.71611800	H	5.92029300	0.05356500	-2.90876200
C	3.51222800	-2.50709300	-2.83159800	H	4.13958900	-0.02640200	-2.89159400
H	4.39822100	-2.53750800	-2.19297900	C	5.24711300	-1.80201900	-1.10691700
H	3.49206600	-3.42547800	-3.42462700	H	6.13638500	-1.99721100	-1.71158300
H	3.59315600	-1.65873000	-3.51155600	H	5.35777800	-2.33098800	-0.16199800
C	2.18767100	-3.53537700	-0.96848600	H	4.38027000	-2.21582200	-1.62725000
H	2.96179300	-3.42015600	-0.20657200	C	6.25431600	0.36091500	-0.18356800
H	1.21250400	-3.60774300	-0.48757200	H	7.15736600	0.33387800	-0.80012800
H	2.36700000	-4.48186900	-1.48437700	H	6.00912300	1.40263700	0.02752300
Cl	-1.89079700	2.14273200	-3.01328100	H	6.48138400	-0.13735600	0.75950100
Cl	0.41392400	-1.28815400	4.77729300	Cl	-1.99776300	-2.08233000	3.36920600
<b>[L(HCl<sub>2</sub>)<sup>-</sup>]<sup>-</sup>, 7Cl, E<sub>0</sub>=-2652.044458 au</b>				<b>[L(HCl<sub>2</sub>)<sup>-</sup>]<sup>-</sup>, 8Cl, E<sub>0</sub>=-2652.031149 au</b>			
N	-0.49697400	-0.02153800	1.39229200	N	1.37543700	-0.19927800	-1.66551100
C	-0.34063000	1.40306100	1.89288500	C	0.32604700	-0.29110900	-2.67914700
H	0.72015300	1.61721700	1.83295000	H	-0.18115300	-1.23817000	-2.53031100
H	-0.67184500	1.37985400	2.93373100	H	0.76052100	-0.30306300	-3.69990600
C	0.37848600	-0.96209200	2.19243700	C	2.18649800	-1.41296400	-1.61141900
H	0.14830300	-1.95577500	1.83162100	H	2.94576800	-1.25760800	-0.85394400
H	0.03874500	-0.86311500	3.22561600	H	2.72149300	-1.56754600	-2.57168400
C	-1.95454000	-0.45129900	1.44896100	C	2.21146700	0.98724200	-1.85790200
H	-2.50408900	0.32519600	0.93503900	H	1.54363700	1.83783100	-1.95370400
H	-2.21094400	-0.45573100	2.51171600	H	2.80051400	0.90882300	-2.79491700
C	-1.15033200	2.35372400	1.06166400	C	-0.67069800	0.83698300	-2.58702900
C	-2.35295300	2.85890400	1.56377100	C	-0.59693500	1.89806300	-3.49426700
C	-0.73723600	2.69731800	-0.23378200	C	-1.65034900	0.87231800	-1.58117500
C	-3.15693400	3.67669800	0.77663500	C	-1.44610400	2.99528300	-3.39980300
H	-2.65410200	2.58259400	2.56874800	H	0.15553300	1.86142600	-4.27567200
C	-1.57225800	3.47926600	-1.03452800	C	-2.47728800	1.99467100	-1.46582900
C	-2.77235000	3.97044500	-0.53000700	C	-2.37913500	3.04726500	-2.36883400
H	-4.08772200	4.06503800	1.17360000	H	-1.36627000	3.80942000	-4.11196500
H	-1.28513200	3.68255800	-2.05561000	H	-3.18276100	2.05878100	-0.64788100
H	-3.41127600	4.57741800	-1.16196100	H	-3.02841100	3.90807800	-2.25600900
C	-2.15827300	-1.78315100	0.79197000	C	3.15233400	1.20712000	-0.69883800
C	-2.21406900	-2.94232000	1.57311600	C	4.48950200	0.80972400	-0.78962400
C	-2.24941700	-1.88696500	-0.60423800	C	2.68218100	1.72913300	0.51532300
C	-2.29213600	-4.19558500	0.97720100	C	5.34016200	0.86915500	0.30924700
H	-2.17410400	-2.84337700	2.65232000	H	4.85307200	0.41812200	-1.73423600
C	-2.26182700	-3.15171200	-1.19838800	C	3.52444200	1.73702700	1.63183300
C	-2.28151100	-4.29826500	-0.41285500	C	4.84388700	1.31080000	1.53338200
H	-2.32669500	-5.08721400	1.59211800	H	6.37075600	0.54413300	0.21915800
H	-2.24008800	-3.22604800	-2.27584800	H	3.12588200	2.06000100	2.58245000
H	-2.29072600	-5.27312500	-0.88713600	H	5.48160900	1.32239700	2.41047800
C	1.83731800	-0.63788600	2.04641300	C	1.40272400	-2.66935300	-1.31080100
C	2.51243900	-0.12234400	3.15760300	C	1.17027800	-3.57275200	-2.35432400
C	2.52664100	-0.80444300	0.83254600	C	0.86018800	-2.95256300	-0.04479100
C	3.85026200	0.24434000	3.07057400	C	0.39543100	-4.71343400	-2.18451600
H	1.96235800	0.00838300	4.08315400	H	1.58837200	-3.34740800	-3.33007700
C	3.86557900	-0.41137500	0.74510700	C	0.06025500	-4.09160100	0.11446200
C	4.51942400	0.10830300	1.85674100	C	-0.17414600	-4.96432600	-0.93913500
H	4.35876200	0.64995500	3.93783100	H	0.21890800	-5.38340300	-3.01853000
H	4.38813000	-0.47787400	-0.20301700	H	-0.40214700	-4.26014200	1.07577300
H	5.55576300	0.41295400	1.76409000	H	-0.80396300	-5.83414000	-0.78777400
N	0.55312400	2.22583500	-0.65081100	N	-1.76457500	-0.25680300	-0.69461200
N	1.79948600	-1.31927700	-0.30638200	N	1.06862500	-2.04234000	1.04986200
N	-2.32964800	-0.66709800	-1.36326100	N	1.33352900	2.21640000	0.56477400
O	0.39807100	1.49632500	-1.89165400	O	-1.57470100	0.17319600	0.66230500
H	1.05920300	0.76313500	-1.77177100	H	-2.35526000	0.68938800	1.00658600
O	-1.40260100	-0.74908400	-2.45938800	O	0.68002200	1.59355300	1.67962000
H	-0.82916200	0.02271500	-2.29976400	H	-0.02781500	1.07881300	1.24796800
O	2.03654100	-0.49353500	-1.44762300	O	-0.16363500	-1.96546200	1.78736500

H	2.98561700	-0.52961900	-1.80367100	H	-0.59806500	-1.16301800	1.43806400
C	1.60494000	3.29502800	-0.81585300	C	-2.97993500	-1.13026900	-0.87561100
C	-3.69168200	-0.34821000	-1.91743700	C	1.16374800	3.69932000	0.67722300
C	2.04134300	-2.77005000	-0.66046500	C	2.12639900	-2.41086900	2.04651400
C	-3.57664100	1.00575800	-2.62334300	C	-0.33706200	3.97724700	0.55073400
H	-4.56395500	1.33159500	-2.96201000	H	-0.52127300	5.05542100	0.57034400
H	-3.17720100	1.75096500	-1.93905300	H	-0.71117200	3.57585800	-0.38874000
H	-2.91656100	0.93775800	-3.48784600	H	-0.89704300	3.51644300	1.36402400
C	-4.19881100	-1.40185300	-2.91689700	C	1.68242000	4.27809300	2.00636600
H	-4.43878600	-2.34658100	-2.42660400	H	2.77209700	4.24648000	2.06830000
H	-5.10829300	-1.03578800	-3.40091700	H	1.37265300	5.32293200	2.09651400
H	-3.44793500	-1.57918900	-3.68847600	H	1.25704900	3.72186100	2.84290800
C	-4.67029600	-0.22343500	-0.74356500	C	1.90072200	4.34829400	-0.50103700
H	-4.74208400	-1.15009500	-0.17156100	H	2.97368100	4.14646700	-0.47111100
H	-4.37650100	0.58382300	-0.07028400	H	1.50185000	3.98906300	-1.45183500
H	-5.66464200	0.00937800	-1.13250100	H	1.75734900	5.43117800	-0.46053600
C	1.32947500	-3.02902500	-1.99402400	C	2.13868000	-1.30062400	3.10512400
H	1.26665700	-4.10824500	-2.16110200	H	3.02393200	-1.40567300	3.73991400
H	0.32456400	-2.60976500	-1.98175700	H	2.15337900	-0.32543700	2.62177900
H	1.87671000	-2.57982600	-2.82161500	H	1.24758000	-1.35226500	3.72902700
C	1.40013800	-3.62827000	0.43452800	C	3.48514900	-2.44692900	1.34045900
H	1.82979900	-3.41605500	1.41648900	H	3.49021300	-3.15133900	0.50539600
H	0.32182000	-3.48256900	0.46892000	H	3.76456600	-1.45698400	0.98098000
H	1.58853400	-4.68194000	0.21502400	H	4.24633300	-2.77073000	2.05525700
C	3.52842100	-3.13925000	-0.78438300	C	1.85812100	-3.76844200	2.72187500
H	3.60319500	-4.17681700	-1.12355300	H	2.58295800	-3.92714000	3.52554000
H	4.04776600	-2.50984900	-1.50892700	H	0.85754900	-3.78188500	3.15601200
H	4.04094500	-3.06483900	0.17743700	H	1.94942800	-4.59653200	2.01520000
C	1.33644500	4.23441000	-2.00358600	C	-4.31764600	-0.38103600	-1.01640600
H	0.50952600	4.91977300	-1.80892000	H	-4.35324600	0.21681600	-1.92921600
H	2.22807800	4.83626000	-2.19581100	H	-5.12786400	-1.11349400	-1.05947100
H	1.12088200	3.64959000	-2.89870000	H	-4.51146700	0.26625400	-0.16201800
C	2.94968300	2.59142500	-1.01758300	C	-3.07341800	-2.09018200	0.31461400
H	3.75007400	3.33553500	-1.04016500	H	-3.83623300	-2.84185500	0.09662100
H	3.14497400	1.89959200	-0.20030100	H	-2.12336300	-2.58887100	0.48784800
H	2.99904400	2.03110700	-1.94984000	H	-3.37062900	-1.57173600	1.22561000
C	1.65595600	4.09745600	0.49153400	C	-2.71545700	-1.94145000	-2.15347700
H	0.72011800	4.62223100	0.69227700	H	-2.56867900	-1.28696500	-3.01649400
H	1.88468000	3.44980100	1.34035700	H	-1.83581000	-2.57531800	-2.03215300
H	2.45247300	4.84117100	0.41561300	H	-3.57767600	-2.58030300	-2.36252400
Cl	4.69416100	-0.30011700	-2.72698500	H	-5.11659500	0.61364500	2.34508200
H	-0.16708500	-0.06688000	0.41968800	Cl	-6.09091000	-0.33604700	2.59664400
Cl	-1.68262400	0.10646900	4.82053200	Cl	-3.77609900	1.85876500	1.93034600
<b>[L(HCl<sub>2</sub>)<sup>-</sup>]<sup>-</sup>, 9Cl, E<sub>0</sub>=-2652.027081 au</b>				<b>[L(HBr<sub>2</sub>)<sup>-</sup>]<sup>-</sup>, 1Br, E<sub>0</sub>=-6879.917667 au</b>			
N	0.78551800	-0.00849200	-1.73740400	O	-3.68935900	-0.66234400	0.10548000
C	0.99995700	-1.39787200	-2.14250800	H	-3.40388300	-0.40024000	-0.80466500
H	1.72922600	-1.81418000	-1.46204200	O	-1.39080300	2.87701900	-2.09268400
H	1.44769400	-1.43660200	-3.15818400	H	-1.79588400	2.01094200	-2.33764800
C	2.04523600	0.73494000	-1.75003400	O	3.85720500	-2.01901600	0.20767800
H	1.81777800	1.74383500	-1.43626300	H	3.74695100	-1.60363500	1.09693700
H	2.44173200	0.80173000	-2.78536800	N	-2.62933900	-1.50900800	0.57562400
C	-0.20625600	0.63543200	-2.59970200	N	-1.14051000	2.75410400	-0.68802300
H	-1.11082600	0.04774100	-2.53087300	N	3.07971300	-1.15711400	-0.63567800
H	0.12400200	0.59638400	-3.65930200	N	0.70437000	-0.17794100	0.55121200
C	-0.25332400	-2.24104300	-2.16356100	H	1.74198300	-0.25552700	0.56220000
C	-0.87255200	-2.47185300	-3.39788700	C	0.20360900	-1.39462800	1.34806700
C	-0.86040900	-2.75444900	-1.00287300	H	-0.07243500	-2.13153800	0.60736100
C	-2.08473100	-3.14157100	-3.50500300	H	1.07263200	-1.73526800	1.90698100
H	-0.39654600	-2.07728300	-4.28961700	C	-0.92225000	-1.07159600	2.29014800
C	-2.09812000	-3.40535400	-1.11326900	C	-0.59108800	-0.69589700	3.59852000
C	-2.70821300	-3.59471200	-2.34544500	H	0.45281000	-0.72924500	3.89375900
H	-2.54658700	-3.28527500	-4.47548100	C	-1.55896700	-0.22412000	4.47511700
H	-2.58357500	-3.73073600	-0.20542100	H	-1.28019500	0.07967700	5.47748800
H	-3.66822000	-4.09705300	-2.39794300	C	-2.87776600	-0.10788300	4.03903700
C	-0.48152700	2.08151500	-2.26035600	H	-3.63821400	0.29647700	4.69854300
C	0.13869200	3.07039000	-3.03368200	C	-3.22771500	-0.51887000	2.75946700

C	-1.27955400	2.48288000	-1.17335700	H	-4.24382300	-0.42323600	2.40647800
C	0.03339900	4.42206200	-2.73150700	C	-2.26662500	-1.04084000	1.88475300
H	0.74858200	2.75405600	-3.87360800	C	-3.13236100	-2.93614500	0.53188500
C	-1.35998400	3.84709700	-0.85592500	C	-3.46824900	-3.25094300	-0.92958900
C	-0.71033400	4.80715600	-1.61910600	H	-2.59901100	-3.08741000	-1.56445500
H	0.54305000	5.16030800	-3.34067400	H	-4.27381000	-2.61614500	-1.29438000
H	-1.92100000	4.13183000	0.02155700	H	-3.77502900	-4.29746300	-1.01508400
H	-0.78834700	5.85409900	-1.34584300	C	-2.01973400	-3.88080300	1.00004000
C	3.12998300	0.13755800	-0.88425200	H	-1.16197000	-3.84398800	0.32659700
C	4.12069900	-0.63144500	-1.50691700	H	-2.40216300	-4.90462800	0.99266500
C	3.16388600	0.26583600	0.51653500	H	-1.68814400	-3.65638000	2.01540500
C	5.09656900	-1.30817800	-0.78648600	C	-4.38516600	-3.13387400	1.40129900
H	4.09176900	-0.72234200	-2.58777900	H	-4.78548500	-4.13913300	1.24373900
C	4.13526100	-0.44066200	1.24124600	H	-5.15110600	-2.40969300	1.12150400
C	5.08798800	-1.22255200	0.60311400	H	-4.16136900	-3.02202900	2.46420300
H	5.83663100	-1.91133000	-1.30056600	C	0.32901800	1.14130100	1.18315800
H	4.10519800	-0.38506700	2.31908600	H	0.67806600	1.08544500	2.21014000
H	5.82302700	-1.76122300	1.19161300	H	-0.75036300	1.19126400	1.15206700
N	-0.25646000	-2.56195900	0.28298100	C	0.95879900	2.30951900	0.47826800
N	2.18383700	1.05668600	1.20215100	C	2.29286500	2.62891800	0.74941500
N	-1.95070100	1.51062300	-0.36188100	H	2.82245800	2.04560100	1.49655800
O	-1.33123600	-2.43743500	1.22619300	C	2.93404600	3.64414900	0.04965300
H	-1.15864000	-1.59558300	1.69560300	H	3.97306000	3.87061100	0.25853900
O	-1.96519600	2.03532100	0.97454000	C	2.24315300	4.33820100	-0.94231200
H	-1.58153600	1.32331700	1.52615500	H	2.74454200	5.10928800	-1.51762300
O	1.95385200	0.41738300	2.46762700	C	0.90698000	4.05209000	-1.19634000
H	0.98667600	0.28322200	2.50821900	H	0.36554600	4.56854800	-1.97570500
C	0.63319700	-3.66823400	0.79577700	C	0.24023200	3.06227300	-0.46575400
C	-3.38445900	1.19469400	-0.71429300	C	-2.14224300	3.61220400	0.04261400
C	2.54941500	2.48883800	1.50869300	C	-2.11742800	5.06400200	-0.46413600
C	-3.84175600	0.10576600	0.26479000	H	-2.24650500	5.08221600	-1.54633900
H	-4.83102000	-0.25978500	-0.02615300	H	-1.17647100	5.55832300	-0.21021600
H	-3.14076900	-0.73025800	0.25418200	H	-2.93188100	5.63064600	-0.00434500
H	-3.90369400	0.48809700	1.28247600	C	-3.51684000	2.98203400	-0.20704800
C	-4.28538800	2.43526900	-0.59020400	H	-3.52818900	1.94569100	0.13371000
H	-4.03349200	3.18856500	-1.34134500	H	-3.76050900	2.98704300	-1.26871700
Cl	-4.07215700	0.01501800	4.52363400	H	-4.28522400	3.54275700	0.33391100
H	-2.84392200	0.00072600	3.97195700	C	-1.84933200	3.59248500	1.54862900
H	-5.33083500	2.14797300	-0.73346000	H	-0.84474600	3.95278700	1.77844900
H	-4.18124900	2.87473800	0.40182000	H	-1.97520400	2.59545900	1.97293300
C	-3.47420900	0.63845800	-2.13932500	H	-2.56325900	4.25198900	2.04839900
C	-3.04840100	1.32203900	-2.87707800	C	0.30440400	-0.25004100	-0.90066600
H	-2.98503200	-0.33298200	-2.21763100	H	0.68318800	0.64970100	-1.37653200
H	-4.52921900	0.49580800	-2.38765900	H	-0.78109800	-0.22105900	-0.95145700
C	1.32029700	3.11284200	2.18214000	C	0.82782000	-1.50821300	-1.54586400
H	1.48290900	4.18528400	2.32615700	C	-0.06264300	-2.26626700	-2.31332500
H	0.43515700	2.97012100	1.56056500	H	-1.05243400	-1.86287400	-2.49661600
Cl	-1.05296000	-0.00521500	3.10024200	C	0.31377800	-3.49956700	-2.83032200
H	1.12989500	2.65562400	3.15233400	H	-0.39336700	-4.07341900	-3.41827700
C	2.83951700	3.25862700	0.21599100	C	1.58311500	-4.00532200	-2.55602400
H	3.62831900	2.78893100	-0.37541500	H	1.87218700	-4.98641400	-2.91726200
H	1.94164800	3.36535100	-0.39315800	C	2.48867200	-3.24706900	-1.82497300
H	3.17683200	4.26388800	0.48215500	H	3.47124500	-3.62920600	-1.59002900
C	3.77150300	2.57436500	2.43938400	C	2.13738400	-1.97797500	-1.35571700
H	3.93826200	3.61378000	2.73607600	C	4.03147100	-0.36105400	-1.49926900
H	3.60048100	1.98072500	3.33746300	C	3.21933300	0.62506000	-2.34499100
H	4.67603600	2.21335800	1.94306000	H	2.69059100	1.34229200	-1.71817400
C	-0.14730500	-4.98075700	0.98329800	H	2.50330400	0.11413800	-2.99110800
H	-0.47798700	-5.38729300	0.02400200	H	3.90261100	1.18841800	-2.98508600
H	0.49161600	-5.72565700	1.46622600	C	4.87611700	-1.26456500	-2.41098800
H	-1.01965600	-4.81011700	1.61404800	H	4.26798300	-1.74978100	-3.17672000
C	1.19147800	-3.18204600	2.13951000	H	5.38033500	-2.02942100	-1.81845400
H	1.93205700	-3.89604400	2.51257800	H	5.63697800	-0.66173500	-2.91425500
H	1.66850100	-2.20820700	2.01941500	C	4.95437100	0.41196700	-0.55080700
H	0.39875400	-3.08145300	2.87972000	H	5.62153900	-0.26603300	-0.02052000
C	1.80580400	-3.90637200	-0.16146000	H	4.37554400	0.95686700	0.19213000

H	1.47032800	-4.13413600	-1.17543700	H	5.55438900	1.12248300	-1.12616600
H	2.48079700	-3.05042600	-0.18473700	Br	-2.86623100	0.11859500	-2.89980300
H	2.37730200	-4.76504800	0.20090900	Br	3.22643900	-0.35716400	2.90013800
<b>[L(HBr<sub>2</sub>)]<sup>-</sup>, 2Br, E<sub>0</sub>=-6879.908721 au</b>				<b>[L(HBr<sub>2</sub>)]<sup>-</sup>, 3Br, E<sub>0</sub>=-6879.902183 au</b>			
N	-1.10928800	-0.00060800	-0.00087900	N	1.30538800	0.09098300	-0.67307400
C	-1.59162800	-0.87299600	-1.14675700	C	0.94317100	-0.62911800	-1.95676400
H	-1.09728400	-0.48748500	-2.02510200	H	0.87713100	-1.67749600	-1.69705700
H	-2.66538200	-0.68872700	-1.21023100	H	1.78743300	-0.46758100	-2.63069200
C	-1.59253900	1.42761600	-0.18378100	C	2.51415300	-0.53839900	-0.01697200
H	-1.09886100	1.99597900	0.58937300	H	2.71723500	0.06246900	0.85773600
H	-2.66629500	1.38962100	0.00716800	H	3.32962800	-0.42040800	-0.73530800
C	-1.59372700	-0.55642900	1.32696900	C	1.54710500	1.56656200	-0.94461100
H	-1.09953200	-1.50977600	1.43350400	H	0.65412200	1.91858500	-1.44426700
H	-2.66728100	-0.70354200	1.19745200	H	2.40331300	1.59804900	-1.62295100
C	-1.32327700	-2.33078700	-0.91745600	C	-0.34760300	-0.10394600	-2.50959100
C	-2.37792300	-3.13376900	-0.46805900	C	-0.32293700	0.72917700	-3.63218500
C	-0.04389700	-2.88624100	-1.07349400	C	-1.56849000	-0.37790200	-1.87346200
C	-2.16302800	-4.46356300	-0.12722300	C	-1.49334800	1.31219200	-4.10438900
H	-3.35838200	-2.68141500	-0.35398600	H	0.62921500	0.93015200	-4.11110300
C	0.17125900	-4.21568300	-0.69326600	C	-2.73454800	0.24549100	-2.32585100
C	-0.87807600	-4.99513900	-0.22111500	C	-2.69376000	1.08258200	-3.43559200
H	-2.98563000	-5.07008900	0.23345500	H	-1.46409400	1.95906100	-4.97381800
H	1.17394700	-4.61254300	-0.75020900	H	-3.66556500	0.10071200	-1.78903500
H	-0.69025600	-6.02260800	0.07180800	H	-3.60701500	1.56147300	-3.77010400
C	-1.32721500	0.37127100	2.47499700	C	1.80301700	2.31337600	0.33001900
C	-2.38234900	1.16251600	2.94364100	C	3.11673200	2.62115200	0.69887900
C	-0.04875200	0.51345900	3.03619200	C	0.74424200	2.64213700	1.18893800
C	-2.16872100	2.12257500	3.92515200	C	3.38548500	3.20232400	1.93288400
H	-3.36205200	1.03563900	2.49300500	H	3.92073300	2.37021200	0.01488300
C	0.16520200	1.50748800	3.99766900	C	1.02650500	3.17944000	2.44805700
C	-0.88459700	2.30650600	4.43478200	C	2.33803200	3.45583300	2.81750700
H	-2.99163300	2.73865800	4.26850900	H	4.40719300	3.42994300	2.21374800
H	1.16734200	1.65628500	4.37141400	H	0.21362600	3.35803900	3.13667500
H	-0.69776200	3.07391600	5.17838800	H	2.54238900	3.87120600	3.79811200
C	-1.32420500	1.95800400	-1.56084400	C	2.28639300	-1.98044000	0.32709000
C	-2.37814100	1.96801700	-2.48178900	C	2.93727400	-2.95216300	-0.44125100
C	-0.04521000	2.37286300	-1.96296400	C	1.41454800	-2.37850100	1.35326400
C	-2.16281200	2.33766300	-3.80378000	C	2.71252800	-4.30553200	-0.22093800
H	-3.35826500	1.64134800	-2.14771200	H	3.59963000	-2.62149400	-1.23443400
C	0.17044900	2.70829400	-3.30435700	C	1.17350300	-3.74174700	1.54975300
C	-0.87815700	2.68701200	-4.21624900	C	1.81554800	-4.69651100	0.77098400
H	-2.98479900	2.32680300	-4.51007900	H	3.21394600	-5.04592500	-0.83310900
H	1.17299000	2.95741900	-3.61892700	H	0.45536300	-4.03747900	2.29997900
H	-0.69000200	2.94706700	-5.25246600	H	1.60935000	-5.74815200	0.93682700
N	1.02341400	-2.05946400	-1.56545300	N	-1.54881900	-1.29482800	-0.75876300
N	1.02122700	2.38714900	-1.00003500	N	0.73536700	-1.36751700	2.13172500
N	1.01885400	-0.32658400	2.56801700	N	-0.59263100	2.37968000	0.73048900
O	2.21976800	-2.50581300	-0.90846400	O	-2.12236500	-0.67268100	0.40554600
H	2.67266500	-1.68072400	-0.61688800	H	-3.13224400	-0.57390700	0.34347500
O	2.21549200	0.46501500	2.62748900	O	-1.29511500	1.69908300	1.78401400
H	2.66898000	0.30520400	1.76742000	H	-1.62285400	0.90106400	1.32940300
O	2.21886100	2.04249200	-1.71344600	O	-0.59105400	-1.85011000	2.40697000
H	2.67114500	1.37727000	-1.14437900	H	-1.15956200	-1.37618400	1.76638300
C	1.28379900	-2.14882400	-3.05952300	C	-2.12956500	-2.66772000	-1.04696300
C	1.27730300	-1.57589800	3.39297200	C	-1.39388100	3.59164000	0.32906000
C	1.27927700	3.72602600	-0.33016000	C	1.34269400	-1.06304500	3.48272500
H	-0.08146600	-0.00061100	-0.00020700	C	-2.72412600	3.07922200	-0.22770900
Br	-4.93365200	-0.00103100	-0.00381600	H	-3.32117700	3.92079700	-0.58965300
C	1.71109800	-3.56776100	-3.46831500	H	-2.54545200	2.40145600	-1.05939800
H	0.89332600	-4.28245400	-3.34874000	H	-3.30611100	2.54528000	0.52255400
H	2.01164800	-3.57011500	-4.51949000	C	-1.65885500	4.54480100	1.50621400
H	2.55787200	-3.89282400	-2.86425500	H	-0.74870600	5.04802800	1.83872300
C	2.39962100	-1.14567600	-3.37023000	H	-2.37128000	5.31346300	1.19584900
H	2.57031300	-1.11289400	-4.45036700	H	-2.09371800	3.99437300	2.34149700
H	2.12252100	-0.14762800	-3.02815500	C	-0.62848500	4.32580100	-0.77842400
H	3.33122400	-1.42335600	-2.87918900	H	0.35394800	4.66579600	-0.44450000



C	0.03285300	-1.74768200	-3.85025900	H	-0.50310200	3.69106500	-1.65765900
H	-0.84043000	-2.34474300	-3.58125600	H	-1.20329000	5.20391500	-1.08223900
H	-0.19855600	-0.68860500	-3.72735600	C	0.43971800	-0.02209000	4.15417500
H	0.23188300	-1.91235000	-4.91205100	H	0.93930000	0.37201000	5.04396500
C	2.39390500	3.49446100	0.69550700	H	0.22749700	0.79658700	3.46963200
H	2.56287100	4.41353900	1.26441300	H	-0.50936300	-0.46575000	4.45104600
H	2.11661200	2.69869900	1.38818500	C	2.74006000	-0.46722500	3.29121000
H	3.32649400	3.20905700	0.21077000	H	3.39614500	-1.13109800	2.72441300
C	1.70696300	4.78988800	-1.35404000	H	2.69205100	0.50519600	2.80118700
H	0.88987000	5.04277200	-2.03392600	H	3.19279600	-0.31675700	4.27426400
H	2.00577800	5.70174200	-0.83007700	C	1.43401800	-2.31682200	4.36887700
H	2.55492000	4.43017200	-1.93639200	H	1.75268100	-2.02582400	5.37339100
C	0.02683900	4.20914500	0.41085600	H	0.45864200	-2.79838300	4.44645800
H	-0.84573400	4.27350200	-0.24179400	H	2.15718900	-3.03701800	3.98050600
H	-0.20492800	3.57324500	1.26653900	C	-3.44814500	-2.65538400	-1.84008200
H	0.22432200	5.21137200	0.79901700	H	-3.31688100	-2.24609900	-2.84318800
C	2.39312300	-2.34763600	2.68073900	H	-3.79676700	-3.68695200	-1.94449500
H	2.56206000	-3.29981700	3.19232100	H	-4.22320400	-2.08955900	-1.31991600
H	2.11699600	-2.54967800	1.64494500	C	-2.36540800	-3.39882200	0.27758700
H	3.32538800	-1.78463600	2.67702700	H	-2.64544100	-4.43144600	0.05352300
C	0.02564200	-2.46026500	3.43987700	H	-1.46952800	-3.40538400	0.89238200
H	-0.84775700	-1.92803800	3.82116300	H	-3.17867700	-2.94054900	0.84084300
H	-0.20481800	-2.88376300	2.46119900	C	-1.05536400	-3.41486400	-1.85081900
H	0.22334400	-3.29723900	4.11405600	H	-0.82063900	-2.89749000	-2.78406300
C	1.70334500	-1.22055800	4.82662400	H	-0.14214200	-3.53316100	-1.26543500
H	0.88536400	-0.75875700	5.38472600	H	-1.42601700	-4.40964100	-2.11066600
H	2.00239400	-2.12991600	5.35477300	H	0.51498900	-0.00282100	-0.02330100
H	2.55076500	-0.53567800	4.80699700	Br	-5.17060700	-0.16703500	0.45690900
Br	3.98145500	0.00161200	0.00311700	Br	4.31629800	0.38732400	-2.95678500
<b>[L(HBr<sub>2</sub>)]<sup>-</sup>, 4Br, E<sub>0</sub>=-6879.900396 au</b>				<b>[L(HBr<sub>2</sub>)]<sup>-</sup>, 5Br, E<sub>0</sub>=-6879.903731 au</b>			
O	-1.37057900	1.11476600	0.80465000	N	1.07571600	-0.39189000	0.62234500
O	2.41666700	2.71160200	-1.44778200	C	0.52739000	-1.80606100	0.77678100
O	-3.40001100	0.46386700	-0.90316000	H	-0.46887900	-1.66950000	1.16939300
N	-1.40554100	1.23359100	2.22782200	H	1.17578500	-2.28358300	1.51554600
N	2.54244300	1.71828100	-0.42539000	C	1.08960900	0.29552700	1.98299800
N	-2.70710000	-0.66481200	-1.48534900	H	1.44035800	1.30555700	1.79749300
N	0.31879800	-1.77270100	0.08567500	H	1.80635500	-0.26908900	2.58316600
C	-0.87720000	-1.64207400	1.03238800	C	2.46151700	-0.39832400	0.02139200
C	-0.45428500	-1.12853800	2.38705900	H	2.37966200	-0.96222400	-0.89585200
C	0.26719100	-2.02684200	3.18742800	H	3.08490500	-0.94943800	0.72978100
C	0.83284600	-1.64553400	4.39596900	C	0.49366400	-2.57174100	-0.51212900
C	0.70855100	-0.32415100	4.81541300	C	1.62369900	-3.29818700	-0.90914900
C	-0.00647200	0.57778000	4.04073700	C	-0.64693000	-2.56894900	-1.33208100
C	-0.63721800	0.19642000	2.84690900	C	1.66577000	-3.93012000	-2.14573800
C	-2.83302300	1.37451800	2.68838700	H	2.47141700	-3.34608100	-0.23349300
C	-3.65292100	0.09527300	2.44806900	C	-0.57812500	-3.16389400	-2.59752800
C	-2.84144500	1.70358900	4.18803400	C	0.57154100	-3.82866900	-3.00449900
C	-3.43703000	2.56760800	1.93473200	H	2.55117400	-4.47921000	-2.44437000
C	1.30308200	-0.65677600	0.27616300	H	-1.43511100	-3.08467400	-3.25044900
C	2.52499300	-0.70471300	-0.59434000	H	0.60637300	-4.28551200	-3.98764000
C	3.10376400	-1.89788900	-1.03503500	C	2.99881100	0.97925700	-0.23177300
C	4.13692300	-1.87400400	-1.96639100	C	4.02467900	1.46221100	0.58658200
C	4.59576300	-0.65531500	-2.46603500	C	2.48652000	1.79387400	-1.25420200
C	4.07400700	0.53725600	-1.97796100	C	4.52568800	2.74769500	0.41625600
C	3.07140500	0.52384500	-1.00502800	H	4.40442300	0.81833900	1.37282200
C	3.32915100	2.30023300	0.71825900	C	2.97385500	3.09601300	-1.39957700
C	4.71229900	2.79460800	0.26188100	C	3.98676500	3.56811500	-0.57331000
C	2.51053800	3.46874200	1.27713300	H	5.31402600	3.11314200	1.06411200
C	3.49001400	1.24247200	1.81674500	H	2.51883100	3.73835700	-2.13929700
C	-0.13343800	-2.05503800	-1.34102400	H	4.35153900	4.58183300	-0.69893400
C	-0.37459200	-0.85138700	-2.21617100	C	-0.28042400	0.30387500	2.59038700
C	0.67227500	-0.39573400	-3.02565900	C	-0.61862800	-0.62113900	3.58077300
C	0.55535800	0.76807700	-3.77374000	C	-1.25109800	1.19347900	2.10363000
C	-0.62830300	1.49474000	-3.72893700	C	-1.92292600	-0.68714700	4.06016600
C	-1.70418400	1.01996500	-2.99221600	H	0.14547700	-1.29788100	3.94827600
C	-1.60113300	-0.16527500	-2.26252200	C	-2.57114400	1.08328300	2.54776900

C	-3.75349900	-1.44140100	-2.22203900	C	-2.90093400	0.14952500	3.52585900
C	-3.09312200	-2.62201200	-2.94277600	H	-2.18120500	-1.40939500	4.82615300
C	-4.51105200	-0.57961200	-3.24847400	H	-3.34242400	1.68774600	2.09410500
C	-4.72737700	-1.97586600	-1.16318400	H	-3.92974600	0.06570600	3.85709300
H	0.76635500	-2.69539300	0.36846200	N	-1.85147400	-1.96832400	-0.84213500
H	-1.61235400	-1.03214600	0.53426000	N	-0.79741000	2.14721600	1.13379400
H	-1.24965300	-2.66360900	1.12102900	N	1.39717500	1.29286200	-2.05256200
H	0.41558400	-3.03714000	2.81718000	O	-2.50606000	-1.35876500	-1.96459100
H	1.39099600	-2.36585500	4.98220500	H	-2.85257300	-0.50477600	-1.62308300
H	1.18390200	0.01246700	5.73012800	O	0.46854900	2.37230400	-2.24536700
H	-0.07786800	1.61595800	4.33337800	H	-0.20378100	2.17975600	-1.55785600
H	-3.22463100	-0.74974800	2.99302500	O	-1.09284700	1.67139200	-0.18366800
H	-3.70480400	-0.15348700	1.38933500	H	-2.08446500	1.59775200	-0.32813900
H	-4.67716600	0.24042200	2.80345500	C	-2.82683100	-2.94191800	-0.20463600
H	-2.45599200	0.88246900	4.79306100	C	1.72027400	0.76990700	-3.42468900
H	-3.87227900	1.89444000	4.49623600	C	-1.04503100	3.60047000	1.32864000
H	-2.25090200	2.59917400	4.39114200	H	0.44909300	0.13563600	-0.00554400
H	-2.78467100	3.43813500	2.02150000	C	-2.13678000	-3.72190000	0.92190000
H	-4.41447800	2.80700100	2.36221700	H	-1.81913700	-3.06553300	1.73302300
H	-3.57461000	2.36735500	0.87412000	H	-2.85726800	-4.42961400	1.33924900
H	1.58262000	-0.70462300	1.32403600	H	-1.27622000	-4.29223200	0.56907500
H	0.78470400	0.28470300	0.11743700	C	-3.95388100	-2.09834800	0.39810800
H	2.72950700	-2.85070500	-0.67257300	H	-3.54611100	-1.36629900	1.09644100
H	4.56451400	-2.80702500	-2.31517400	H	-4.50085300	-1.55061500	-0.36742800
H	5.37481500	-0.63393300	-3.22068200	H	-4.65287800	-2.74756200	0.93405900
H	4.41811800	1.49154000	-2.35138700	C	-3.39612600	-3.93144900	-1.23424000
H	4.60068900	3.47693500	-0.58169500	H	-4.18695900	-4.52675400	-0.76990700
H	5.35577700	1.96327200	-0.03558800	H	-3.81876800	-3.38911500	-2.07965500
H	5.20499300	3.32872700	1.07925500	H	-2.62775700	-4.61735500	-1.59845600
H	3.00930800	3.87537800	2.16241600	C	-2.50592100	4.05604600	1.16376200
H	1.50758900	3.13759900	1.54854800	H	-3.12680200	3.74314000	2.00435900
H	2.40037800	4.26104800	0.53861300	H	-2.54134000	5.14869400	1.11883600
H	2.52274500	0.95805900	2.23284000	H	-2.94792800	3.65996500	0.24835600
H	4.08551100	1.66833500	2.62830000	C	-0.54194200	3.92737200	2.74305400
H	4.00383300	0.34828100	1.45892100	H	-1.12909700	3.41734500	3.50850000
H	-1.01397400	-2.67546000	-1.22578700	H	0.50453000	3.63518700	2.85783400
H	0.64812200	-2.67790100	-1.76892700	H	-0.62206000	5.00368400	2.91334500
H	1.60486900	-0.94239500	-3.03750600	C	-0.16730600	4.34268500	0.31054200
H	1.40328900	1.12663800	-4.34349700	H	-0.18608300	5.41411500	0.52815400
H	-0.71192900	2.44321400	-4.24448700	H	0.86301400	3.98821500	0.36134000
H	-2.61397500	1.59576500	-2.91951300	H	-0.52554000	4.19845300	-0.70738800
H	-2.65063800	-3.32837900	-2.23875700	C	0.40402800	0.24249700	-4.00952800
H	-2.32269600	-2.29007600	-3.64037600	H	0.60143600	-0.28000100	-4.95001900
H	-3.85696800	-3.15734300	-3.51177800	H	-0.07269900	-0.45285900	-3.31815200
H	-3.85248700	-0.26364400	-4.05964700	H	-0.29083800	1.05909900	-4.19884600
H	-4.92528800	0.30730800	-2.76976900	C	2.29985500	1.86982600	-4.33097700
H	-5.33049200	-1.15985700	-3.68191100	H	3.28739100	2.18983500	-3.99013200
H	-5.47018700	-2.62801600	-1.63089100	H	2.40198400	1.48773600	-5.35029400
H	-5.24207900	-1.15523100	-0.66509300	H	1.63383500	2.73272900	-4.35118500
H	-4.18267200	-2.54988800	-0.41004000	C	2.72274000	-0.38298900	-3.31671800
H	-1.04193600	1.99547400	0.45506600	H	3.62658500	-0.09203200	-2.77664800
H	1.47492000	2.98906200	-1.35880500	H	2.27746500	-1.25493600	-2.83865200
H	-2.75239800	0.77362500	-0.23523800	H	3.02034500	-0.68188800	-4.32475600
Br	-0.62538700	3.72948200	-0.73488600	Br	-4.08399700	1.37219500	-0.99829600
Br	1.15950200	-4.74150200	0.70035200	Br	3.43231300	-2.33897500	2.89165700
<b>[L(HBr<sub>2</sub>)], 6Br, E<sub>0</sub>=-6879.898174 au</b>				<b>[L(HBr<sub>2</sub>)], 7Br, E<sub>0</sub>=-6879.897767 au</b>			
N	-0.43765600	-0.12343500	0.04159600	N	1.09803400	-0.25589000	0.90054700
C	-0.79203600	0.43928400	-1.31127200	C	1.18222200	-1.77038400	0.95566600
H	-0.01542100	0.10853400	-1.99381800	H	0.18543300	-2.10729200	1.21494800
H	-0.70969700	1.51770800	-1.27107100	H	1.88526600	-1.99267300	1.76205100
C	-1.15774000	0.51711800	1.23990200	C	0.57071500	0.29500800	2.20808000
H	-0.37045300	0.78369400	1.93330300	H	0.61628800	1.37149200	2.11190000
H	-1.76307000	-0.26882600	1.69365800	H	1.28331800	-0.03146000	2.96885500
C	1.04993500	-0.11662900	0.22454800	C	2.45314500	0.34368000	0.56044500
H	1.31010700	0.89916900	0.50945800	H	2.77883400	-0.16909600	-0.33398900
H	1.51246100	-0.27392900	-0.74878700	H	3.10291300	0.08561900	1.40098600

C	-2.15962200	0.01425700	-1.76904000	C	1.63642700	-2.32679000	-0.36108800
C	-2.97365400	0.98661800	-2.35669400	C	2.95314600	-2.77233700	-0.50670000
C	-2.65036000	-1.29585700	-1.63366800	C	0.76691000	-2.34947400	-1.46123600
C	-4.25552200	0.68521000	-2.79248300	C	3.41531000	-3.21053800	-1.74329600
H	-2.59818700	2.00058200	-2.42825900	H	3.60961800	-2.74752700	0.35685300
C	-3.95881000	-1.58319200	-2.03302800	C	1.25156400	-2.74533500	-2.70947700
C	-4.75249600	-0.60452700	-2.61532900	C	2.56674700	-3.17803200	-2.84804700
H	-4.87481900	1.45935900	-3.23013200	H	4.43755800	-3.55502500	-1.84835700
H	-4.34438500	-2.57249900	-1.83784500	H	0.60020600	-2.69329500	-3.56936900
H	-5.76508600	-0.84676400	-2.91848400	H	2.93073100	-3.48332200	-3.82286800
C	1.57553800	-1.14783400	1.18051000	C	2.35624300	1.82191300	0.33304500
C	0.76995400	-1.85937800	2.06518800	C	2.68441800	2.70682500	1.36560200
C	2.96533800	-1.42812700	1.11510500	C	1.89607700	2.32889600	-0.89146800
C	1.30297100	-2.84487000	2.89437600	C	2.49677000	4.07536100	1.21139200
H	-0.30030600	-1.70178500	2.12097200	H	3.06839700	2.30067600	2.29510700
C	3.48664100	-2.39648000	1.97926800	C	1.64861400	3.69847200	-1.01662800
C	2.66373800	-3.10645000	2.85158200	C	1.94565500	4.56545500	0.02851800
H	0.63962800	-3.38908500	3.55519700	H	2.74704900	4.75147800	2.02040600
H	4.54355300	-2.60543600	1.97911800	H	1.20929300	4.07183800	-1.93014900
H	3.10062000	-3.85795800	3.50051000	H	1.74833700	5.62574800	-0.08193900
C	-2.03421400	1.68857900	0.91214100	C	-0.82183700	-0.18276400	2.50191000
C	-3.41939200	1.50672500	0.96630100	C	-1.00251500	-1.08164400	3.55817900
C	-1.51097400	2.93410200	0.53173900	C	-1.92958900	0.21683300	1.73439100
C	-4.28332100	2.53189100	0.60272000	C	-2.26054300	-1.59870700	3.84447900
H	-3.80185500	0.53954600	1.27439600	H	-0.13507400	-1.38599500	4.13390600
C	-2.38531300	3.94545100	0.12421300	C	-3.18787100	-0.32484200	2.01274900
C	-3.76140800	3.74515700	0.15983000	C	-3.34898500	-1.22542900	3.05977700
H	-5.35469200	2.37224800	0.63319000	H	-2.38499600	-2.30083500	4.66099100
H	-1.97149500	4.87098000	-0.24904900	H	-4.03857200	-0.07146000	1.38859400
H	-4.42626900	4.54013000	-0.16102400	H	-4.33259000	-1.63848500	3.25272800
N	-1.83568400	-2.30559900	-0.98494400	N	-0.59684700	-1.97130800	-1.21928700
N	-0.08023900	3.09475400	0.48136900	N	-1.71008000	1.13146800	0.63617300
N	3.71769300	-0.74812200	0.12389000	N	1.70322200	1.39775600	-1.97143400
O	-2.70056900	-3.18646100	-0.26638400	O	-0.95210500	-0.91506100	-2.14413000
H	-2.72156900	-2.84527600	0.66927000	H	-1.53787300	-0.34806300	-1.57777000
O	3.75136700	0.65458300	0.42130100	O	0.42123600	1.65249900	-2.57103100
H	3.41637100	1.09161000	-0.40027900	H	-0.02474300	0.79193000	-2.47194400
O	0.21651600	3.79012300	-0.74244700	O	-2.34340700	0.63296800	-0.54402300
H	0.90999900	3.23648600	-1.17861400	H	-3.35072000	0.63656500	-0.50574300
C	-1.01152700	-3.20198100	-1.88483500	C	-1.60108000	-3.09380000	-1.31852100
C	5.04697800	-1.19911500	-0.36315300	C	2.74990200	1.44607800	-3.05145600
C	0.54922600	3.85655500	1.61827300	C	-2.11002900	2.57215900	0.86775000
H	-0.77922300	-1.11207700	-0.02192200	C	2.40139300	0.34370700	-4.05551200
C	-0.09399300	-2.36782600	-2.78207300	H	3.18682600	0.27107100	-4.81275900
H	-0.65021800	-1.65610200	-3.39432500	H	2.31686700	-0.61326600	-3.54534700
H	0.66432100	-1.83511400	-2.20783600	H	1.45597700	0.55724700	-4.55382200
H	0.43453200	-3.04344500	-3.45811900	C	2.80362700	2.79989500	-3.77972300
C	-1.91793700	-4.07934600	-2.76270900	H	3.19318100	3.59225000	-3.13868000
H	-2.48871200	-3.47290600	-3.46980600	H	3.46174900	2.71923300	-4.64906700
H	-1.30322200	-4.77863200	-3.33546500	H	1.80799500	3.07827100	-4.12873000
H	-2.61155300	-4.64724300	-2.14407900	C	4.11049400	1.13745400	-2.41525400
C	-0.15405400	-4.07244800	-0.95843800	H	4.37744400	1.86683000	-1.64862000
H	0.48271500	-4.73041400	-1.55603600	H	4.12068000	0.14037100	-1.97134600
H	0.48688500	-3.45192600	-0.32860200	H	4.88043100	1.16727900	-3.19013200
H	-0.78516300	-4.67750500	-0.31019300	C	-1.97931100	3.29484800	-0.47872600
C	2.06787600	3.76428600	1.42419900	H	-2.01438500	4.37471600	-0.30816900
H	2.40257100	2.72533500	1.42890500	H	-1.03813400	3.03917900	-0.96318700
H	2.36876900	4.20977600	0.47661000	H	-2.79373600	3.02230300	-1.14866200
H	2.57516300	4.29281200	2.23641800	C	-1.11701300	3.17314300	1.86762800
C	0.11062500	5.33042500	1.63860700	H	-1.12558100	2.63411800	2.81799500
H	-0.94834800	5.42886900	1.88700900	H	-0.10639000	3.18310300	1.46277500
H	0.68519700	5.87466500	2.39298000	H	-1.40457000	4.20670200	2.07467700
H	0.29250900	5.78761900	0.66573800	C	-3.53762000	2.73957300	1.41207900
C	0.16980100	3.19012500	2.94562800	H	-3.76700500	3.80792500	1.46679800
H	-0.91144800	3.14098400	3.08715500	H	-4.28174300	2.27002800	0.76577500
H	0.58337800	2.18341800	3.01975900	H	-3.63410100	2.32509500	2.41809700

H	0.59010400	3.77673100	3.76609800	C	-1.77857100	-3.62556700	-2.75045700
C	5.35027000	-0.36934600	-1.62465200	H	-0.91894200	-4.21046300	-3.08253900
H	5.49401900	0.68277500	-1.38328800	H	-2.65646400	-4.27523500	-2.78700900
H	6.26276900	-0.74547400	-2.09556100	H	-1.94109900	-2.79499100	-3.43852400
H	4.52474500	-0.43179300	-2.33449300	C	-2.94035200	-2.56009500	-0.80395600
C	4.94445700	-2.66957900	-0.79655300	H	-3.66724100	-3.37541700	-0.76475700
H	5.86670500	-2.95360100	-1.30955400	H	-2.82849700	-2.14996900	0.19807300
H	4.79317800	-3.35805000	0.03267100	H	-3.35963500	-1.78201500	-1.43997400
H	4.11228000	-2.79108000	-1.49369400	C	-1.12637000	-4.22113800	-0.39149500
C	6.17982100	-0.95970900	0.65419000	H	-0.16802200	-4.63938600	-0.70477300
H	7.15132200	-1.09030500	0.16904300	H	-1.03726700	-3.87077900	0.63884400
H	6.11177800	0.06436700	1.02376400	H	-1.86785600	-5.02312300	-0.40735200
H	6.14169600	-1.63654900	1.50818200	H	0.42037200	0.00787300	0.17411800
Br	-2.96246800	-2.17940200	2.70833500	Br	3.60937900	-1.19179100	3.57493300
Br	2.46491800	2.02793700	-2.24840800	Br	-5.44828800	0.40688400	-0.85320000
<b>[L(HBr<sub>2</sub>)], 8Br, E<sub>0</sub>=-6879.876299 au</b>				<b>[L(HBr<sub>2</sub>)], 9Br, E<sub>0</sub>=-6879.870047 au</b>			
N	2.18211700	0.24406500	1.53603900	N	-1.68190900	-0.01275700	1.62290500
C	1.32325600	0.40008300	2.70874400	C	-3.05797800	-0.05053600	1.13051200
H	0.82648800	1.35985500	2.61700500	H	-3.20596600	0.84277900	0.53990600
H	1.92462400	0.42424900	3.64066200	H	-3.77343800	0.00145900	1.97837200
C	3.00725300	1.42733900	1.30468500	C	-1.42898600	1.21529600	2.37772300
H	3.62096100	1.22436400	0.43491000	H	-0.39568800	1.18196600	2.69208300
H	3.70250900	1.58980600	2.15457100	H	-2.04590400	1.23117400	3.30090600
C	3.00496200	-0.96380000	1.62556900	C	-1.39095600	-1.19022300	2.44210200
H	2.33975500	-1.78839600	1.86243800	H	-1.58735400	-2.05851000	1.82813000
H	3.74639500	-0.87757100	2.44646700	H	-2.08870600	-1.23955400	3.30464300
C	0.29234000	-0.69484000	2.82191500	C	-3.39108900	-1.28398900	0.32460800
C	0.48607000	-1.73340300	3.73746600	C	-4.09759900	-2.31515300	0.95500300
C	-0.84317200	-0.72301100	1.99600600	C	-2.97528100	-1.47275100	-1.00577000
C	-0.39902000	-2.80280800	3.82127800	C	-4.35352300	-3.52829700	0.32857800
H	1.36003400	-1.70230900	4.38036300	H	-4.41884000	-2.16163300	1.98000500
C	-1.71101000	-1.81820400	2.05699600	C	-3.21250500	-2.70869000	-1.62473000
C	-1.49360900	-2.84963100	2.96346700	C	-3.88820500	-3.72810600	-0.96829100
H	-0.22457000	-3.60016900	4.53548900	H	-4.88642800	-4.31331800	0.85345300
H	-2.54700900	-1.87959300	1.37236400	H	-2.82763800	-2.86107300	-2.62199000
H	-2.17822600	-3.68982200	2.98852600	H	-4.05172000	-4.67527800	-1.47107600
C	3.72928900	-1.24853300	0.33280100	C	0.01715900	-1.22687600	2.98673600
C	5.07327900	-0.89392400	0.18401100	C	0.22450000	-0.85008700	4.31898300
C	3.04600100	-1.78832000	-0.76693200	C	1.13620900	-1.55222100	2.20010900
C	5.72362600	-1.01218700	-1.03979300	C	1.49675200	-0.73723300	4.86519000
H	5.60241400	-0.48856100	1.04046100	H	-0.64332700	-0.60422300	4.92228200
C	3.68641600	-1.85515900	-2.00849900	C	2.42013500	-1.40479700	2.74490400
C	5.01497100	-1.47059400	-2.14770000	C	2.60222200	-0.99883500	4.05977600
H	6.76336900	-0.71947100	-1.13519100	H	1.62372200	-0.42361700	5.89541500
H	3.12373500	-2.19112900	-2.86721500	H	3.27027800	-1.58421200	2.10360300
H	5.49432900	-1.52774000	-3.11880300	H	3.60707600	-0.88806500	4.45280700
C	2.22117100	2.70120800	1.09956900	C	-1.71495600	2.48907200	1.61747500
C	2.19221900	3.63871700	2.13846500	C	-2.93221600	3.13774400	1.85963700
C	1.48438000	2.97006000	-0.06746700	C	-0.85105400	3.02703500	0.64535600
C	1.43353600	4.80024900	2.06357700	C	-3.33384100	4.25585200	1.14030900
H	2.76025200	3.42484800	3.03806100	H	-3.59033900	2.72105000	2.61506400
C	0.70269600	4.13106100	-0.12788300	C	-1.27258500	4.14194700	-0.09523700
C	0.67237200	5.03812200	0.92236100	C	-2.49821800	4.74829200	0.14154900
H	1.41788800	5.49728900	2.89391500	H	-4.29248800	4.72094400	1.34147000
H	0.09178300	4.29043900	-1.00409800	H	-0.62652800	4.50308000	-0.88116400
H	0.05173700	5.92453200	0.85033400	H	-2.79668600	5.60608300	-0.45170300
N	-1.07064700	0.38538400	1.10517900	N	-2.26527900	-0.43818700	-1.70082900
N	1.48167600	2.02470400	-1.15229700	N	0.41536100	2.41421600	0.36796700
N	1.69532900	-2.23210400	-0.57276500	N	0.96891800	-1.96886500	0.83815100
O	-1.12624200	-0.08919200	-0.24974600	O	-1.33525100	-1.09906400	-2.57471500
H	-1.97067800	-0.57792900	-0.44104100	H	-0.46717600	-0.70679900	-2.36383000
O	0.88098000	-1.62470300	-1.58588000	O	2.10244400	-1.46164500	0.11814900
O	0.27387800	-1.06982200	-1.06151400	H	1.72492700	-0.95696500	-0.62686100
H	0.14153700	1.96861700	-1.67174800	O	0.66573000	2.62229100	-1.03189100
H	-0.25089800	1.19267000	-1.22736600	H	0.89482100	1.73966900	-1.38515000
C	-2.21257300	1.30524400	1.45673700	C	-3.08186200	0.48838300	-2.56840700

C	1.46963800	-3.71168100	-0.60087300	C	0.93123300	-3.45522900	0.57998200
C	2.36740100	2.33227000	-2.32237900	C	1.61894800	2.96076500	1.10183700
C	0.00182200	-3.93660600	-0.22603900	C	0.70753000	-3.62471500	-0.92816600
H	-0.21010300	-5.00827500	-0.16858800	H	0.55864700	-4.68306100	-1.16272000
H	-0.20791000	-3.48641200	0.74199400	H	-0.17401900	-3.06543900	-1.24475900
H	-0.66819900	-3.49105100	-0.96078700	H	1.56320900	-3.25875200	-1.49426200
C	1.75201000	-4.35025400	-1.97305800	C	2.24173900	-4.14000900	1.00394600
H	2.81800000	-4.35613500	-2.20928800	H	2.37465600	-4.10977900	2.08838400
H	1.40371000	-5.38681600	-1.97336000	H	3.75596900	-0.02589500	-2.10155600
H	1.21294100	-3.80830400	-2.75144700	H	2.22812500	-5.18836700	0.69235600
C	2.36890200	-4.34509900	0.46802100	H	3.09133900	-3.64853200	0.52973900
H	3.42787300	-4.17546300	0.26145200	C	-0.24615900	-4.09346500	1.32433800
H	2.13499500	-3.94508500	1.45662100	H	-0.20616900	-3.90132600	2.39865400
H	2.19526200	-5.42409600	0.48885400	H	-1.20087600	-3.74594400	0.92812600
C	2.17223000	1.19448600	-3.33276900	H	-0.20261100	-5.17592800	1.17747200
H	2.93968700	1.25596600	-4.11049100	C	2.81662400	2.11050000	0.66094200
H	2.24447700	0.23234300	-2.82889300	H	3.69866800	2.37539400	1.25055800
H	1.19004700	1.25645500	-3.79905200	H	2.60478400	1.05042400	0.80702700
C	3.82547200	2.34314900	-1.85346700	H	3.05055600	2.26750500	-0.39055300
H	3.98927100	3.06878200	-1.05338900	C	1.44174300	2.80508400	2.61561700
H	4.13370500	1.35453300	-1.51447400	H	0.53346600	3.29148600	2.97801500
H	4.46513800	2.62319700	-2.69463200	H	1.43614900	1.75510400	2.90906000
C	2.02719000	3.67919500	-2.98627600	H	2.29316200	3.27880700	3.11122100
H	2.61165000	3.79314000	-3.90380400	C	1.86077300	4.44200700	0.76527700
H	0.96893000	3.71341000	-3.24838100	H	2.80137100	4.77284300	1.21436200
H	2.25786700	4.52235200	-2.33110800	H	1.92817500	4.57438500	-0.31454100
C	-3.52870500	0.60522500	1.84035900	H	1.05776800	5.07556900	1.15119200
H	-3.43062700	0.03797100	2.76802600	C	-3.78788300	-0.27143100	-3.70465000
H	-4.30183000	1.36369000	1.98543900	H	-4.55565800	-0.94577500	-3.31681500
H	-3.87833700	-0.06185700	1.05302800	H	-4.27043900	0.44025900	-4.38048900
C	-2.47334200	2.23549900	0.26805900	H	-3.06224000	-0.85220600	-4.27430300
H	-3.16729400	3.01829400	0.58384500	C	-2.10096700	1.51736100	-3.14456500
H	-1.55043100	2.69571000	-0.07529600	H	-2.65342600	2.28774200	-3.69094800
H	-2.93427800	1.70441600	-0.56391600	H	-1.53503200	1.99202100	-2.34172400
C	-1.71480600	2.14013900	2.64656300	H	-1.39278900	1.04730300	-3.82586700
H	-1.44573400	1.50426700	3.49393000	C	-4.12466900	1.22859400	-1.72423400
H	-0.84956000	2.74026200	2.36102000	H	-4.78153500	0.54220900	-1.18572700
H	-2.51126400	2.81322200	2.97473700	H	-3.65120100	1.91006200	-1.01701500
H	-5.03487400	-0.36735100	-1.26344000	H	-4.74668700	1.82909700	-2.39324400
Br	-3.67615200	-1.82261100	-1.17624200	Br	5.19740300	-0.05876000	-1.70023500
Br	-6.07056200	0.78092300	-1.29501800	Br	1.71290600	0.05792000	-2.71851800
<b>[L(HI<sub>2</sub>)<sup>-</sup>, 1I, E<sub>0</sub>=-15570.688571 au</b>				<b>[L(HI<sub>2</sub>)<sup>-</sup>, 2I, E<sub>0</sub>=-15570.679936 au</b>			
O	-3.47372200	-0.95753700	1.20583800	N	1.09699400	0.00025900	-0.00022300
H	-3.54092400	-0.57859300	0.29946900	C	1.57822900	0.53654500	1.33607800
O	-2.04740000	3.09120100	-1.07652300	H	1.09428600	1.49422000	1.44943900
H	-2.51613200	2.26226300	-1.32100900	H	2.65315700	0.67963000	1.21746900
O	3.73531200	-1.75718100	-1.40672000	C	1.57845000	0.88924800	-1.13276300
H	3.95891000	-1.49211500	-0.48567000	H	1.09502500	0.50818300	-2.01890900
N	-2.27627300	-1.75233400	1.17702500	H	2.65346300	0.71530000	-1.19708200
N	-1.34657100	2.76068200	0.12943300	C	1.57767500	-1.42532900	-0.20364500
N	2.68526600	-0.84579000	-1.76360300	H	1.09425600	-2.00178500	0.56985000
N	0.84219600	-0.19089300	0.27736300	H	2.65280100	-1.39432900	-0.02121200
H	1.81291200	-0.20953600	-0.09968000	C	1.29684500	-0.39991400	2.47306500
C	0.67000300	-1.51868700	1.03369200	C	2.34305000	-1.20216900	2.94287400
H	0.21567800	-2.19710600	0.32543400	C	0.01353800	-0.53801700	3.02430700
H	1.68381600	-1.84622600	1.25681500	C	2.11695200	-2.16909800	3.91443200
C	-0.11777600	-1.38613100	2.30824500	H	3.32873000	-1.07761300	2.50518500
C	0.59854300	-1.14213700	3.48769200	C	-0.21272600	-1.53783800	3.97694400
H	1.68276200	-1.14283100	3.44174000	C	0.82846600	-2.34794000	4.41404900
C	-0.05241800	-0.84147400	4.67612500	H	2.93399200	-2.79255300	4.25803300
H	0.52279800	-0.63781200	5.57171800	H	-1.21742600	-1.68221200	4.34511100
C	-1.44376800	-0.76690700	4.69149200	H	0.63116100	-3.11939900	5.15053300
H	-1.96766000	-0.49457700	5.60135600	C	1.29524300	-1.94222900	-1.58286000
C	-2.16898900	-1.05393300	3.54281900	C	2.34123500	-1.94860800	-2.51274900
H	-3.24698500	-0.99326700	3.54132300	C	0.01167500	-2.35025600	-1.97777100
C	-1.52203600	-1.40466900	2.35094500	C	2.11487700	-2.30670700	-3.83580700

C	-2.70073000	-3.20690000	1.11149500	H	3.32710100	-1.63238500	-2.18611600
C	-3.51797300	-3.38328700	-0.17241800	C	-0.21483400	-2.67544800	-3.31990100
H	-2.94233000	-3.06703900	-1.04065100	C	0.82618300	-2.64943400	-4.24023600
H	-4.43308600	-2.79454000	-0.14345000	H	2.93186000	-2.29317400	-4.54761700
H	-3.78085700	-4.43809000	-0.29250300	H	-1.21969700	-2.92169900	-3.62878400
C	-1.45388400	-4.09425400	1.03132300	H	0.62860500	-2.90163300	-5.27650000
H	-0.89300800	-3.90336700	0.11499000	C	1.29672900	2.34216700	-0.89040100
H	-1.76880300	-5.14056000	1.01398300	C	2.34302500	3.15005800	-0.43061900
H	-0.79555800	-3.96002600	1.89141000	C	0.01329200	2.88864500	-1.04586200
C	-3.55539300	-3.61416000	2.32273400	C	2.11708600	4.47481300	-0.07847100
H	-3.93779800	-4.62767100	2.17490900	H	3.32870100	2.70860500	-0.31996100
H	-4.40482600	-2.93802300	2.42606200	C	-0.21276100	4.21342800	-0.65581500
H	-2.97725000	-3.60279300	3.24884700	C	0.82855200	4.99688600	-0.17278000
C	0.69931100	1.01673300	1.17359500	H	2.93426900	5.08401000	0.28950900
H	1.38293400	0.85101500	2.00208500	H	-1.21746800	4.60446600	-0.71458200
H	-0.32258200	1.00440000	1.52464600	H	0.63127900	6.02032300	0.12746500
C	1.03169500	2.30332000	0.47219500	N	-1.04733100	0.31286500	2.55783800
C	2.37262100	2.67733900	0.34035700	N	-1.04780700	2.05943900	-1.54952700
H	3.13417800	2.04501200	0.78572100	N	-1.04920700	-2.37149100	-1.00757200
C	2.72577500	3.81717500	-0.37126200	O	-2.24841200	-0.47442600	2.62352300
H	3.77047000	4.08473800	-0.47717100	H	-2.72698300	-0.29210000	1.78628400
C	1.73116500	4.58747300	-0.97075900	O	-2.25037100	-2.03482100	-1.72213100
H	1.99670300	5.46138400	-1.55596300	H	-2.72867000	-1.40044800	-1.14595000
C	0.39284000	4.24689500	-0.81562000	O	-2.24891600	2.51026700	-0.90074100
H	-0.38647200	4.82569400	-1.28946900	H	-2.72747000	1.69429400	-0.63929700
C	0.02565300	3.12487500	-0.06419300	C	-1.29645700	1.56088000	3.39172700
C	-2.06115300	3.43436100	1.27725800	C	-1.29834900	-3.71750500	-0.34350500
C	-2.20896400	4.94597000	1.03784400	C	-1.29671000	2.15728400	-3.04732100
H	-2.68463800	5.12664900	0.07402800	H	0.06919200	0.00052300	-0.00043400
H	-1.23886200	5.44871200	1.05538300	C	-1.71083300	1.20040600	4.82702600
H	-2.83125500	5.38458300	1.82261500	H	-0.88952400	0.73479000	5.37690600
C	-3.43876600	2.77067000	1.37868600	H	-2.00285400	2.10884400	5.36037100
H	-3.33364700	1.69337200	1.51689600	H	-2.56082400	0.51867300	4.81314200
H	-4.02179500	2.93656200	0.47365300	C	-0.04247700	2.44206700	3.43049700
H	-3.98710500	3.18452100	2.23018400	H	0.83286600	1.90807400	3.80473300
C	-1.29649200	3.19874700	2.58636400	H	0.18041600	2.86842400	2.45116800
H	-0.26912400	3.56461500	2.53726000	H	-0.23357300	3.27757000	4.10816600
H	-1.28737100	2.14503900	2.86810400	C	-2.41618200	2.33827200	2.69237700
H	-1.80576300	3.74346100	3.38512800	H	-2.57245400	3.29197200	3.20469800
C	-0.04474000	-0.11701100	-0.93997800	H	-2.15154500	2.53918900	1.65321600
H	0.10777400	0.86257600	-1.38341700	H	-3.35348000	1.78373000	2.70092900
H	-1.07643400	-0.17561000	-0.60334900	C	-1.71137700	3.58040600	-3.45292800
C	0.26217800	-1.24238500	-1.89666500	H	-0.89030900	4.28960500	-3.32411900
C	-0.81550700	-1.96546100	-2.41711400	H	-2.00293900	3.58813700	-4.50645600
H	-1.81931500	-1.62248500	-2.19664400	H	-2.56170300	3.90891800	-2.85589400
C	-0.60954800	-3.08967900	-3.20596000	C	-0.04238800	1.75069900	-3.82952700
H	-1.46166100	-3.63430300	-3.59577200	H	0.83268400	2.34204500	-3.55384200
C	0.68928500	-3.52632600	-3.45759000	H	0.18084700	0.68948000	-3.70912100
H	0.86302100	-4.42707500	-4.03615100	H	-0.23319000	1.91981000	-4.89198100
C	1.77009700	-2.80022900	-2.97443000	C	-2.41604600	1.16257900	-3.37111100
H	2.78314400	-3.13239400	-3.14644400	H	-2.57248100	1.12994000	-4.45319200
C	1.56887300	-1.63292200	-2.23203600	H	-2.15113700	0.16197300	-3.02618500
C	3.24556400	0.13453300	-2.77382500	H	-3.35343100	1.44671500	-2.89496800
C	2.16218700	1.16141200	-3.11748500	C	-2.41948300	-3.50079200	0.67796000
H	1.87454000	1.74346800	-2.24279000	H	-2.57535600	-4.42092500	1.24849300
H	1.27579700	0.69144500	-3.54696000	H	-2.15691400	-2.70024400	1.37109300
C	2.56023300	1.85853800	-3.85846100	H	-3.35658600	-3.23265100	0.19204600
H	3.72559700	-0.56972400	-4.05168100	C	-1.71103000	-4.78100100	-1.37321800
H	2.89412100	-0.99318900	-4.61792600	H	-0.88879900	-5.02414100	-2.05035100
H	4.42951100	-1.36493600	-3.80238500	H	-2.00303400	-5.69704500	-0.85303200
H	4.23714600	0.15408600	-4.69170500	H	-2.56063800	-4.42889900	-1.95770700
C	4.42952400	0.83823800	-2.10256900	C	-0.04475100	-4.19052100	0.40166700
H	5.25653900	0.14703100	-1.94727100	H	0.83130500	-4.24663500	-0.24707200
H	4.14304400	1.23847400	-1.13214500	H	0.17677600	-3.55528600	1.26069900
H	4.77023500	1.66109300	-2.73680900	H	-0.23518000	-5.19532300	0.78628300
I	-3.95113000	0.33476800	-1.96691500	I	5.20556300	-0.00107600	-0.00095500

I	4.26759200	-0.54093600	1.79676600	I	-4.42092600	0.00047000	-0.00005500
<b>[L(HI<sub>2</sub>)<sup>-</sup>, 3I, E<sub>0</sub>=-15570.678009</b>				<b>[L(HI<sub>2</sub>)<sup>-</sup>, 4I, E<sub>0</sub>=-15570.673146 au</b>			
N	-1.43295300	-0.07571600	-0.27533500	O	-1.38096200	-1.12411900	0.96298300
C	-1.29868200	0.47050600	-1.68259000	O	-2.24932600	3.13518000	-1.11467200
H	-1.16186800	1.53816300	-1.57230500	O	-1.40578300	-3.16683300	-0.87307300
H	-2.25537400	0.27285000	-2.16985600	N	-1.32123900	-1.21052600	2.39016800
C	-2.47842500	0.68558200	0.50864000	N	-1.16125700	2.94091000	-0.20305600
H	-2.53296700	0.19907700	1.47189900	N	-0.20945200	-2.72771600	-1.55794300
H	-3.41852500	0.52993500	-0.02476300	N	1.72974900	-0.08754600	-0.09576300
C	-1.76006500	-1.55898700	-0.31034800	C	1.43168600	-1.25293400	0.85338400
H	-0.99377500	-2.01028400	-0.92650800	C	1.18654700	-0.76912900	2.26134800
H	-2.73176700	-1.63252200	-0.80295800	C	2.30472000	-0.27876700	2.95153600
C	-0.14984600	-0.17584800	-2.39640900	C	2.19592500	0.31848200	4.19953700
C	-0.40705400	-1.13528900	-3.38035700	C	0.93694100	0.46144300	4.77560000
C	1.17580400	0.11969100	-2.04313400	C	-0.18016000	-0.02750100	4.11351800
C	0.63861100	-1.82053400	-3.98849200	C	-0.08227900	-0.68552300	2.87890700
H	-1.43705400	-1.35008700	-3.64388200	C	-1.67672000	-2.60633300	2.83095500
C	2.21978000	-0.60046100	-2.62899800	C	-0.63303100	-3.64585800	2.38843500
C	1.95006900	-1.56284800	-3.59573100	C	-1.78787700	-2.62311800	4.36219100
O	0.42909900	-2.56509900	-4.74781400	C	-3.05861100	-2.92963800	2.24699400
H	3.24111900	-0.43070200	-2.30799700	C	0.89045800	1.11746300	0.21658500
H	2.77265300	-2.11540200	-4.03492900	C	1.15099400	2.32718800	-0.63387700
C	-1.78160400	-2.14027900	1.07126200	C	2.39922800	2.61209700	-1.19325100
C	-3.00535100	-2.34406600	1.71725000	C	2.54241800	3.65675700	-2.10031500
C	-0.58372700	-2.41475500	1.74675800	C	1.43367500	4.42279200	-2.45811800
C	-3.04247900	-2.76579500	3.04136900	C	0.20436200	4.19169000	-1.85172600
H	-3.92219500	-2.14119400	1.17366600	C	0.06397500	3.17704200	-0.90164200
C	-0.62833200	-2.78983500	3.09241000	C	-1.39693500	3.80247800	1.01172700
C	-1.84911200	-2.96191300	3.73498300	C	-1.53862600	5.28710800	0.63678400
H	-3.99512000	-2.91389700	3.53621200	C	-2.68435200	3.30249500	1.67388200
O	0.29861100	-2.92579900	3.63010300	C	-0.23553800	3.62222400	1.99650700
H	-1.86836800	-3.25216700	4.77953500	C	1.74744800	-0.55160000	-1.55038700
C	-2.15306300	2.14497500	0.62618100	C	0.43483500	-0.47656800	-2.28546400
C	-2.91455100	3.05237200	-0.11879200	C	0.15224700	0.67493200	-3.02931700
C	-1.09229400	2.61523500	1.41688000	C	-1.07779600	0.85262100	-3.64850900
C	-2.61870000	4.40986600	-0.10863400	C	-2.04869200	-0.13574200	-3.53828100
H	-3.72584600	2.66745600	-0.72788100	C	-1.76192000	-1.31666700	-2.86756900
C	-0.78516400	3.97913000	1.39964700	C	-0.51682100	-1.51200200	-2.26816800
C	-1.54002900	4.86825200	0.64464500	C	0.23128500	-3.89817400	-2.38320800
H	-3.20983800	5.09844200	-0.70068600	C	1.45599400	-3.50026000	-3.21458200
H	0.06888700	4.32460900	1.96281800	C	-0.87831300	-4.40210400	-3.32344400
H	-1.28065800	5.92111500	0.64206100	C	0.62802000	-5.00406600	-1.39615900
N	1.38956100	1.16081300	-1.06669800	H	2.74404700	0.13295700	0.08423600
N	-0.30269900	1.66831800	2.17164700	H	0.61413500	-1.80627500	0.42153500
N	0.64469700	-2.26928200	1.01456200	H	2.34023400	-1.85601000	0.81595300
O	2.16857100	0.65322400	0.03299900	H	3.27607400	-0.34545500	2.47048700
H	3.13652400	0.51808000	-0.20456900	H	3.08243600	0.69216900	4.69787200
O	1.56071700	-1.52683600	1.83809400	H	0.81891500	0.96735700	5.72733900
H	1.82978600	-0.80290100	1.24497200	H	-1.16854600	0.10376200	4.53148100
O	1.06281300	2.11941600	2.13705200	H	0.34870000	-3.41880000	2.81148600
H	1.49063400	1.54759900	1.46979900	H	-0.55196000	-3.69489700	1.30392500
C	1.92713900	2.46724600	-1.62324800	H	-0.92864000	-4.63793900	2.74124800
C	1.31297800	-3.55912500	0.60532200	H	-0.83016200	-2.43281900	4.84754500
C	-0.65015900	1.54891200	3.63945100	H	-2.13386300	-3.61120200	4.67476900
C	2.54220300	-3.17871700	-0.22253200	H	-2.51134300	-1.88136000	4.70608500
H	3.02011100	-4.08236300	-0.61015900	H	-3.76487500	-2.13161400	2.48198000
H	2.24923500	-2.55669700	-1.06534300	H	-3.42170300	-3.86696500	2.67683700
H	3.27806500	-2.62978400	0.36344300	H	-3.04080500	-3.04315800	1.16490400
C	1.74584400	-4.41042700	1.80994000	H	1.08776200	1.33560700	1.26121500
H	0.89078000	-4.82410600	2.34829100	H	-0.15471200	0.83126900	0.13440200
H	2.35710400	-5.24619500	1.46016200	H	3.26246100	2.00151400	-0.94722200
H	2.34869100	-3.81133400	2.49366900	H	3.51315500	3.85277800	-2.54055700
C	0.33408000	-4.34864800	-0.27174400	H	1.53140300	5.21373800	-3.19389800
H	-0.59115600	-4.58919600	0.25581100	H	-0.66562600	4.77692200	-2.11400100
H	0.09083200	-3.79933900	-1.18323400	H	-2.30542000	5.40460900	-0.12986600
H	0.80555700	-5.28864400	-0.56783800	H	-0.59736200	5.69823400	0.26484300

C	0.33963400	0.55207800	4.25285100	H	-1.83600000	5.86436400	1.51661600
H	0.00772600	0.28417700	5.26005100	H	-2.85244100	3.84828500	2.60722400
H	0.40098800	-0.34815900	3.64487000	H	-2.61496700	2.23593400	1.89009200
H	1.33726500	0.98395900	4.31498000	H	-3.54524600	3.44606100	1.02309600
C	-2.07197700	0.99970600	3.78333400	H	-0.18717900	2.59637000	2.36404700
H	-2.80828000	1.62488900	3.27394100	H	-0.40428000	4.27268000	2.85829700
H	-2.14090600	-0.02310600	3.41310600	H	0.72652700	3.89327900	1.55774900
H	-2.33315700	0.98183700	4.84410300	H	2.15149900	-1.55529100	-1.50619700
C	-0.54303900	2.89892600	4.36806600	H	2.48864000	0.07487900	-2.03993500
H	-0.67249100	2.73953500	5.44179400	H	0.89602400	1.45701500	-3.09176200
H	0.44029600	3.34148200	4.20556300	H	-1.28779600	1.77827600	-4.16933600
H	-1.30988900	3.60203100	4.03637600	H	-3.03837600	0.01574800	-3.95019500
C	3.06812700	2.30878300	-2.64273400	H	-2.52177400	-2.07281200	-2.74353800
H	2.74086800	1.79016200	-3.54522700	H	2.31294000	-3.25871000	-2.58397500
H	3.40912200	3.30561000	-2.93587100	H	1.24517900	-2.65025700	-3.86538200
H	3.92149400	1.77938100	-2.21513500	H	1.73999900	-4.34571800	-3.84556100
C	2.42336600	3.33742000	-0.46521700	H	-1.11170400	-3.66081400	-4.08995700
H	2.66967200	4.32593100	-0.86106900	H	-1.78579400	-4.62048200	-2.76121900
H	1.66238600	3.44804200	0.30234700	H	-0.54743300	-5.31616500	-3.82424700
H	3.32371600	2.92006100	-0.01348100	H	1.04340000	-5.85847500	-1.93743200
C	0.73169300	3.15726900	-2.29600300	H	-0.23638400	-5.33643900	-0.82279700
H	0.31406000	2.54506300	-3.09873900	H	1.38295200	-4.63160700	-0.69992900
H	-0.05004400	3.38014400	-1.56814700	H	-2.20654200	-0.60854800	0.75635200
H	1.06295500	4.09920300	-2.73994200	H	-2.75883900	2.30083500	-1.02541600
I	5.42346700	-0.03495900	-0.34530800	H	-1.48664100	-2.50081500	-0.16009400
H	-0.53231800	0.05412700	0.20249700	I	5.12822400	-0.11833900	0.11084400
I	-5.07229200	-0.51088700	-2.04303700	I	-4.18642400	0.26783600	-0.30722400
<b>[L(HI<sub>2</sub>)]<sup>-</sup>, 5I, E<sub>0</sub>=-15570.67788 au</b>				<b>[L(HI<sub>2</sub>)]<sup>-</sup>, 6I, E<sub>0</sub>=-15570.670122 au</b>			
N	-1.30608700	0.02318700	-0.18833700	N	0.40854600	0.04903300	0.06413300
C	-1.32831600	-1.49685700	-0.07656400	C	0.32131800	0.87560000	1.32037600
H	-0.49618600	-1.82818300	-0.67904800	H	-0.49096700	0.46065900	1.90929200
H	-2.27414800	-1.80581500	-0.52650500	H	0.01465700	1.87942500	1.05555900
C	-1.43774900	0.43157500	-1.65099900	C	1.22030100	0.67609100	-1.07883300
H	-1.37078700	1.51394800	-1.65974200	H	0.60320100	0.56815400	-1.96154800
H	-2.43196800	0.10151400	-1.95730200	H	2.10379800	0.05167400	-1.21134700
C	-2.40101500	0.65753900	0.63616900	C	-0.95638000	-0.38576900	-0.38221000
C	-2.28935800	0.25645200	1.63288100	H	-1.38122900	0.45678800	-0.92148100
H	-3.33961700	0.29687200	0.21102000	H	-1.57375700	-0.51377800	0.50591000
C	-1.19687100	-1.98628600	1.33433300	C	1.61923400	0.88616000	2.07945600
C	-2.34858200	-2.15780900	2.11280400	C	2.05582300	2.10894800	2.59643600
C	0.06082500	-2.27024300	1.89145700	C	2.40415400	-0.26145100	2.28743600
C	-2.25571000	-2.51017900	3.45331900	C	3.24898400	2.20982000	3.29672900
H	-3.31691000	-1.99910700	1.64964800	H	1.46032100	2.99380700	2.40488200
C	0.14918500	-2.57228300	3.25531300	C	3.62618000	-0.14644100	2.95579800
C	-0.99802900	-2.68117600	4.03086500	C	4.04208300	1.07652200	3.46395300
H	-3.15500900	-2.63000600	4.04592000	H	3.57492900	3.17131800	3.67551500
H	1.12812700	-2.71030200	3.69061300	H	4.25233000	-1.02284300	3.02841900
H	-0.91063300	-2.91887200	5.08538000	H	4.99375300	1.14618600	3.97878900
C	-2.33807500	2.15623800	0.63575100	C	-0.97001000	-1.66574600	-1.17047400
C	-3.32969100	2.86806300	-0.04643600	C	0.16753600	-2.20901400	-1.76196500
C	-1.30375300	2.85280700	1.28137100	C	-2.20201900	-2.36462900	-1.25549200
C	-3.29213800	4.25594800	-0.11239900	C	0.12647800	-3.42590300	-2.43837900
H	-4.11749000	2.31193000	-0.54350900	H	1.13394700	-1.72804700	-1.69177700
C	-1.25679400	4.24659000	1.18525700	C	-2.23186900	-3.56739500	-1.96951700
C	-2.24352600	4.94237100	0.49693500	C	-1.07987900	-4.10003500	-2.54413000
H	-4.06193100	4.79432200	-0.65278200	H	1.04123000	-3.81918300	-2.86425000
H	-0.41709300	4.76596000	1.62306300	H	-3.15916000	-4.10285200	-2.08313000
H	-2.18909400	6.02355500	0.43148400	H	-1.14017500	-5.04106600	-3.08005600
C	-0.35466000	-0.19607200	-2.47519700	C	1.65718100	2.09579300	-0.86938600
C	-0.62612100	-1.32225400	-3.25592100	C	3.01815100	2.33090100	-0.65089000
C	0.95682000	0.29298800	-2.38604000	C	0.75887100	3.17427500	-0.86681000
C	0.40799100	-1.98386300	-3.91023700	C	3.48523700	3.61171400	-0.38616600
H	-1.64651200	-1.68552900	-3.31825400	H	3.69967400	1.48756900	-0.67178000
C	1.99872500	-0.40995000	-2.99609000	C	1.22963800	4.45322800	-0.55616800
C	1.72079300	-1.54203100	-3.75666300	C	2.58249300	4.67011700	-0.31785500
H	0.19345300	-2.86017100	-4.51099500	H	4.54087100	3.77483200	-0.20435900



H	3.02314900	-0.10356300	-2.83796800	H	0.51809400	5.26163200	-0.47274600
H	2.53677400	-2.08599700	-4.21832700	H	2.92991400	5.66938000	-0.07811000
N	1.21427300	-2.25933600	1.04027500	N	1.98948300	-1.52903600	1.71403800
N	1.13068900	1.49766800	-1.62260800	N	-0.64148800	2.91453200	-1.08647000
N	-0.26392900	2.09977400	1.93746400	N	-3.30891500	-1.82758500	-0.54931200
O	2.30588400	-1.74609400	1.82239100	O	3.16217800	-2.26182500	1.34895400
H	2.80621000	-1.16849600	1.21283300	H	3.33081100	-2.05815100	0.39568000
O	0.98160300	2.76303300	1.66954800	O	-3.66945100	-0.56114800	-1.12205400
H	1.37200100	2.19886000	0.96879800	H	-3.67750600	0.06077400	-0.35871200
O	1.74096100	1.19496700	-0.36524900	O	-1.36256000	3.72012800	-0.13668300
H	2.66829100	0.84486000	-0.47448400	H	-1.95126200	3.08569600	0.33192100
C	1.61851600	-3.62713900	0.51629400	C	1.20526300	-2.46423200	2.61344600
C	-0.34743400	1.96909300	3.43665200	C	-4.53355300	-2.60624900	-0.21954400
C	1.69826200	2.70070100	-2.29768600	C	-1.17609900	3.23342000	-2.45994300
H	-0.40290700	0.36500700	0.17237300	H	0.94307100	-0.79490300	0.38427700
C	0.44486800	-4.26529500	-0.23752800	C	-0.04804700	-1.76875700	3.15016700
H	0.17140800	-3.68794100	-1.12177900	H	0.18708000	-0.85492000	3.69800400
H	0.75501200	-5.25577100	-0.57888700	H	-0.76277300	-1.54177600	2.35889400
H	-0.43730300	-4.39225500	0.39183400	H	-0.54818100	-2.44856800	3.84314300
C	2.76901900	-3.39516800	-0.46643000	C	2.06787400	-2.93652300	3.79405900
H	2.46920600	-2.68556500	-1.23832100	H	2.32029600	-2.10467700	4.45558900
H	3.65059300	-2.99191100	0.02910400	H	1.51150100	-3.67517200	4.37665200
H	3.04073300	-4.34055400	-0.94492800	H	2.98845900	-3.39512100	3.43551600
C	2.07076600	-4.56307200	1.64831600	C	0.78652100	-3.65413100	1.74177800
H	2.47912800	-5.48166300	1.21879900	H	0.19058900	-4.35210500	2.33582500
H	2.84805400	-4.08344400	2.24290500	H	0.18260200	-3.32085000	0.89541800
H	1.23901900	-4.83764000	2.30092200	H	1.66107500	-4.17283600	1.35356500
C	3.16624400	2.57358100	-2.74019900	C	-2.63599700	2.76392400	-2.48601100
H	3.27764400	1.89240600	-3.58494700	H	-2.70966900	1.69374800	-2.28324200
H	3.53354800	3.55388500	-3.05722100	H	-3.22965300	3.29142600	-1.74028400
H	3.80352700	2.22153300	-1.92688000	H	-3.06551900	2.95507400	-3.47336500
C	0.80117300	2.96030000	-3.51750000	C	-1.10240600	4.73746100	-2.77099100
H	0.84771600	2.13905100	-4.23482200	H	-0.06824800	5.07638000	-2.86238400
H	-0.23878000	3.09710400	-3.21234900	H	-1.60846400	4.94130300	-3.71834800
H	1.13447600	3.87042100	-4.02171800	H	-1.59606500	5.30793200	-1.98398000
C	1.56229500	3.87567300	-1.32170300	C	-0.37778700	2.45272200	-3.50988400
H	1.82298900	4.80414200	-1.83667000	H	0.69061600	2.67108900	-3.46179100
H	0.54032300	3.95144000	-0.95009700	H	-0.52677100	1.37695100	-3.40708100
H	2.22871200	3.76304800	-0.46770500	H	-0.73324700	2.73649700	-4.50322100
C	0.83799500	1.09458100	3.86291900	C	-5.33995800	-1.75202500	0.77539300
H	0.74309900	0.83689800	4.92162000	H	-5.71713300	-0.84362000	0.30788100
H	0.86669100	0.17273700	3.28187000	H	-6.19224600	-2.33117600	1.14090000
H	1.78069000	1.61782900	3.71153500	H	-4.71949000	-1.45332400	1.62072000
C	-0.26998700	3.33934500	4.13086400	C	-4.12014800	-3.89007200	0.51706400
H	-1.15593200	3.94443200	3.92434800	H	-5.01631100	-4.37790600	0.90828900
H	-0.20401700	3.19604900	5.21267400	H	-3.59384100	-4.60518000	-0.11190100
H	0.61643800	3.88137500	3.80092300	H	-3.47165400	-3.63819800	1.35917100
C	-1.65466300	1.27360700	3.82559100	C	-5.42647000	-2.88290100	-1.44506900
H	-2.53020700	1.79119900	3.42698600	H	-6.40491500	-3.24531500	-1.11772900
H	-1.66477400	0.23398800	3.50055300	H	-5.56924600	-1.95209800	-1.99577500
H	-1.73860100	1.27323700	4.91495800	H	-5.00974100	-3.62427200	-2.12691300
I	4.84829500	-0.04440500	-0.11668500	I	4.12961500	-1.64824200	-1.86560600
I	-4.93361800	-1.28490700	-1.52762800	I	-3.48181300	1.62600200	1.64282800
<b>[L(HI<sub>2</sub>)<sup>-</sup>, 7], E<sub>0</sub>=-15570.674099 au</b>				<b>[L(HI<sub>2</sub>)<sup>-</sup>, 8], E<sub>0</sub>=-15570.641910 au</b>			
N	-1.34741100	-0.49180100	-0.07269500	N	2.77010000	0.37545700	1.47321700
C	-1.55876100	-1.07535600	1.31211800	C	1.97679500	0.55793100	2.68741300
H	-0.67609600	-1.67033800	1.51500600	H	1.45510000	1.50394000	2.59095800
H	-2.43823900	-1.71720200	1.23008600	H	2.62936900	0.62779900	3.58166900
C	-1.07388400	-1.58915700	-1.07850000	C	3.55402300	1.56603900	1.15161900
H	-1.01826700	-1.09806500	-2.04068100	H	4.12248700	1.34250100	0.25651400
H	-1.95396300	-2.23463000	-1.05593900	H	4.29182500	1.77497700	1.95396400
C	-2.54463700	0.34730400	-0.48965500	C	3.62406900	-0.81108000	1.55935100
H	-2.71162100	1.03801600	0.32530700	H	2.99274000	-1.63953800	1.86523200
H	-3.38068500	-0.35142000	-0.56430800	H	4.40907300	-0.67810000	2.33192900
C	-1.74854900	0.01228900	2.32719200	C	0.97752900	-0.55178800	2.89908100
C	-3.02797800	0.28879700	2.81668000	C	1.24510000	-1.55261200	3.83767600

C	-0.65844500	0.78861700	2.74612900	C	-0.20283400	-0.63207600	2.14266000
C	-3.23152200	1.34911300	3.69373000	C	0.38897100	-2.63477200	4.01098000
H	-3.85885200	-0.32516900	2.48495700	H	2.15384700	-1.48169800	4.42685000
C	-0.87793800	1.87997500	3.58852000	C	-1.04282200	-1.73977600	2.29410300
C	-2.15675600	2.15519600	4.06296100	C	-0.75262900	-2.73364300	3.22164900
H	-4.22638500	1.55684400	4.06995800	H	0.62132300	-3.40216700	4.74121200
H	-0.04780300	2.51841100	3.85236800	H	-1.91767600	-1.84204800	1.66554000
H	-2.31403100	3.00528700	4.71746100	H	-1.41754400	-3.58444800	3.31657800
C	-2.28631300	1.07293300	-1.77509000	C	4.27940100	-1.13045800	0.23820000
C	-2.76763200	0.54790000	-2.97896400	C	5.60379400	-0.75283100	-0.00171100
C	-1.52751200	2.25276300	-1.78847300	C	3.54774800	-1.72794000	-0.79879700
C	-2.44624500	1.14818800	-4.19067300	C	6.18575500	-0.90497200	-1.25580200
H	-3.38031600	-0.34669700	-2.94946200	H	6.17116300	-0.30276600	0.80655300
C	-1.15395300	2.81252800	-3.01299600	C	4.11762400	-1.83009000	-2.07188600
C	-1.60942500	2.26284100	-4.20585100	C	5.42630500	-1.42216800	-2.30244500
H	-2.81882200	0.73005000	-5.11825800	H	7.21097900	-0.59362800	-1.42243600
H	-0.49540200	3.66872000	-3.02068200	H	3.51512800	-2.21204100	-2.88307200
H	-1.31234600	2.70768400	-5.14876300	H	5.85067900	-1.50716700	-3.29677600
C	0.18047500	-2.35126700	-0.76358600	C	2.72919200	2.81485400	0.94419600
C	0.05817300	-3.67380000	-0.32521200	C	2.73563200	3.78995300	1.94831700
C	1.45648300	-1.77171200	-0.87019500	C	1.92471100	3.02486900	-0.18968400
C	1.18157300	-4.41370000	0.02490400	C	1.94817500	4.93217700	1.87291300
H	-0.93401700	-4.10448700	-0.24312700	H	3.35655500	3.62206600	2.82234900
C	2.57947800	-2.51474000	-0.49660900	C	1.11544700	4.16678000	-0.24962900
C	2.44110200	-3.82465800	-0.05195000	C	1.12146200	5.11167500	0.76719500
H	1.07129000	-5.43501600	0.37062800	H	1.96193200	5.65948900	2.67686000
H	3.56496600	-2.06239600	-0.51865200	H	0.45491900	4.28115700	-1.09638000
H	3.32622200	-4.37815400	0.23976700	H	0.47833300	5.98200400	0.69703300
N	0.64043900	0.38609600	2.28530200	N	-0.50376400	0.43678400	1.22560600
N	1.55260900	-0.39639200	-1.30558900	N	1.88432900	2.03911700	-1.23737700
N	-1.17328500	2.83456300	-0.52091900	N	2.22116500	-2.19313200	-0.51064200
O	1.27891400	1.52783400	1.66204800	O	-0.62954100	-0.09416200	-0.10403300
H	1.77397400	1.09637400	0.92165400	H	-1.47552800	-0.59269200	-0.22524900
O	0.22622800	3.16538800	-0.54678500	O	1.33747800	-1.65004300	-1.50275000
H	0.56966900	2.66296700	0.21395000	H	0.74814200	-1.08564100	-0.97000600
O	2.39934300	0.33378100	-0.41378300	O	0.51880800	1.93570100	-1.67876500
H	3.36074600	0.06830400	-0.46411700	H	0.17084300	1.16936600	-1.18566700
C	1.54644800	-0.18423200	3.35150800	C	-1.64315800	1.34834300	1.60545500
C	-1.94685100	4.07191100	-0.14951300	C	2.03157000	-3.67748500	-0.46362200
C	1.99082500	-0.16781600	-2.73590600	C	2.69672500	2.32024400	-2.46594800
C	-1.47378700	4.48720700	1.24621500	C	0.59058300	-3.91945600	-0.00493800
H	-2.07282300	5.32871400	1.60454000	H	0.41031900	-4.99159600	0.11513900
H	-1.58492100	3.65756700	1.94079500	H	0.41618100	-3.42646800	0.94918500
H	-0.42663600	4.78870400	1.22797800	H	-0.12553500	-3.52856300	-0.72716400
C	-1.72784400	5.23714400	-1.12911600	C	2.26029700	-4.36952800	-1.81966400
H	-2.18656500	5.04534800	-2.10028400	H	3.31232100	-4.35855400	-2.11159900
H	-2.17917500	6.14501700	-0.72013300	H	1.94167400	-5.41362200	-1.75612000
H	-0.66047100	5.41741500	-1.26593400	H	1.66667000	-3.87772600	-2.59163900
C	-3.43502600	3.70731200	-0.09025600	C	2.99878700	-4.24252200	0.58401400
H	-3.80681800	3.34956800	-1.05190500	H	4.04135700	-4.05531200	0.31803800
H	-3.62416400	2.94394500	0.66671200	H	2.80266900	-3.80770200	1.56611100
H	-4.00848500	4.59687000	0.18132500	H	2.85580000	-5.32368600	0.65716200
C	2.21379100	1.34056900	-2.90089900	C	2.47383900	1.13949100	-3.41972700
H	2.28262000	1.57541800	-3.96675400	H	3.19535300	1.18710600	-4.24109400
H	1.38969000	1.90151100	-2.46293100	H	2.59752700	0.19971600	-2.88451900
H	3.13733000	1.65590000	-2.41690500	H	1.46628700	1.16115100	-3.83244000
C	0.84461000	-0.61747300	-3.64705400	C	4.17744100	2.38175600	-2.07921900
H	0.60472600	-1.67362700	-3.50295600	H	4.36679600	3.14181700	-1.31768200
H	-0.04722200	-0.01437800	-3.48558600	H	4.52773100	1.41437100	-1.72039500
H	1.14970500	-0.49031600	-4.68828500	H	4.76332500	2.64263500	-2.96451200
C	3.26860800	-0.92949100	-3.12040000	C	2.28818900	3.63226400	-3.16028300
H	3.55455800	-0.64140500	-4.13601800	H	2.81822200	3.72263300	-4.11276800
H	4.10647900	-0.69055100	-2.46282000	H	1.21661800	3.63340800	-3.36393100
H	3.11147900	-2.01017100	-3.11056900	H	2.53470400	4.50535100	-2.55178200
C	1.99224200	0.85746400	4.39059600	C	-2.92125300	0.63790100	2.08480500
H	1.18197600	1.14023700	5.06494900	H	-2.76290700	0.10613200	3.02483700

H	2.79791700	0.43737500	4.99743400	H	-3.70304800	1.38429900	2.24200200
H	2.37435700	1.74669400	3.88775700	H	-3.29912500	-0.06497700	1.34229800
C	2.77723900	-0.76034000	2.64803400	C	-1.98611100	2.22879000	0.39993700
H	3.40819900	-1.27513900	3.37664200	H	-2.68351800	3.00552300	0.72160400
H	2.48056400	-1.47576200	1.88313800	H	-1.09318400	2.69630900	-0.00676700
H	3.39002100	0.00607700	2.17605600	H	-2.47415700	1.65761200	-0.38917800
C	0.78761600	-1.32631100	4.04077200	C	-1.09965600	2.23520800	2.73581800
H	-0.10988000	-0.97737800	4.55463700	H	-0.77326600	1.63594700	3.58963200
H	0.50483800	-2.09989500	3.32394500	H	-0.26334500	2.84023600	2.38267000
H	1.44540800	-1.78532700	4.78211900	H	-1.89117400	2.90499800	3.08168900
H	-0.51057300	0.10472500	-0.05022700	H	-4.85098500	-0.36722800	-0.82792600
I	5.74602700	-0.13831200	-0.07174800	I	-3.39279900	-2.01427500	-0.98228200
I	-4.67316100	-2.82583000	-0.19370800	I	-5.99282400	0.97021500	-0.67484800
<b>[L(HI<sub>2</sub>)<sup>-</sup>, 9I, E<sub>0</sub>=-15570.633594 au</b>							
N	2.13859400	0.10466600	1.67757700				
C	3.46277000	0.34222900	1.10652000				
H	3.68288200	-0.49775600	0.46268000				
H	4.23486000	0.34707900	1.90475700				
C	2.08446100	-1.18831700	2.36138800				
H	1.07679100	-1.30310000	2.73476700				
H	2.75518600	-1.18108000	3.24620200				
C	1.75979200	1.18238500	2.59281100				
H	1.82766100	2.10930100	2.03856100				
H	2.48596400	1.25003600	3.43009100				
C	3.57985700	1.64118900	0.34456700				
C	4.17625400	2.73226400	0.98787400				
C	3.07071700	1.82575100	-0.95351100				
C	4.23444400	3.99318900	0.40810500				
H	4.57164300	2.58178300	1.98709100				
C	3.11045700	3.10579000	-1.52496300				
C	3.67874100	4.18006400	-0.85445000				
H	4.68579600	4.82112800	0.94332500				
H	2.65737200	3.24564200	-2.49497700				
H	3.68811900	5.15971200	-1.31992900				
C	0.38044800	1.01377000	3.18307500				
C	0.25976700	0.53643500	4.49307500				
C	-0.79040000	1.23811600	2.44021400				
C	-0.97482200	0.22956900	5.05215200				
H	1.16698200	0.36782300	5.06423500				
C	-2.03172900	0.89169100	2.99190600				
C	-2.12508100	0.38970000	4.28309800				
H	-1.03551600	-0.15705900	6.06345700				
H	-2.91478100	0.99156300	2.37726500				
H	-3.09637200	0.12339500	4.68540900				
C	2.47491300	-2.37054700	1.50578500				
C	3.77117300	-2.88101100	1.64944500				
C	1.62960400	-2.95238300	0.54272000				
C	4.26161700	-3.90106900	0.84474900				
H	4.41571800	-2.43110300	2.39740400				
C	2.13759300	-3.96723100	-0.28255500				
C	3.43653800	-4.43481200	-0.14123200				
H	5.27759300	-4.25796200	0.97167000				
H	1.49742100	-4.36080800	-1.05756300				
H	3.80029800	-5.21691600	-0.79899600				
N	2.46682200	0.73398100	-1.66434500				
N	0.28698300	-2.48032500	0.35992900				
N	-0.70184600	1.75404000	1.10515900				
O	1.41526200	1.30570400	-2.46349400				
H	0.62018500	0.78738200	-2.24887600				
O	-1.75146800	1.11610300	0.36221500				
H	-1.31182700	0.71657000	-0.40590600				
O	-0.00464500	-2.64421400	-1.04003100				
H	-0.38675700	-1.79405500	-1.32500300				
C	3.35337100	-0.03367800	-2.61607400				
C	-0.90088400	3.23871800	0.93460000				
C	-0.80619000	-3.21000200	1.10943900				

C	-0.74180500	3.52435600	-0.56415800				
H	-0.74650600	4.60464800	-0.73692400				
H	0.19965900	3.11255100	-0.93017200				
H	-1.55382200	3.07694600	-1.13635500				
C	-2.28973700	3.69161400	1.41537600				
H	-2.39075100	3.58920100	2.49870500				
H	-3.66904600	-0.05714500	-1.44899000				
H	-2.44314500	4.74360600	1.15824200				
H	-3.06712900	3.10047200	0.93045500				
C	0.18787500	3.99748800	1.70049200				
H	0.19851100	3.73824500	2.76145700				
H	1.17389000	3.81241300	1.27232000				
H	-0.01255600	5.06917500	1.62063800				
C	-2.11737300	-2.49072500	0.76958700				
H	-2.93107400	-2.88806800	1.38196000				
H	-2.02690300	-1.42159700	0.96518800				
H	-2.38394400	-2.62285800	-0.27815100				
C	-0.57468000	-3.11202800	2.62040800				
H	0.40020500	-3.50628700	2.91546100				
H	-0.67614200	-2.08518200	2.97197700				
H	-1.34054900	-3.70749900	3.12399300				
C	-0.88438200	-4.68961300	0.69789300				
H	-1.75545800	-5.15544700	1.16681200				
H	-0.98899800	-4.77326600	-0.38384200				
H	0.00632400	-5.23990800	1.01224700				
C	3.90267300	0.86674300	-3.73569200				
H	4.59537300	1.61524900	-3.34286000				
H	4.43997600	0.25751200	-4.46789500				
H	3.08340600	1.37524800	-4.24420000				
C	2.48639400	-1.15116500	-3.20992900				
H	3.10839900	-1.81840100	-3.81397100				
H	2.01789000	-1.73193200	-2.41408500				
H	1.69842200	-0.74467000	-3.84305200				
C	4.51972800	-0.67281000	-1.85542000				
H	5.10991800	0.06668600	-1.31012700				
H	4.17004900	-1.44101200	-1.16525600				
H	5.17975000	-1.15707800	-2.57985400				
I	-5.08515400	0.02107100	-0.49499500				
I	-1.74568900	-0.20058900	-2.81332400				
<b>[L(HClBr)]<sup>-</sup>, 1a, E<sub>0</sub>=-4765.992206 au</b>				<b>[L(HClBr)]<sup>-</sup>, 1b, E<sub>0</sub>=-4765.991182 au</b>			
O	3.77553600	-0.66338700	0.57390100	O	-3.52028700	-0.61956300	-0.25952300
H	3.35101100	-0.40213200	1.43089600	H	-3.09236200	-0.38434300	-1.11956300
O	1.25435700	2.78600500	2.46798400	O	-0.90116200	2.85325100	-2.18731600
H	1.62059800	1.90477400	2.72672500	H	-1.25903100	1.98036300	-2.47711000
O	-3.65608900	-2.01558500	-0.58847400	O	3.87841300	-2.03110900	1.08513400
H	-3.43258700	-1.58288200	-1.44774300	H	3.60548600	-1.57303200	1.91873400
N	2.79611400	-1.50022100	-0.05792100	N	-2.56859600	-1.48544300	0.37744600
N	1.18436500	2.71869200	1.03961000	N	-0.87439100	2.75125300	-0.75965500
N	-3.00842100	-1.16215100	0.36580400	N	3.28376100	-1.20174300	0.07718600
N	-0.50349300	-0.15705000	-0.47887400	N	0.74303900	-0.18765900	0.81562700
H	-1.52983800	-0.23471700	-0.63011200	H	1.75937600	-0.25415000	1.02465100
C	0.10047500	-1.36356900	-1.21732400	C	0.11227100	-1.39563900	1.53059600
H	0.26934000	-2.11304700	-0.45729000	H	-0.08400700	-2.12156900	0.75488900
H	-0.68317500	-1.69148100	-1.89702800	H	0.88985900	-1.76099500	2.19676800
C	1.34734000	-1.03063400	-1.98778300	C	-1.12313300	-1.04996200	2.31212600
C	1.20290200	-0.63260600	-3.32314100	C	-0.97185200	-0.66533300	3.65012900
H	0.21064200	-0.65764900	-3.76222400	H	0.02123600	-0.70305800	4.08626300
C	2.28447100	-0.14963300	-4.04757900	C	-2.04899400	-0.17742600	4.37854300
H	2.14928200	0.17144100	-5.07394100	H	-1.91072500	0.13345300	5.40763300
C	3.52916400	-0.04438600	-3.42887800	C	-3.29296300	-0.05368500	3.76160300
H	4.37479900	0.36848000	-3.96853800	H	-4.13363200	0.36313800	4.30594400
C	3.69600500	-0.47709400	-2.11981900	C	-3.46561100	-0.47199600	2.44824900
H	4.65247400	-0.38989600	-1.62595900	H	-4.42150800	-0.36933700	1.95599300
C	2.62160700	-1.01090500	-1.39724600	C	-2.39645300	-1.00984800	1.72179300
C	3.28824100	-2.92803800	0.03502300	C	-3.09011100	-2.90125200	0.26763400
C	3.41065800	-3.26556700	1.52477900	C	-3.17385700	-3.23441900	-1.22555200

H	2.45670900	-3.11820700	2.02831800	H	-2.20174800	-3.10589700	-1.69923500
H	4.14970300	-2.63151700	2.01142600	H	-3.88269500	-2.58450900	-1.73578900
H	3.71030300	-4.31156100	1.63785200	H	-3.49239800	-4.27351100	-1.35020700
C	2.25588400	-3.86386600	-0.60365100	C	-2.09848500	-3.86053900	0.93604000
H	1.30940500	-3.83576000	-0.06132900	H	-1.13479200	-3.85328600	0.42421700
H	2.63356600	-4.88845800	-0.55702900	H	-2.49742200	-4.87621600	0.87477300
H	2.07467400	-3.62283900	-1.65265200	H	-1.94450300	-3.62532700	1.99063900
C	4.65381300	-3.11366900	-0.64742000	C	-4.47869200	-3.05691100	0.90981400
H	5.02867400	-4.12177000	-0.45011600	H	-4.87087800	-4.05539900	0.69799400
H	5.36996000	-2.39448700	-0.24828200	H	-5.16612100	-2.31986800	0.49335100
H	4.58546400	-2.98439900	-1.72953900	H	-4.43795200	-2.93316400	1.99400000
C	-0.04943300	1.17000600	-1.03987500	C	0.25250800	1.14243300	1.33448500
H	-0.27397400	1.13201700	-2.10198900	H	0.40043100	1.11523300	2.40964300
H	1.01839400	1.21336600	-0.87814600	H	-0.80161600	1.18768400	1.09738100
C	-0.75403700	2.32912400	-0.39356800	C	1.00516100	2.29366100	0.72894400
C	-2.04155500	2.66796700	-0.82069700	C	2.28487900	2.59582100	1.20457900
H	-2.47749000	2.10879200	-1.64292200	H	2.67966600	2.01371000	2.03162700
C	-2.75872300	3.67111900	-0.17939300	C	3.04542100	3.59187600	0.60365600
H	-3.76191900	3.91326200	-0.51030200	H	4.04215200	3.80561100	0.97153700
C	-2.19320500	4.33187200	0.90999400	C	2.53197600	4.28302700	-0.49280500
H	-2.75802100	5.09224800	1.43894900	H	3.13120300	5.03875000	-0.98958000
C	-0.90140300	4.02568500	1.32188300	C	1.24836700	4.01339200	-0.95243400
H	-0.45932800	4.51499400	2.17774300	H	0.84590400	4.52671100	-1.81379300
C	-0.15452900	3.04935100	0.65357800	C	0.45822400	3.04324500	-0.32584700
C	2.27617700	3.58951300	0.47318600	C	-1.96572700	3.63092900	-0.20617000
C	2.19314900	5.02588500	1.01662900	C	-1.84561200	5.07346700	-0.72582600
H	2.17666400	5.00933100	2.10651100	H	-1.80853300	5.07406300	-1.81522700
H	1.29799100	5.53805900	0.65524400	H	-0.94766800	5.56219200	-0.33965900
H	3.06556700	5.59757500	0.68796400	H	-2.71286900	5.65675300	-0.40402700
C	3.60377700	2.94092100	0.88075600	C	-3.29285600	3.00928000	-0.65483600
C	3.65256600	1.91293500	0.51884700	H	-3.37127900	1.98144500	-0.29747800
H	3.70858200	2.91891800	1.96481500	H	-3.36604600	2.99196200	-1.74155200
H	4.43840600	3.50783100	0.45699800	H	-4.12905200	3.59027300	-0.25390800
C	2.18141500	3.61527900	-1.05794500	C	-1.90762900	3.63421600	1.32702600
H	1.21716500	3.99141400	-1.40528700	H	-0.94897300	3.99713300	1.70259500
H	2.35470400	2.62877100	-1.49010500	H	-2.09932400	2.64354000	1.74131900
H	2.95808600	4.28129600	-1.44226900	H	-2.68790700	4.30157600	1.70152000
C	-0.30189500	-0.24564900	1.01213100	C	0.61497100	-0.28847300	-0.68330400
H	-0.74733500	0.64601600	1.44299200	H	1.09342100	0.59399300	-1.09800000
H	0.76610100	-0.21197600	1.20987800	H	-0.44238100	-0.24199500	-0.93369100
C	-0.89986300	-1.51204400	1.56943000	C	1.22152500	-1.56949700	-1.19529300
C	-0.11839400	-2.26961600	2.44807700	C	0.46322600	-2.34659200	-2.07707400
H	0.83435100	-1.86113300	2.76621900	H	-0.47733400	-1.94351600	-2.43668900
C	-0.55412300	-3.50966300	2.89861700	C	0.90538900	-3.60085000	-2.47963900
H	0.06867000	-4.08452800	3.57444600	H	0.30099900	-4.19065300	-3.15929100
C	-1.76912800	-4.02151600	2.44666000	C	2.10216700	-4.10640400	-1.97481000
H	-2.09750600	-5.00779800	2.75654900	H	2.43425400	-5.10244400	-2.24736400
C	-2.57107500	-3.26277800	1.60346900	C	2.88042100	-3.33008800	-1.12524200
H	-3.50922700	-3.64900300	1.23262500	H	3.80220900	-3.71220800	-0.71148800
C	-2.16776600	-1.98727000	1.19790400	C	2.47239700	-2.04196400	-0.76727800
C	-4.07499500	-0.38292300	1.10100900	C	4.38701000	-0.44997900	-0.62869500
C	-3.39369900	0.59042000	2.06834300	C	3.75548000	0.51084700	-1.64152500
H	-2.78607200	1.31966500	1.53366100	H	3.13668900	1.25761300	-1.14473800
H	-2.77219800	0.07036100	2.79939600	H	3.15551300	-0.01744200	-2.38475800
H	-4.16277200	1.14083600	2.61566800	H	4.55099300	1.04093200	-2.17099500
C	-5.03445600	-1.30385600	1.87043000	C	5.36740800	-1.39537300	-1.34018200
H	-4.53660500	-1.80005300	2.70557500	H	4.89897400	-1.90312600	-2.18540700
H	-5.44668800	-2.05992100	1.20055000	H	5.74297700	-2.14225500	-0.63903900
H	-5.86138500	-0.71188000	2.27218800	H	6.21697900	-0.82035400	-1.71876200
C	-4.85948100	0.40508600	0.04621100	C	5.13744300	0.35099300	0.44132400
H	-5.44153000	-0.26452700	-0.58539900	H	5.68942700	-0.31219200	1.10575300
H	-4.18491300	0.96557200	-0.59795500	H	4.44274800	0.92725800	1.04887700
H	-5.53876100	1.10255500	0.54424800	H	5.84056900	1.03477000	-0.04254700
Cl	2.50144300	0.08332400	3.23915600	Br	-2.22180500	0.05675000	-3.12470900
Br	-2.68918100	-0.29166400	-3.14103300	Cl	2.77040400	-0.31657600	3.37046200
<b>[L(HClBr)]<sup>-</sup>, 2a, E<sub>0</sub>=-4765.988652 au</b>				<b>[L(HClBr)]<sup>-</sup>, 2b, E<sub>0</sub>=-4765.987683 au</b>			

N	-0.46293600	-0.54634200	0.34273700	N	-0.58449300	-0.81194700	0.52506800
C	-0.38450700	-0.10108200	-1.10225800	C	-1.08348500	-0.59308200	-0.89226000
H	-0.29215200	-0.99751400	-1.70716800	H	-1.39150100	-1.57647100	-1.22984900
H	0.53728700	0.45585400	-1.24213400	H	-0.21626500	-0.27517900	-1.47555700
C	0.12379600	0.47308600	1.28895600	C	0.23098800	0.33359400	1.06874900
H	1.18446900	0.47699600	1.08361700	H	1.08835800	0.46189000	0.41195400
H	-0.07424100	0.09268700	2.28914800	H	0.57484200	0.00716500	2.04641100
C	0.09478600	-1.94923500	0.59709200	C	0.19730100	-2.14102800	0.53182300
H	0.05105900	-2.45922200	-0.35531200	H	0.48946000	-2.30627200	-0.49694200
H	-0.61710300	-2.39474500	1.29108300	H	-0.52908900	-2.88232200	0.86047100
C	-1.58209100	0.72704900	-1.50914400	C	-2.21095100	0.39097700	-1.03899800
C	-1.34716900	1.90304600	-2.22791300	C	-1.95800400	1.62422800	-1.64611400
C	-2.90478500	0.38081100	-1.18800400	C	-3.50303900	0.09765600	-0.58056500
C	-2.39504800	2.73840600	-2.58955700	C	-2.96151100	2.57818200	-1.74848700
H	-0.32696900	2.16354100	-2.47824600	H	-0.95777500	1.83588000	-2.00490500
C	-3.94937500	1.24704500	-1.51674500	C	-4.49807200	1.07476600	-0.65612200
C	-3.69831400	2.41872300	-2.21735800	C	-4.22841400	2.30817500	-1.23561400
H	-2.18558500	3.65389500	-3.13029900	H	-2.74193400	3.54060700	-2.19485800
H	-4.94678800	1.00357000	-1.18098500	H	-5.46436900	0.86810200	-0.21902400
H	-4.51766700	3.08617700	-2.46175100	H	-5.00573000	3.06384100	-1.27786500
C	1.46857100	-1.97810100	1.20647700	C	1.42437100	-2.13876000	1.39940900
C	1.55777300	-2.10955900	2.59769300	C	1.31689000	-2.32532200	2.78172600
C	2.64037200	-1.79956700	0.45464300	C	2.67857000	-1.85405100	0.83272400
C	2.78135300	-2.01706200	3.24857400	C	2.42775400	-2.16886100	3.60220000
C	0.64064900	-2.23499300	3.16375800	H	0.33900600	-2.52611300	3.20512900
C	3.86453200	-1.67139100	1.12142600	C	3.77936200	-1.65341800	1.67110200
C	3.93493500	-1.77579300	2.50478100	C	3.65394000	-1.80516600	3.04676800
H	2.82876500	-2.10210000	4.32797600	H	2.32740100	-2.29698200	4.67380200
H	4.74716500	-1.45547700	0.53765100	H	4.71894500	-1.35087100	1.23118400
H	4.89249000	-1.66583200	3.00230400	H	4.51461700	-1.64019200	3.68609700
C	-0.45050000	1.84815600	1.10983000	C	-0.50313800	1.64005400	1.18883400
C	-1.77313000	2.09405200	1.49106100	C	-1.77193600	1.71777100	1.77265600
C	0.31054700	2.87666200	0.53139100	C	0.10894800	2.80732200	0.70822100
C	-2.35934700	3.32953500	1.25877300	C	-2.45876300	2.92186800	1.80679600
H	-2.34459000	1.29072400	1.94257300	H	-2.23602100	0.82353300	2.17124700
C	-0.29119800	4.11831400	0.29921800	C	-0.60217300	4.01262500	0.72476400
C	-1.61493300	4.33957800	0.65156100	C	-1.87893000	4.06832100	1.26307900
H	-3.39572400	3.49386500	1.52858700	H	-3.45563200	2.95634500	2.22950000
H	0.28249900	4.87891700	-0.20979300	H	-0.14812500	4.88443300	0.27537600
H	-2.07089800	5.30186700	0.44401700	H	-2.42594800	5.00520400	1.25840300
N	-3.14942400	-0.83031200	-0.43896000	N	-3.73031300	-1.18167500	0.03551200
N	1.65316400	2.60523500	0.09972900	N	1.42595300	2.71121900	0.15566800
N	2.55002400	-1.68450500	-0.97234200	N	2.77157100	-1.73341400	-0.59284700
O	-4.15382800	-0.54942400	0.54662300	O	-4.47341600	-0.96525600	1.24495500
H	-3.71038100	-0.80697000	1.39254500	H	-3.82985200	-1.25058200	1.93622700
O	3.50867700	-0.69727500	-1.37354400	O	3.54585200	-0.56689800	-0.89529800
H	3.00290300	-0.07800500	-1.96117200	H	2.95946500	-0.05819800	-1.50895600
O	1.88454500	3.34168000	-1.10761300	O	1.47654000	3.49367900	-1.04242100
H	2.00479000	2.64276300	-1.79620700	H	1.55436200	2.79712700	-1.73511800
C	-3.61258600	-2.02415800	-1.23442800	C	-4.46994200	-2.20469400	-0.77206900
C	2.84447300	-2.94128700	-1.75513700	C	3.36301700	-2.90598100	-1.32024500
C	2.76675900	2.95431600	1.04928900	C	2.57044800	3.11002700	1.03300600
H	-1.47493000	-0.66951300	0.54147300	H	-1.37832900	-0.99000500	1.18038400
C	-2.58910100	-2.33139400	-2.33202800	C	-3.75419000	-2.41233600	-2.11178600
H	-2.43045500	-1.47898600	-2.99442100	H	-3.65388200	-1.47935400	-2.66914700
H	-1.63044400	-2.63212300	-1.90761200	H	-2.76279900	-2.84672600	-1.97171700
H	-2.95703300	-3.16470800	-2.93518600	H	-4.33531300	-3.10934700	-2.72076300
C	-4.99118300	-1.78469700	-1.87038000	C	-5.93219700	-1.80102800	-1.03330000
H	-4.94472500	-1.01641400	-2.64459000	H	-5.99372600	-0.94471800	-1.70800400
H	-5.34840200	-2.70995000	-2.33083500	H	-6.47003000	-2.63415100	-1.49494300
H	-5.70593600	-1.47739800	-1.10679500	H	-6.42146700	-1.54836000	-0.09236700
C	-3.68400900	-3.20503400	-0.25988500	C	-4.42478500	-3.50722600	0.03655200
H	-3.93335900	-4.11981200	-0.80512300	H	-4.87080800	-4.32421200	-0.53834500
H	-2.72896800	-3.34369500	0.24907300	H	-3.39131200	-3.76194000	0.27962800
H	-4.43968700	-3.03289400	0.50494100	H	-4.96825100	-3.39525600	0.97385700
C	4.05937200	2.43727500	0.40565500	C	3.85463300	2.74500500	0.27837700

H	3.96194900	1.37777500	0.16216500	H	3.87182800	1.67719500	0.05651100
H	4.27094300	2.97687500	-0.51686000	H	3.91363000	3.29380000	-0.66101500
H	4.89876800	2.57222800	1.09469600	H	4.72781300	2.99565100	0.88883300
C	2.84968600	4.47280000	1.28079400	C	2.55090500	4.61469200	1.35429600
H	1.96778900	4.84004700	1.81159900	H	1.68604600	4.87800000	1.96755900
H	3.73189300	4.71002800	1.88230400	H	3.45437600	4.89143200	1.90540100
H	2.92811100	4.99187800	0.32548800	H	2.51667700	5.19186700	0.42927100
C	2.56030000	2.24655900	2.39475100	C	2.50787700	2.29880800	2.33309200
H	1.59520600	2.49004800	2.84326700	H	1.58341000	2.48168600	2.88440300
H	2.64777600	1.16357300	2.30234300	H	2.59960900	1.23016200	2.13553800
H	3.34089700	2.57916800	3.08368900	H	3.34452300	2.59153000	2.97277700
C	2.56523400	-2.60896800	-3.22538700	C	3.16653400	-2.63536100	-2.81647100
H	3.23792800	-1.83278100	-3.58674200	H	3.72220700	-1.75202800	-3.12857700
H	2.69239900	-3.50484200	-3.84035800	H	3.51091700	-3.49472000	-3.39956100
H	1.54582000	-2.23718400	-3.34485000	H	2.11409100	-2.44896800	-3.03603600
C	1.90872100	-4.07018300	-1.30768500	C	2.59467900	-4.17379000	-0.92611400
H	2.17775800	-4.98213600	-1.84620000	H	3.00652400	-5.02292900	-1.47709600
H	1.99095400	-4.27542100	-0.23880500	H	2.68017000	-4.38834000	0.14058600
H	0.86757500	-3.84699700	-1.54712600	H	1.53617800	-4.09343300	-1.18147900
C	4.30433200	-3.39388800	-1.58428100	C	4.85889800	-3.09289400	-1.01411800
H	4.51511400	-4.22489500	-2.26310400	H	5.27800700	-3.86225700	-1.66871400
H	4.97763700	-2.57033600	-1.82080500	H	5.39128200	-2.15784400	-1.19057700
H	4.50037600	-3.73268100	-0.56428800	H	5.02052200	-3.40618200	0.01960800
Br	-2.39669300	-1.43269300	3.07212600	Cl	-2.15703600	-1.78868500	3.02738800
Cl	2.10816300	1.19511300	-3.27555700	Br	1.62711800	0.93109200	-3.01078600
<b>[L(HClBr)]<sup>-</sup>, 3a, E<sub>0</sub>=-4765.984915 au</b>				<b>[L(HClBr)]<sup>-</sup>, 3b, E<sub>0</sub>=-4765.981148 au</b>			
N	-0.01988200	-0.00422900	-0.90019200	N	0.00121900	0.00038900	1.36400100
C	0.02920200	1.43532000	-1.38329100	C	-1.03170600	1.00295800	1.84884700
H	-0.78340800	1.93240000	-0.87585100	H	-0.78576100	1.92838200	1.35113000
H	-0.17442800	1.38354700	-2.45415400	H	-0.85376000	1.09284400	2.92142800
C	-1.29978300	-0.67471400	-1.36798600	C	1.38660800	0.39433300	1.84650900
H	-1.31239500	-1.63633000	-0.87818500	H	2.06394800	-0.28270300	1.34919000
H	-1.17488500	-0.80495000	-2.44437600	H	1.37684800	0.19719800	2.91946200
C	1.19218600	-0.77245800	-1.39764400	C	-0.34901500	-1.39541300	1.85003000
H	2.03985100	-0.30549700	-0.92015300	H	-1.27543400	-1.64491500	1.35595500
H	1.22135800	-0.59127600	-2.47350800	H	-0.51184300	-1.28630300	2.92326100
C	1.35832000	2.08422000	-1.13402100	C	-2.43920900	0.55521300	1.58768600
C	2.26070300	2.17335500	-2.20012300	C	-3.15871300	-0.01051400	2.64656700
C	1.74024600	2.53282000	0.14002800	C	-3.01857300	0.62361300	0.31132300
C	3.54874900	2.65585300	-2.00222200	C	-4.42227400	-0.54996400	2.43875200
H	1.94345700	1.81792200	-3.17586300	H	-2.68808200	-0.05420200	3.62390000
C	3.05070300	2.98192800	0.33800500	C	-4.27569700	0.04517700	0.10307300
C	3.94688800	3.03942100	-0.72280000	C	-4.96873400	-0.53910100	1.15661300
H	4.24217300	2.70595900	-2.83367000	H	-4.96248400	-0.99842900	3.26440600
H	3.35584700	3.25639600	1.33690300	H	-4.68167500	0.03985700	-0.89758600
H	4.95953700	3.38718700	-0.54823000	H	-5.94059900	-0.98522600	0.97431300
C	1.10016500	-2.24271300	-1.11555200	C	0.74140900	-2.39061600	1.58474100
C	0.70398300	-3.09175200	-2.15524400	C	1.59384900	-2.73222800	2.64092900
C	1.33040900	-2.77086700	0.16452400	C	0.96831200	-2.92513400	0.30711200
C	0.48785100	-4.44485900	-1.92445300	C	2.69174700	-3.55727100	2.42934600
H	0.53102600	-2.66008400	-3.13640100	H	1.39944300	-2.30333600	3.61912000
C	1.07393600	-4.12692500	0.39646900	C	2.09648700	-3.72547500	0.09513700
C	0.65340800	-4.95461200	-0.63782300	C	2.95155300	-4.03521800	1.14611900
H	0.16753800	-5.08846500	-2.73552500	H	3.35240500	-3.80198100	3.25293600
H	1.18457400	-4.50746000	1.40106400	H	2.30129600	-4.07339700	-0.90645300
H	0.45654300	-6.00236500	-0.43703600	H	3.82282900	-4.65436900	0.96088400
C	-2.52162900	0.14520000	-1.07764400	C	1.70359200	1.83625300	1.58231000
C	-3.08092700	0.89015100	-2.12200300	C	1.57585100	2.74431000	2.63968100
C	-3.06718500	0.23718200	0.21250500	C	2.05269600	2.30076500	0.30493500
C	-4.14143200	1.75709400	-1.88779500	C	1.74353000	4.10757900	2.42945400
H	-2.63983100	0.80483800	-3.11048100	H	1.30261300	2.36078000	3.61787000
C	-4.11039900	1.14002000	0.44660200	C	2.18347900	3.67799600	0.09422100
C	-4.63983600	1.89477600	-0.59354000	C	2.02672500	4.57250400	1.14636000
H	-4.55593200	2.33876400	-2.70297700	H	1.62741700	4.80134900	3.25399000
H	-4.47475400	1.25550400	1.45663000	H	2.38217600	4.03011300	-0.90713300
H	-5.44606900	2.59181400	-0.39106700	H	2.12885300	5.63666800	0.96220000

N	0.79455600	2.46311600	1.21866200	N	-2.28155800	1.23506700	-0.75990500
N	-2.50046100	-0.55292900	1.26958200	N	2.21076700	1.35437600	-0.76458700
N	1.76581300	-1.89418400	1.21559600	N	0.06832400	-2.58971200	-0.76162000
O	1.54558500	2.17430300	2.40679000	O	-2.62474600	0.51522100	-1.95417400
H	1.04655900	1.44352800	2.84403200	H	-1.76535200	0.35297800	-2.40807300
O	1.17260600	-2.37942200	2.42876800	O	0.86086800	-2.52659400	-1.95749400
H	0.79680200	-1.57521000	2.86095200	H	0.57186000	-1.70031900	-2.40980100
O	-2.59845000	0.23151000	2.46727500	O	1.75907400	2.00998100	-1.95965700
H	-1.70667600	0.16025300	2.88481800	H	1.18572600	1.34761700	-2.41072400
C	0.01499900	3.73731800	1.49033700	C	-2.60003700	2.69720900	-1.02092400
C	3.26505400	-1.84503000	1.44940700	C	-1.04089400	-3.59440000	-1.02167600
C	-3.19926600	-1.87186500	1.54905600	C	3.63485600	0.89535500	-1.02628800
H	-0.00796800	-0.00431800	0.12769300	H	-0.00006600	-0.00066400	0.33632800
Br	-0.06827100	-0.01213800	-4.72502600	Cl	0.00542900	0.00293400	5.02714700
Cl	0.05256100	0.01035900	3.93188100	Br	-0.00485500	0.00109900	-3.71444900
C	0.94872700	4.88452400	1.90942000	C	-4.06569100	2.88294700	-1.44586200
H	1.59313200	5.19815000	1.08458300	H	-4.75201400	2.65523500	-0.62676500
H	0.35261700	5.74683500	2.22010400	H	-4.23011200	3.92118700	-1.74646500
H	1.57165600	4.57246700	2.74746400	H	-4.29559600	2.23578300	-2.29197200
C	-0.97118700	3.41426300	2.61806200	C	-2.32318500	3.54077400	0.22912700
H	-1.61448400	4.28046000	2.79950900	H	-2.87075600	3.18379100	1.10329600
H	-1.59624100	2.56228700	2.34737800	H	-1.25754800	3.58136700	0.45925200
H	-0.44829700	3.16934100	3.54158700	H	-2.64878900	4.56472300	0.02995800
C	-0.78142600	4.15730200	0.24934300	C	-1.65823700	3.15734800	-2.13862700
H	-0.14797100	4.28054700	-0.63103400	H	-1.79196000	4.22951700	-2.31027800
H	-1.58051700	3.44898900	0.02560000	H	-0.61911900	2.97278000	-1.86277700
H	-1.25347800	5.12122500	0.45507500	H	-1.85844800	2.62842300	-3.06937000
C	-2.39375500	-2.56838900	2.65108600	C	4.53074100	2.06907500	-1.45403600
H	-2.80900000	-3.56420400	2.83257600	H	4.67936100	2.77824300	-0.63619400
H	-1.34937200	-2.67183700	2.35391000	H	5.51084500	1.68968000	-1.75534300
H	-2.42521900	-2.00302200	3.58148900	H	4.08525800	2.59143500	-2.30034800
C	-4.65009600	-1.64920000	2.00642700	C	4.22701200	0.23403200	0.22397100
H	-5.26710300	-1.24652100	1.19949600	H	4.19391400	0.88763100	1.09755200
H	-5.08459800	-2.60172000	2.32167900	H	3.72793700	-0.70801800	0.45566000
H	-4.67491500	-0.95967700	2.85000100	H	5.27590400	0.00174700	0.02388700
C	-3.19071600	-2.76225500	0.30085800	C	3.55886200	-0.15201300	-2.14215200
H	-3.63841000	-2.27131900	-0.56522400	H	4.55330800	-0.57411400	-2.31486800
H	-2.18181300	-3.09329700	0.04997500	H	2.87876400	-0.95808900	-1.86351800
H	-3.77968500	-3.65756600	0.51481900	H	3.19992500	0.28486400	-3.07297300
C	3.50118800	-0.80778600	2.55252000	C	-1.91185100	-3.00593500	-2.13656100
H	4.57647300	-0.67373200	2.70366800	H	-2.77446500	-3.65671800	-2.30777900
H	3.06277500	0.15175400	2.27530200	H	-2.27011000	-2.01397500	-1.85798800
H	3.05409000	-1.12411700	3.49398200	H	-1.35539200	-2.91358700	-3.06820000
C	3.99445200	-1.38515000	0.18160700	C	-0.47185400	-4.95678500	-1.44970200
H	3.76709600	-2.01338800	-0.68166000	H	0.06862600	-5.43974300	-0.63209400
H	3.76937000	-0.34454000	-0.05679400	H	-1.29032900	-5.61631500	-1.75045800
H	5.07022600	-1.44888300	0.36303700	H	0.20278800	-4.83198300	-2.29638000
C	3.80843400	-3.21700600	1.88083600	C	-1.90774400	-3.77675900	0.22987000
H	3.74134000	-3.94724700	1.07078800	H	-1.32349700	-4.07315500	1.10293300
H	4.86009900	-3.12137700	2.16421800	H	-2.47505200	-2.87411300	0.46138800
H	3.24938500	-3.58758000	2.73985900	H	-2.63239800	-4.57027800	0.03152200
<b>[L(HClBr)]<sup>-</sup>, 4a, E<sub>0</sub>=-4765.978875 au</b>				<b>[L(HClBr)]<sup>-</sup>, 4b, E<sub>0</sub>=-4765.976076 au</b>			
N	0.40107500	-0.58436600	0.79704900	N	0.82342900	-0.52735400	1.22561300
C	-0.89820900	-1.35312800	1.00490800	C	-0.22820600	-1.55462600	1.62981300
H	-1.64933300	-0.58800300	1.12992400	H	-1.15200500	-0.99748400	1.66873400
H	-0.75356200	-1.91128300	1.93323500	H	0.07060100	-1.88694800	2.62686600
C	0.66308000	0.29652800	2.01221700	C	0.86443900	0.58628000	2.26604100
H	1.57382300	0.84298200	1.78767500	H	1.59747200	1.29949300	1.90327700
H	0.81142700	-0.39539100	2.84409800	H	1.20075200	0.10456600	3.18658400
C	1.56295300	-1.52048700	0.56062200	C	2.18716400	-1.16152700	1.08042600
H	1.26894100	-2.14498200	-0.26974200	H	2.05599800	-1.98265100	0.39138000
H	1.63627600	-2.12921600	1.46522800	H	2.43057100	-1.55395200	2.07082400
C	-1.24176900	-2.25703800	-0.14144100	C	-0.33619700	-2.70027400	0.66805500
C	-0.73503500	-3.56283800	-0.16233100	C	0.48817400	-3.81970200	0.83977100
C	-2.05464300	-1.81631700	-1.19916500	C	-1.24245000	-2.67030400	-0.40484300
C	-0.94228600	-4.39039400	-1.25891500	C	0.49120700	-4.85209700	-0.08993200



H	-0.16533200	-3.91038700	0.69317800	H	1.13522000	-3.85593600	1.70986200
C	-2.21669200	-2.63757700	-2.32159700	C	-1.19671500	-3.68904400	-1.36416600
C	-1.65652800	-3.90802900	-2.35536900	C	-0.33052600	-4.76424100	-1.21330600
H	-0.53412800	-5.39441000	-1.26569300	H	1.14288600	-5.70666400	0.05033200
H	-2.77678300	-2.25402900	-3.16192800	H	-1.84249600	-3.61245300	-2.22674200
H	-1.79381000	-4.53071700	-3.23285200	H	-0.31025500	-5.54524300	-1.96570500
C	2.84935800	-0.80407400	0.27329200	C	3.23181000	-0.20227600	0.59096200
C	3.83945100	-0.77282200	1.26026100	C	4.20976800	0.24151800	1.48654700
C	3.07215200	-0.15688200	-0.95244200	C	3.23994300	0.26837800	-0.73186200
C	5.02971000	-0.08539300	1.05184900	C	5.17362900	1.16162800	1.09049600
H	3.64749800	-1.27877600	2.20062100	H	4.18446400	-0.13184300	2.50470700
C	4.25829000	0.55745800	-1.14333800	C	4.19363300	1.21617300	-1.11459900
C	5.23014400	0.59102600	-0.15036300	C	5.15403100	1.65723200	-0.21206500
H	5.78493100	-0.06031800	1.82890100	H	5.91957100	1.50479900	1.79801900
H	4.38511600	1.11478000	-2.06001900	H	4.14190400	1.62738100	-2.11211800
H	6.14386800	1.15217300	-0.31387100	H	5.88499600	2.39471500	-0.52557300
C	-0.47591700	1.24050900	2.25113800	C	-0.48286300	1.22613600	2.41410500
C	-1.42382000	0.96695700	3.23957500	C	-1.30706800	0.89348000	3.49154600
C	-0.62142100	2.37652400	1.43758700	C	-0.95002500	2.10191600	1.42158900
C	-2.52716700	1.79858400	3.40216200	C	-2.60112100	1.39881300	3.56511700
H	-1.29107000	0.08936100	3.86330200	H	-0.92835100	0.21831000	4.25132600
C	-1.75711900	3.17829400	1.57390900	C	-2.26908500	2.55966300	1.47148000
C	-2.70044300	2.89216000	2.55626500	C	-3.08660600	2.21203200	2.54294100
H	-3.26094300	1.57956500	4.16939200	H	-3.23800700	1.13415100	4.40145400
H	-1.92322000	3.99253400	0.88493700	H	-2.66762700	3.13930400	0.65218500
H	-3.58215400	3.51641300	2.64665300	H	-4.11139600	2.56471700	2.56751500
N	-2.69930500	-0.54206000	-1.09564500	N	-2.19557300	-1.60329600	-0.47927600
N	0.42587100	2.60521600	0.48870900	N	-0.01406300	2.43434600	0.38689600
N	2.01769000	-0.16756600	-1.93302100	N	2.19435300	-0.16503800	-1.62292600
O	-2.73343700	0.02394800	-2.41279600	O	-2.37956000	-1.29974200	-1.87012500
H	-2.51733100	0.97622800	-2.28018700	H	-2.43380300	-0.31935500	-1.91106800
O	1.94083600	1.14826500	-2.50712400	O	1.77895100	0.97553600	-2.39202100
H	1.22775400	1.55275300	-1.96936400	H	0.97921200	1.26373000	-1.90308400
O	0.08704900	1.98409000	-0.75707200	O	-0.24982400	1.60889600	-0.75870800
H	-0.74679900	2.40417600	-1.14255700	H	-1.15726600	1.78515200	-1.15186800
C	-4.12344000	-0.59237800	-0.57324400	C	-3.55594300	-1.93130300	0.11034200
C	2.14365900	-1.12203100	-3.08570200	C	2.52752900	-1.24101500	-2.61867200
C	1.07479000	3.93415400	0.34686500	C	0.27908200	3.85637500	0.06441000
H	0.29344500	0.02892300	-0.02745900	H	0.55241500	-0.11949700	0.31727400
C	-4.16687600	-1.29817600	0.78811700	C	-3.40551200	-2.38635800	1.56760600
H	-3.61419200	-0.74489800	1.54842700	H	-3.00845300	-1.59168000	2.20043100
H	-5.20845700	-1.34832700	1.11498600	H	-4.39646200	-2.64280700	1.95026900
H	-3.78339500	-2.31860600	0.74202600	H	-2.77203000	-3.26914900	1.66643200
C	-4.57187200	0.86090300	-0.38976100	C	-4.36867500	-0.63364700	0.08024600
H	-3.87755700	1.39180400	0.26286500	H	-3.83763500	0.15742400	0.61115800
H	-4.60093100	1.39394900	-1.33848100	H	-4.53786800	-0.28763000	-0.93803300
H	-5.56965700	0.88352000	0.05899000	H	-5.33732800	-0.79525000	0.56286000
C	-5.06030600	-1.31796400	-1.55279200	C	-4.27498700	-3.02652800	-0.69390200
H	-6.09453200	-1.21837700	-1.21213700	H	-5.29726800	-3.13997500	-0.32306400
H	-4.97570200	-0.87651300	-2.54552400	H	-4.31510500	-2.75066900	-1.74737700
H	-4.82702000	-2.38347400	-1.61531900	H	-3.77224300	-3.99153900	-0.59649900
C	0.25485400	4.99731200	-0.40446500	C	-0.85385300	4.62864200	-0.63499600
H	-0.59442800	5.35109900	0.18095600	H	-1.67366500	4.85522400	0.04806600
H	0.89162600	5.86159600	-0.61644800	H	-0.46552900	5.58091800	-1.00851200
H	-0.12955400	4.61109800	-1.34844700	H	-1.25894000	4.06816500	-1.47883300
C	1.39757200	4.41176600	1.77096200	C	0.63383800	4.52657200	1.40065100
H	0.49412500	4.62050000	2.34552600	H	-0.21718800	4.54135300	2.08358600
H	1.98066900	3.65906300	2.30703000	H	1.45973800	4.00305500	1.88796000
H	1.98638500	5.33040600	1.71511700	H	0.93942500	5.55909300	1.21509600
C	2.39814800	3.69893700	-0.39888100	C	1.52350400	3.86240500	-0.83483000
H	2.98675300	4.62062300	-0.40019600	H	1.87591500	4.88995400	-0.95983900
H	2.97475000	2.91012100	0.08676000	H	2.32094600	3.26541800	-0.39070400
H	2.23061900	3.40319400	-1.43281200	H	1.30614700	3.45712200	-1.82164700
C	0.85352300	-0.98627100	-3.90409900	C	1.22835800	-1.55222600	-3.37218800
H	0.82647500	-1.75451500	-4.68229000	H	1.37309200	-2.42788900	-4.01153900
H	-0.02033900	-1.10785700	-3.26329200	H	0.41920100	-1.76170200	-2.67214800

H	0.79429200	-0.00557500	-4.37351700	H	0.92822700	-0.70865700	-3.99173000
C	3.36568900	-0.79912800	-3.96329900	C	3.61666900	-0.78650200	-3.60582800
H	4.30090100	-0.99011400	-3.43162600	H	4.58030900	-0.65794700	-3.10713700
H	3.35124500	-1.42847800	-4.85727700	H	3.73932700	-1.54094400	-4.38764700
H	3.34133200	0.24509700	-4.27567000	H	3.33141600	0.15463100	-4.07645200
C	2.25934600	-2.55591300	-2.55866400	C	2.99884900	-2.49888000	-1.88289000
H	3.08389800	-2.66765200	-1.85106100	H	3.84101600	-2.29407400	-1.21803500
H	1.33185800	-2.88526100	-2.09083200	H	2.18893200	-2.95513200	-1.31459400
H	2.45254800	-3.22289200	-3.40240400	H	3.33028200	-3.23202300	-2.62229300
Cl	-2.30105100	3.08492700	-2.09424500	Cl	1.83640700	-1.99963700	4.40738700
Br	0.85027400	-2.85829400	3.82247100	Br	-2.95949600	1.92502800	-2.26409300
<b>[L(HCIBr)]<sup>-</sup>, 5a, E<sub>0</sub> = -4765.976441 au</b>				<b>[L(HCIBr)]<sup>-</sup>, 5b, E<sub>0</sub> = -4765.974674 au</b>			
N	-0.96507800	0.12764000	0.73925400	N	-1.26145800	0.11016800	1.20636500
C	-0.52662700	-0.62221000	1.98137500	C	-0.61683400	-0.70133300	2.31244800
H	-0.53800900	-1.67018500	1.71193800	H	-0.67428900	-1.73330600	1.99185500
H	-1.29745100	-0.42462600	2.72958200	H	-1.24943900	-0.55046000	3.18980700
C	-2.25802400	-0.43322800	0.19078500	C	-2.62757700	-0.43643100	0.85537700
H	-2.50871600	0.18723900	-0.65755200	H	-3.02282600	0.22880500	0.10114800
H	-2.99843500	-0.28344900	0.98091100	H	-3.21862100	-0.34239800	1.77016100
C	-1.10592900	1.61059600	1.04015200	C	-1.35637000	1.57179600	1.61154200
H	-0.15526400	1.91173000	1.46031800	H	-0.35087300	1.86158800	1.88727100
H	-1.89590400	1.67786400	1.79224900	H	-2.01270100	1.58378800	2.48505400
C	0.83386500	-0.16811500	2.41769400	C	0.79905200	-0.26042100	2.53437000
C	0.95301900	0.65196200	3.54387300	C	1.11017400	0.49695100	3.66774300
C	1.97650800	-0.49484600	1.67062700	C	1.79816400	-0.53684400	1.58796000
C	2.18935200	1.17000800	3.91225900	C	2.39225800	1.00285400	3.84956200
H	0.05951600	0.89462400	4.10876900	H	0.32641200	0.70110100	4.38898100
C	3.20893600	0.06373600	2.02041100	C	3.07348800	0.00983900	1.75435300
C	3.31125200	0.88799800	3.13585200	C	3.36573400	0.77219200	2.88007400
H	2.27168200	1.80708000	4.78552200	H	2.62282100	1.59141400	4.73028200
H	4.07761000	-0.12273300	1.39956600	H	3.82558000	-0.13495100	0.98666900
H	4.27428500	1.31593500	3.39038800	H	4.35900400	1.19227000	2.99060200
C	-1.43531300	2.38330000	-0.20172600	C	-1.88769100	2.40931400	0.48683300
C	-2.75902500	2.76122100	-0.44993900	C	-3.23467100	2.78657700	0.48360700
C	-0.44138200	2.66717500	-1.14945200	C	-1.06589800	2.75851400	-0.59466600
C	-3.10601900	3.36865100	-1.65134600	C	-3.77758600	3.45881500	-0.60545200
H	-3.51091700	2.54391900	0.30151400	H	-3.85104600	2.51782500	1.33491800
C	-0.80643000	3.23154300	-2.37506200	C	-1.63018600	3.38981000	-1.70687000
C	-2.12958300	3.57811100	-2.62429000	C	-2.97666000	3.73584300	-1.71248000
H	-4.13555500	3.65086600	-1.83846400	H	-4.82435800	3.73965300	-0.60225200
H	-0.05003400	3.37609100	-3.13260200	H	-1.00999800	3.58680500	-2.56910500
H	-2.39852700	4.01381700	-3.58018800	H	-3.40102000	4.22385100	-2.58291400
C	-2.13502800	-1.88048300	-0.18325500	C	-2.56578300	-1.85756900	0.37916700
C	-2.76249100	-2.82815800	0.63312400	C	-3.04273300	-2.85914800	1.23220500
C	-1.37977400	-2.30848400	-1.28687900	C	-2.01095300	-2.21178700	-0.86119100
C	-2.62675400	-4.18818000	0.38292500	C	-2.95100600	-4.20053100	0.88161800
H	-3.33364300	-2.47480900	1.48524300	H	-3.45992500	-2.56311900	2.18885400
C	-1.22608200	-3.67947600	-1.51477700	C	-1.89790000	-3.56522400	-1.19394100
C	-1.84302000	-4.61080000	-0.68879200	C	-2.36301200	-4.55058000	-0.33204200
H	-3.10790400	-4.91037400	1.03200900	H	-3.31294400	-4.96494800	1.55915000
H	-0.59369000	-4.00114400	-2.32881500	H	-1.41478800	-3.83141500	-2.12224600
H	-1.70566300	-5.66925400	-0.88063200	H	-2.26006400	-5.59422500	-0.60804400
N	1.80999000	-1.39561800	0.55488800	N	1.44329400	-1.37520800	0.46768700
N	-0.72293500	-1.32264000	-2.11522500	N	-1.50697700	-1.17232500	-1.73006000
N	0.91549400	2.33215800	-0.81340700	N	0.32850400	2.41900200	-0.51136900
O	2.30967000	-0.79069600	-0.65120800	O	1.73207600	-0.69790000	-0.76901400
H	3.33238000	-0.73830400	-0.67763300	H	2.72775200	-0.64220800	-0.96584700
O	1.48463700	1.62397700	-1.92696400	O	0.70366300	1.79101400	-1.74910000
H	1.80563700	0.80427000	-1.50567800	H	1.09642300	0.95277500	-1.44231300
O	0.54885500	-1.86505400	-2.50992800	O	-0.32185100	-1.67780700	-2.36915800
H	1.19461900	-1.42816700	-1.91684200	H	0.41537500	-1.26983300	-1.87109700
C	2.34297400	-2.79925500	0.78148600	C	2.00299300	-2.78562100	0.51847400
C	1.81185300	3.49679300	-0.48041700	C	1.26645400	3.57167900	-0.25916800
C	-1.43148600	-0.97410600	-3.40453800	C	-2.42638000	-0.75638500	-2.85598800
C	3.15842800	2.91078600	-0.04934600	C	2.66830000	2.97747600	-0.10437600
H	3.82967400	3.71719100	0.25874000	H	3.37947000	3.77025600	0.14351100

H	3.02062700	2.23674900	0.79293900	H	2.67738200	2.24400800	0.69853600
H	3.63913400	2.35287300	-0.85201200	H	3.00917100	2.48476900	-1.01414000
C	2.01934500	4.44648300	-1.67195100	C	1.26498000	4.60017000	-1.40229500
H	1.11074300	4.99970000	-1.91794200	H	0.32580200	5.15468200	-1.45323300
H	2.79661600	5.17386900	-1.42392100	H	2.07063000	5.32102900	-1.24102700
H	2.34695100	3.88203200	-2.54597300	H	1.44159000	4.09933800	-2.35510500
C	1.18925100	4.25841800	0.69578100	C	0.85261300	4.24624700	1.05419300
H	0.19975500	4.65172700	0.45399300	H	-0.16590400	4.63772200	1.01294900
H	1.11081200	3.62193600	1.57919600	H	0.93196200	3.55364600	1.89420200
H	1.83405100	5.10279400	0.95092700	H	1.52724800	5.08331700	1.24914900
C	-0.54097100	0.02867000	-4.14715800	C	-1.67728400	0.29924800	-3.67710200
H	-1.09871000	0.45951700	-4.98380500	H	-2.37006700	0.77283200	-4.37882000
H	-0.22431000	0.82610000	-3.47808100	H	-1.25295000	1.05886800	-3.02394700
H	0.35265200	-0.45888800	-4.53377700	H	-0.86179300	-0.15342600	-4.23907800
C	-2.77552800	-0.31371800	-3.08530900	C	-3.69647900	-0.13153200	-2.27231000
H	-3.41046000	-0.95178300	-2.46709200	H	-4.21586000	-0.81251100	-1.59486900
H	-2.63708500	0.64953200	-2.59452600	H	-3.47664600	0.80189500	-1.75438800
H	-3.30575100	-0.13054200	-4.02304900	H	-4.37934500	0.10181700	-3.09284800
C	-1.66313800	-2.21183800	-4.28787500	C	-2.80411900	-1.94197300	-3.76003600
C	-2.05415200	-1.89412600	-5.25817600	H	-3.35594500	-1.57163900	-4.62817000
H	-0.72362300	-2.73973300	-4.45498800	H	-1.90642300	-2.44793400	-4.11699600
H	-2.38426700	-2.90010200	-3.84204700	H	-3.43731700	-2.66392900	-3.24013900
C	3.72679700	-2.86373800	1.45203800	C	3.47878600	-2.87798700	0.94455800
H	3.70778700	-2.45948900	2.46558400	H	3.62978400	-2.53380900	1.96909400
H	4.02840500	-3.91319600	1.51828600	H	3.78566100	-3.92686900	0.89695600
H	4.47941800	-2.33244000	0.86736700	H	4.12548000	-2.30788900	0.27508000
C	2.42043500	-3.52710700	-0.56342900	C	1.85409900	-3.43263200	-0.86137100
H	2.66832200	-4.57456800	-0.37247100	H	2.12460100	-4.48828300	-0.77542400
H	1.47286200	-3.48352800	-1.09325400	H	0.83261600	-3.36238800	-1.22490200
H	3.19979500	-3.10236900	-1.19628900	H	2.52165100	-2.96856800	-1.58779500
C	1.30863100	-3.50038100	1.67411800	C	1.13015600	-3.54491700	1.52837300
H	1.18665000	-2.98336500	2.62889200	H	1.17151200	-3.08546400	2.51882000
H	0.34136100	-3.56397000	1.17309900	H	0.09238700	-3.58595500	1.19372800
H	1.64852700	-4.51616700	1.89143900	H	1.49885900	-4.56918100	1.62550200
H	-0.24122900	-0.00012300	0.02123500	H	-0.66952400	0.03303400	0.37026600
Cl	5.20212200	-0.47436100	-0.89883000	Br	4.68848700	-0.30928000	-1.58251100
Br	-3.74607200	0.55227300	3.28287700	Cl	-3.47558700	0.34235500	4.07710800
<b>[L(HClBr)]<sup>-</sup>, 6a, E<sub>0</sub>=-4765.974568 au</b>				<b>[L(HClBr)]<sup>-</sup>, 6b, E<sub>0</sub>=-4765.974664 au</b>			
O	1.25425800	-1.59584300	-0.15615800	O	-1.17799200	1.14114200	-0.70193700
O	-2.55407100	-1.40606200	-2.71979500	O	2.83044200	-0.59784300	-2.41044500
O	3.37048200	-0.29898700	-1.27228900	O	-3.26461400	-0.59886500	-0.97683600
N	1.24385700	-2.50162700	0.94639600	N	-1.20917000	2.51934800	-0.32760000
N	-2.63368500	-1.13131400	-1.31852600	N	2.79544100	0.01846000	-1.11932500
N	2.78824800	1.01696400	-1.12098800	N	-2.74458000	-1.56148900	-0.03017500
N	-0.13695800	1.31797700	0.92831900	N	0.06757800	-0.59200400	1.97627000
C	1.03601000	0.58772800	1.58948600	C	-1.10256600	0.39280500	2.00452600
C	0.55779700	-0.55641900	2.44978700	C	-0.61974700	1.82215400	2.05491200
C	-0.06607700	-0.19788300	3.65410000	C	-0.04478700	2.23522100	3.26609000
C	-0.67714300	-1.13490200	4.47528100	C	0.55999700	3.47623200	3.40810700
C	-0.70157700	-2.46877700	4.07828200	C	0.62727500	4.32741800	2.30880600
C	-0.08542100	-2.84434600	2.89340500	C	0.06001900	3.93879700	1.10382500
C	0.59257400	-1.92210400	2.08141600	C	-0.60899700	2.71427300	0.95759900
C	2.63546400	-3.03376500	1.17469200	C	-2.60432200	3.05912900	-0.50369800
C	3.60066600	-1.94321800	1.67061300	C	-3.60268200	2.43039800	0.48357600
C	2.57630700	-4.16320100	2.21304300	C	-2.57927200	4.57992500	-0.29383700
C	3.11465700	-3.63413900	-0.15453200	C	-3.01667000	2.78490400	-1.95669300
C	-1.22826800	0.36708100	0.53270200	C	1.20636600	-0.07579200	1.14858300
C	-2.42583500	0.97781400	-0.13400800	C	2.41490900	-0.96270900	1.06992600
C	-2.89945800	2.25769300	0.16641800	C	2.81240300	-1.80650300	2.11069200
C	-3.91616600	2.82501200	-0.59517600	C	3.84465100	-2.71912900	1.91780600
C	-4.46371700	2.11599400	-1.66451000	C	4.48437400	-2.79582000	0.68071500
C	-4.04662600	0.81531700	-1.92367400	C	4.14359800	-1.90934800	-0.33453800
C	-3.06119200	0.21907400	-1.13284600	C	3.14279500	-0.95559000	-0.13289900
C	-3.47707000	-2.18997900	-0.66336100	C	3.65115800	1.25633200	-1.15295000
C	-4.87813800	-2.26823600	-1.29341600	C	5.09690000	0.93534200	-1.56852800
C	-2.74217600	-3.52273400	-0.84424000	C	3.01349900	2.21525600	-2.16378900

C	-3.59588700	-1.89225700	0.83620700	C	3.64168900	1.92063900	0.22900500
C	0.34606700	2.29661800	-0.13298500	C	-0.40863200	-2.00722000	1.68269200
C	0.48683700	1.75346300	-1.53258100	C	-0.45900500	-2.41014200	0.23018600
C	-0.58905100	1.89965900	-2.41569600	C	0.65210700	-3.05983600	-0.31954500
C	-0.56956300	1.32981300	-3.68152300	C	0.71913500	-3.36036500	-1.67343100
C	0.54414600	0.60571100	-4.08948200	C	-0.34133400	-3.01868800	-2.50392100
C	1.65152600	0.51374500	-3.25856600	C	-1.48319300	-2.44222800	-1.96590600
C	1.64821100	1.11130100	-1.99719500	C	-1.56744300	-2.16691700	-0.60023000
C	3.90672500	1.98173800	-1.36046100	C	-3.88875300	-2.47444200	0.28237200
C	3.36131500	3.41274900	-1.29589700	C	-3.40744900	-3.58251700	1.22564500
C	4.59337800	1.76092700	-2.72053100	C	-4.49529400	-3.11140200	-0.98110500
C	4.91486800	1.77274200	-0.22230200	C	-4.94414300	-1.62209400	0.99999700
H	-0.49468800	1.96814000	1.69099900	H	0.36880000	-0.65961800	3.00092100
H	1.71594600	0.30153400	0.80458300	H	-1.73205100	0.16663200	1.16007600
H	1.49945800	1.35363000	2.21295000	H	-1.62912800	0.14584100	2.92740400
H	-0.10327600	0.85525200	3.91692100	H	-0.04097200	1.53499600	4.09597800
H	-1.15705400	-0.81782900	5.39353500	H	1.00185300	3.75632300	4.35698900
H	-1.21778600	-3.21345000	4.67413300	H	1.13866000	5.28114500	2.37871000
H	-0.13392300	-3.86884300	2.55233600	H	0.13981500	4.57137300	0.23086500
H	3.26090900	-1.52679200	2.62227800	H	-3.30903700	2.63411100	1.51643000
H	3.70011400	-1.13669700	0.94570900	H	-3.68123300	1.35373600	0.34180200
H	4.59496800	-2.37182200	1.82620600	H	-4.59728800	2.85748100	0.32599600
H	2.27760400	-3.80363100	3.19804900	H	-2.32612400	4.85100400	0.73148000
H	3.57183600	-4.60467800	2.30336700	H	-3.57345200	4.97747600	-0.51206500
H	1.88181000	-4.94396300	1.89644500	H	-1.86438400	5.05232900	-0.97046500
H	2.36314700	-4.31821600	-0.55225300	H	-2.24324800	3.13759200	-2.64109100
H	4.04655000	-4.18122400	0.01224400	H	-3.95236000	3.30827400	-2.17130300
H	3.30117000	-2.87712900	-0.91347200	H	-3.17076800	1.72641500	-2.15612600
H	-1.51961400	-0.12453400	1.45596100	H	1.46771600	0.87878500	1.59459800
H	-0.80040900	-0.38670400	-0.12192000	H	0.83885600	0.12029200	0.14512400
H	-2.45444900	2.82471700	0.97875900	H	2.29774800	-1.76939000	3.06584300
H	-4.26222000	3.82626300	-0.36533900	H	4.13124000	-3.38181800	2.72637900
H	-5.23024000	2.56975500	-2.28377800	H	5.26355500	-3.53211200	0.51438400
H	-4.45940000	0.24996400	-2.74748500	H	4.62977500	-1.95123700	-1.29911800
H	-4.78991900	-2.38781600	-2.37391500	H	5.09681500	0.38214000	-2.50853600
H	-5.46157900	-1.36904100	-1.08143800	H	5.60927800	0.34270900	-0.80698100
H	-5.42146200	-3.12747900	-0.89000900	H	5.65822900	1.86323300	-1.71027200
H	-3.28678500	-4.31585600	-0.32234100	H	3.56114500	3.16286500	-2.16587400
H	-1.72949000	-3.45752200	-0.44465300	H	1.97011900	2.40243200	-1.90776300
H	-2.65828600	-3.78513400	-1.89752500	H	3.02935500	1.79592300	-3.16837600
H	-2.62119900	-1.93513500	1.32369800	H	2.63884000	2.25505100	0.49730100
H	-4.22841200	-2.65595100	1.29595000	H	4.28602700	2.80295200	0.19755200
H	-4.05139700	-0.91937000	1.03031400	H	4.01997000	1.25828100	1.00987300
H	1.27692200	2.68404900	0.26364900	H	-1.37407300	-2.07347000	2.17003100
H	-0.37581200	3.10944300	-0.11910000	H	0.27500500	-2.65621200	2.22446500
H	-1.46923200	2.43572200	-2.08922500	H	1.49209800	-3.29696500	0.31840400
H	-1.44102900	1.40991200	-4.31889600	H	1.61667100	-3.80990000	-2.07906600
H	0.54742100	0.09145600	-5.04245200	H	-0.27583400	-3.17495300	-3.57334800
H	2.50670400	-0.07684800	-3.54941200	H	-2.29601300	-2.13717000	-2.60685000
H	2.97468500	3.65256400	-0.30421800	H	-3.08239400	-3.18097400	2.18665800
H	2.57243900	3.57823900	-2.03123600	H	-2.58943800	-4.15769900	0.78928200
H	4.17571000	4.10885600	-1.51051100	H	-4.23800000	-4.26626600	1.41679800
H	3.91608300	1.99105300	-3.54504900	H	-3.78766100	-3.79299100	-1.45670100
H	4.92264200	0.72669600	-2.81755400	H	-4.77457300	-2.34118200	-1.69953100
H	5.46506300	2.41623300	-2.80301200	H	-5.38898500	-3.68165800	-0.71240600
H	5.71820700	2.51147900	-0.29141300	H	-5.77180200	-2.25288900	1.33606300
H	5.34794600	0.77447900	-0.27098300	H	-5.33420400	-0.85288000	0.33472500
H	4.41697700	1.88645600	0.74341300	H	-4.50066400	-1.13316700	1.87047200
H	0.83843400	-2.08347600	-0.93463300	H	-0.71705800	1.09908700	-1.59154300
H	-1.63353100	-1.75169600	-2.81211400	H	1.94079400	-0.37859500	-2.77365600
H	2.68388400	-0.86834500	-0.86269400	H	-2.58407600	0.10625300	-0.94035100
Cl	0.26045600	-2.73988600	-2.69545700	Br	-0.03212700	0.55476100	-3.54953500
Br	-0.72165400	3.50460500	3.11150700	Cl	0.50822500	-0.97967100	4.90330300
<b>[L(HClBr)]<sup>-</sup>, 7a, E<sub>0</sub>=-4765.972285 au</b>				<b>[L(HClBr)]<sup>-</sup>, 7b, E<sub>0</sub>=-4765.972479 au</b>			
N	-0.30674900	-0.07051100	-0.05900800	N	-0.52159700	-0.31425600	0.24830400
C	-0.78249500	0.34292200	-1.42833500	C	-1.06252400	0.05913600	-1.10814900

H	-0.02341700	0.00655300	-2.12758600	H	-0.32355800	-0.26887600	-1.83293000
H	-0.77893400	1.42410800	-1.48439300	H	-1.09110900	1.13855000	-1.18372500
C	-1.01738700	0.60132500	1.12805700	C	-1.19895900	0.36799300	1.44970600
H	-0.22158200	0.99321200	1.74864100	H	-0.38992500	0.81186800	2.01532000
H	-1.52055700	-0.19460800	1.67894800	H	-1.64155400	-0.43075800	2.04599000
C	1.18038600	0.09277700	0.02555100	C	0.96329900	-0.11656400	0.27085300
H	1.35130500	1.14907000	0.21331400	H	1.11709800	0.95034400	0.40856300
H	1.59954100	-0.09856800	-0.96098000	H	1.35267600	-0.34105100	-0.72150200
C	-2.13625700	-0.21788600	-1.76486000	C	-2.41435000	-0.54172600	-1.37680200
C	-3.04961400	0.63715400	-2.38817500	C	-3.37143400	0.27539000	-1.98519800
C	-2.51995100	-1.54086900	-1.48598200	C	-2.75577500	-1.86436000	-1.04692400
C	-4.32652000	0.20901800	-2.71956400	C	-4.65078900	-0.18954500	-2.25082700
H	-2.75483400	1.66383400	-2.57028000	H	-3.10774700	1.30258400	-2.20759700
C	-3.82278800	-1.95334900	-1.78129700	C	-4.06025600	-2.31280600	-1.27442000
C	-4.71643800	-1.09004800	-2.39993600	C	-4.99809900	-1.48678200	-1.87842000
H	-5.02353000	0.89477200	-3.18677300	H	-5.38176900	0.46731000	-2.70757200
H	-4.12315900	-2.94494600	-1.47802900	H	-4.32449200	-3.30166800	-0.93104800
H	-5.72261700	-1.42895800	-2.62060700	H	-6.00487500	-1.85295100	-2.04677600
C	1.86687000	-0.79897600	1.01716500	C	1.70458200	-0.94638700	1.27840600
C	1.19959900	-1.51217900	2.00864000	C	1.08169700	-1.65995000	2.29861000
C	3.27138500	-0.94083900	0.87065300	C	3.11268000	-1.02921800	1.12032100
C	1.88818600	-2.36948100	2.86566900	C	1.81831600	-2.45463500	3.17588300
H	0.12457300	-1.45521000	2.13239600	H	0.00666600	-1.65226700	2.43179300
C	3.94824500	-1.78110200	1.76030200	C	3.83664900	-1.80502600	2.03117300
C	3.26315700	-2.49769800	2.74012100	C	3.19658800	-2.51987000	3.04188000
H	1.33203800	-2.92148500	3.61328100	H	1.29608200	-3.00790000	3.94656600
H	5.01923000	-1.88256200	1.69663000	H	4.91039300	-1.85777700	1.95954900
H	3.81807800	-3.14809700	3.40784000	H	3.78853700	-3.11933000	3.72527900
C	-2.01287600	1.66010100	0.76025200	C	-2.25643200	1.37260700	1.10346000
C	-3.37149600	1.36558500	0.90757500	C	-3.59209000	1.02029800	1.31955000
C	-1.62292700	2.90757700	0.24903700	C	-1.94884300	2.62525300	0.55062600
C	-4.34100800	2.27688900	0.50874400	C	-4.62007000	1.87759300	0.94871400
H	-3.64994100	0.39987900	1.31535400	H	-3.80603300	0.05117900	1.75685600
C	-2.60357100	3.79983500	-0.19309800	C	-2.98904700	3.46342800	0.13968300
C	-3.95266000	3.48617700	-0.06366300	C	-4.31473900	3.09154700	0.33735200
H	-5.39089800	2.02953200	0.61253000	H	-5.65152400	1.58446100	1.10484800
H	-2.29314800	4.72079200	-0.66499600	H	-2.74385300	4.38798500	-0.36261100
H	-4.70146200	4.18936200	-0.41268000	H	-5.11037700	3.75275300	0.01065200
N	-1.60095500	-2.42956800	-0.80082500	N	-1.78765800	-2.71339400	-0.37989500
N	-0.21648400	3.18515600	0.11025800	N	-0.56490500	2.96376700	0.33794800
C	3.87683500	-0.26327800	-0.21764600	N	3.67981400	-0.36789300	0.00085000
O	-2.36270700	-3.29539600	0.04143200	O	-2.48879400	-3.56931300	0.52177000
H	-2.32614200	-2.89293400	0.95221600	H	-2.42132600	-3.13210900	1.41865500
O	3.78752500	1.15337500	-0.01621300	O	3.53183700	1.05094600	0.15161000
H	3.34137300	1.49545900	-0.83244800	H	3.07585900	1.34375000	-0.67593400
O	-0.03475000	3.77971100	-1.18651000	O	-0.47752600	3.55100800	-0.97251800
H	0.69938600	3.25495700	-1.59648700	H	0.24817900	3.04923100	-1.41910600
C	-0.76215600	-3.34673400	-1.66553000	C	-0.96845600	-3.63417600	-1.25874200
C	5.20334600	-0.61651500	-0.78294300	C	5.01987100	-0.68434700	-0.55714400
C	0.38790100	4.10219600	1.14090300	C	0.04935800	3.92241000	1.32417100
H	-0.55930800	-1.08584900	-0.01934700	H	-0.75110000	-1.33457500	0.31832000
Cl	2.21821300	2.15531300	-2.48930000	Cl	-2.40111200	-2.29913100	3.22087700
Br	-2.42694900	-2.11393100	2.95880600	Br	1.85996300	1.93815700	-2.50786000
C	0.04802400	-2.53637700	-2.68009200	C	5.10056700	0.02948500	-1.91948600
H	-0.58802700	-1.92394800	-3.32139800	H	5.10793300	1.11200300	-1.80105400
H	0.79016900	-1.90223300	-2.19430400	H	6.01869400	-0.27006400	-2.43256700
H	0.59324900	-3.23214100	-3.32157000	H	4.24013800	-0.22538800	-2.53916200
C	-1.64644900	-4.35736600	-2.41252200	C	5.10180800	-2.19479300	-0.82579800
H	-2.29330800	-3.85641200	-3.13652000	H	6.01582700	-2.40674900	-1.38623600
H	-1.01341300	-5.06379600	-2.95582100	H	5.11338700	-2.79740000	0.08050300
H	-2.26629500	-4.91146100	-1.70885600	H	4.24775100	-2.50848500	-1.43034900
C	0.20022200	-4.07154000	-0.71703300	C	6.18018800	-0.17659500	0.32141000
H	0.85121300	-4.73757800	-1.28989700	H	6.31220900	-0.75441300	1.23663300
H	0.82655500	-3.35571200	-0.18039200	H	7.11906000	-0.22059400	-0.23790800
H	-0.35311500	-4.65563500	0.01596300	H	5.98779800	0.86180900	0.59456800
C	1.89936700	4.12375100	0.88134700	C	1.54365900	4.00364100	0.98859100

H	2.32690600	3.12251900	0.95919700	H	2.01670100	3.02280000	1.06295100
H	2.11907600	4.50576100	-0.11501800	H	1.69743600	4.37504600	-0.02402300
H	2.38964100	4.76594000	1.61871800	H	2.04165000	4.68028300	1.68904200
C	-0.17993000	5.52860900	1.05014300	C	-0.58497800	5.32103700	1.24181600
H	-1.23126300	5.56042500	1.34429200	H	-1.62198900	5.31030400	1.58439700
H	0.37689300	6.18951200	1.71993700	H	-0.02798800	6.01535100	1.87673300
H	-0.08322000	5.90382800	0.03105100	H	-0.55263000	5.68582600	0.21495500
C	0.12484700	3.53237800	2.53954400	C	-0.11847300	3.36625200	2.74284200
H	-0.94103600	3.40773800	2.73931000	H	-1.16645300	3.19750000	2.99740200
H	0.62612100	2.57379000	2.68074000	H	0.43283400	2.43423900	2.87448900
H	0.52792000	4.22437400	3.28296500	H	0.28833200	4.08937000	3.45389300
C	5.31952900	0.14587400	-2.11637100	C	0.05407700	-4.31063800	-0.33800500
H	5.37215400	1.22147200	-1.95470600	H	-0.45120000	-4.88650500	0.43504800
H	6.22548800	-0.17242600	-2.63978300	H	0.69396200	-4.97702800	-0.92289100
H	4.45052500	-0.04720900	-2.74657700	H	0.68686600	-3.56613100	0.15004100
C	5.22127900	-2.11786000	-1.10786900	C	-0.22658200	-2.83351300	-2.33174500
H	6.12886500	-2.34896600	-1.67123400	H	-0.90629700	-2.25283300	-2.95753100
H	5.20071000	-2.75323800	-0.22424700	H	0.52193700	-2.16908800	-1.89901300
H	4.35824300	-2.37162000	-1.72770100	H	0.30456400	-3.53358500	-2.98035200
C	6.37965900	-0.19447300	0.11913100	C	-1.86198200	-4.68534900	-1.93546000
H	7.31961100	-0.25944300	-0.43640300	H	-1.23834100	-5.39349200	-2.48739200
H	6.23138900	0.84029800	0.43080300	H	-2.43609300	-5.23135600	-1.18799100
H	6.47859800	-0.81226000	1.01227900	H	-2.55259500	-4.21990800	-2.64251400
<b>[L(HClBr)]-, 8a, E<sub>0</sub>=-4765.971867 au</b>				<b>[L(HClBr)]-, 8b, E<sub>0</sub>=-4765.970354 au</b>			
N	0.65497700	-0.09468500	0.99957600	N	-1.02958500	0.00452800	1.37601900
C	0.62273800	-1.57295000	1.34279300	C	-1.00304100	1.44250100	1.86159000
H	-0.42287200	-1.81245800	1.49735200	H	0.04482900	1.68408000	1.99637300
H	1.18118000	-1.66541300	2.27740000	H	-1.52337700	1.43107600	2.82221600
C	-0.01553400	0.71687800	2.08710100	C	-0.29468600	-0.89585700	2.34622100
H	0.11705800	1.75247700	1.80411300	H	-0.42857700	-1.90179400	1.97132800
H	0.55566800	0.51328500	2.99561500	H	-0.82341300	-0.78806500	3.29571700
C	2.08402300	0.37113600	0.77010800	C	-2.46162300	-0.46536200	1.17343300
H	2.49863900	-0.31700700	0.04648900	H	-2.92527700	0.28405800	0.54674500
H	2.58557600	0.25291300	1.73434600	H	-2.91009200	-0.45506400	2.17043500
C	1.22678500	-2.39054600	0.23988000	C	-1.66321900	2.35359900	0.86946900
C	2.51498800	-2.91143700	0.39086600	C	-2.95010700	2.83613800	1.12361400
C	0.53037000	-2.58933300	-0.96110700	C	-1.02163300	2.68152200	-0.33379000
C	3.12226300	-3.60075200	-0.65355300	C	-3.60995100	3.61519700	0.17891500
H	3.03623300	-2.74777500	1.32834500	H	-3.42866100	2.57281000	2.06096100
C	1.16509100	-3.23956300	-2.02128400	C	-1.70870000	3.42294900	-1.29705100
C	2.45138000	-3.74697700	-1.86607800	C	-2.99321500	3.89166500	-1.03957600
H	4.12106900	-4.00267400	-0.52879200	H	-4.60742000	3.98626600	0.38408700
H	0.65390300	-3.32707500	-2.96853800	H	-1.23942000	3.61168700	-2.25121800
H	2.93272600	-4.25097500	-2.69692300	H	-3.51553900	4.46734200	-1.79571100
C	2.12498800	1.78025400	0.26109500	C	-2.50680500	-1.81606300	0.52484600
C	2.35477000	2.83520800	1.15053300	C	-2.68181400	-2.95956900	1.31133300
C	1.88957900	2.05765000	-1.09391200	C	-2.32986400	-1.95164400	-0.86037700
C	2.28606200	4.15410700	0.71722300	C	-2.61663400	-4.22673100	0.74385700
H	2.56712100	2.60261700	2.18839100	H	-2.84829400	-2.83700200	2.37591400
C	1.75672300	3.38540800	-1.50861300	C	-2.19969000	-3.22835500	-1.41334600
C	1.95226300	4.42646300	-0.60848400	C	-2.34094100	-4.35827300	-0.61614200
H	2.45820900	4.96407500	1.41622500	H	-2.74593200	-5.10588300	1.36408400
H	1.48477200	3.59125700	-2.53359500	H	-1.97284000	-3.32488400	-2.46507400
H	1.84585600	5.45202500	-0.94355200	H	-2.23747300	-5.34276400	-1.05822000
C	-1.46530500	0.36046400	2.24456500	C	1.15739300	-0.53316200	2.46637000
C	-1.85781400	-0.30699300	3.40931600	C	1.60016700	0.02707000	3.66905500
C	-2.41961900	0.64395800	1.25201500	C	2.06611700	-0.70906700	1.40833200
C	-3.17599700	-0.70979600	3.58798000	C	2.92170900	0.42929900	3.82289000
H	-1.10577300	-0.52609000	4.15964900	H	0.88358300	0.16339400	4.47170900
C	-3.73862500	0.21475300	1.42737600	C	3.38809400	-0.28101000	1.56135400
C	-4.11064900	-0.45636300	2.58699800	C	3.80973600	0.28352900	2.75995900
H	-3.46504400	-1.23337700	4.49214200	H	3.24902500	0.86949700	4.75792400
H	-4.46843400	0.37342600	0.64082000	H	4.08251000	-0.35461700	0.73081700
H	-5.13739700	-0.78606000	2.69871300	H	4.83768500	0.61505200	2.85342500
N	-0.82432600	-2.11670200	-1.01207700	N	0.33501300	2.23806000	-0.48933700
N	-1.98114800	1.31600100	0.04911900	N	1.57778700	-1.27138800	0.16890100

N	1.80045500	0.94272400	-1.99909600	N	-2.29562800	-0.75032500	-1.65180700
O	-0.96318100	-1.23607600	-2.15275100	O	0.43382900	1.48596500	-1.72291000
H	-1.58472800	-0.54730000	-1.79423600	H	1.07869300	0.77539400	-1.46817100
O	0.64057700	1.11865000	-2.83036200	O	-1.17434500	-0.82561800	-2.54890800
H	0.12798400	0.311170200	-2.63970300	H	-0.66372000	-0.03198900	-2.30550200
O	-2.47035900	0.62357700	-1.10033400	O	2.00329500	-0.46330200	-0.93028900
H	-3.47650200	0.66764000	-1.22177100	H	2.99615000	-0.48816900	-1.10190000
C	-1.87855900	-3.19498100	-1.06840800	C	1.37321900	3.33359100	-0.47636100
C	2.99720400	0.74565600	-2.88926600	C	-3.53506900	-0.48545100	-2.46297100
C	-2.30866000	2.78911900	-0.05764400	C	1.91767600	-2.72176500	-0.09472800
C	2.73869500	-0.52532800	-3.70316200	C	-3.32761200	0.86113500	-3.16159100
H	3.61909900	-0.76461200	-4.30587600	H	-4.23842700	1.14534600	-3.69568900
H	2.53257400	-1.36014400	-3.03689400	H	-3.09675200	1.63069200	-2.42843100
H	1.88624000	-0.39276900	-4.36916900	H	-2.50758900	0.80480800	-3.87726100
C	3.23690900	1.92478500	-3.84760500	C	-3.80881200	-1.57004800	-3.51894200
H	3.57466100	2.81747800	-3.31892700	H	-4.11106200	-2.51462900	-3.06413300
H	4.00921900	1.65342900	-4.57239500	H	-4.61834200	-1.24138400	-4.17622900
H	2.32099800	2.15655900	-4.39341100	H	-2.91842300	-1.73422200	-4.12787200
C	4.22773300	0.53300800	-1.99934300	C	-4.72420400	-0.37669500	-1.50107400
H	4.42209400	1.39487200	-1.35877700	H	-4.87972600	-1.29875700	-0.93845200
H	4.11170700	-0.35243200	-1.37167100	H	-4.58721100	0.44611900	-0.79713900
H	5.10405500	0.38141900	-2.63434700	H	-5.63093200	-0.17746600	-2.07753300
C	-1.92916600	3.22972300	-1.47677300	C	1.48204700	-3.02927900	-1.53280300
H	-1.91680400	4.32268900	-1.51931600	H	1.47673600	-4.11324300	-1.67925700
H	-0.94518000	2.84988300	-1.74762000	H	0.48443500	-2.63726600	-1.72506900
H	-2.64995500	2.86107200	-2.20522600	H	2.16859200	-2.58475400	-2.25212200
C	-1.43550200	3.53395800	0.95714600	C	1.09750900	-3.57290100	0.87969400
H	-1.62275300	3.19237000	1.97799600	H	1.32568100	-3.32755100	1.91968400
H	-0.37784200	3.42357700	0.72353000	H	0.02974500	-3.45547600	0.70291800
H	-1.67712900	4.59885100	0.91850300	H	1.34818600	-4.62559000	0.72867100
C	-3.78616400	3.11713500	0.21156800	C	3.40880300	-3.05125100	0.07938100
H	-3.94546100	4.18435300	0.03034600	H	3.57227800	-4.09301300	-0.21219600
H	-4.45589200	2.56015000	-0.44581900	H	4.04464400	-2.42415800	-0.54860700
H	-4.05941400	2.91039100	1.24885300	H	3.72443400	-2.94190000	1.11937500
C	-1.88492100	-3.97052100	-2.39644200	C	1.30834100	4.24785500	-1.71111800
H	-1.03081900	-4.64438600	-2.48479200	H	0.44220300	4.91164300	-1.68798600
H	-2.79278900	-4.57582300	-2.45593200	H	2.20447900	4.87233700	-1.74398000
H	-1.88545700	-3.27252500	-3.23459500	H	1.28029900	3.64487200	-2.61959300
C	-3.23829200	-2.52103100	-0.86594900	C	2.74812700	2.66388400	-0.41046000
H	-4.01727900	-3.28510800	-0.80117500	H	3.52125700	3.42800500	-0.29604300
H	-3.24454300	-1.94322400	0.05652300	H	2.80277300	1.98836400	0.44125200
H	-3.50535100	-1.85188300	-1.68227400	H	2.98601400	2.09356400	-1.30704200
C	-1.62080000	-4.15355000	0.10230800	C	1.16032800	4.15605100	0.80191800
H	-0.66083900	-4.66566800	0.01500500	H	0.18955600	4.65489600	0.81712300
H	-1.65079000	-3.62384200	1.05667900	H	1.24706500	3.52835400	1.69115100
H	-2.40890200	-4.90984500	0.11610200	H	1.93660200	4.92249500	0.85845900
Cl	-5.35063100	0.48934500	-1.74781100	H	-0.52545500	-0.04977900	0.48203100
H	0.10856700	0.05527400	0.14176400	Cl	-2.82812300	0.16523100	4.52216700
Br	2.68302100	-0.60748600	4.15687500	Br	4.99769600	-0.19129000	-1.79599400
<b>[L(HClI)]<sup>-</sup>, 1a, E<sub>0</sub>=-9111.378469 au</b>				<b>[L(HClI)]<sup>-</sup>, 1b, E<sub>0</sub>=-9111.376322 au</b>			
O	-3.99804400	-0.72271800	-0.11937800	O	-3.39486300	-0.67282000	0.44023300
H	-3.73003400	-0.42730900	-1.02724500	H	-3.12636100	-0.44205100	-0.47833400
O	-1.85743200	2.82570700	-2.28178600	O	-1.08832100	2.96645200	-1.84827600
H	-2.26103700	1.94897900	-2.49712100	H	-1.47437100	2.10835400	-2.13281700
O	3.55563400	-1.97798000	-0.32825200	O	4.17233600	-1.99215600	0.66879200
H	3.52154400	-1.59721400	0.57843800	H	4.01331100	-1.53740700	1.53334000
N	-2.90236200	-1.53721600	0.32191300	N	-2.33644600	-1.52163800	0.91509400
N	-1.53811400	2.72497100	-0.88943000	N	-0.84871300	2.78869100	-0.44734400
N	2.71640500	-1.09234300	-1.08490700	N	3.42501600	-1.17590000	-0.24366500
N	0.40751800	-0.14145500	0.23396100	N	0.99903800	-0.19454500	0.85304800
H	1.44292700	-0.22349500	0.16541400	H	2.03568000	-0.24787400	0.91551400
C	-0.04499000	-1.36376100	1.04952100	C	0.49004200	-1.40703400	1.65332500
H	-0.30337200	-2.11767600	0.31918800	H	0.18715100	-2.13537000	0.91522300
H	0.84021700	-1.67480500	1.60133300	H	1.36058200	-1.76576800	2.19672100
C	-1.16753500	-1.06480500	2.00486700	C	-0.61803600	-1.06991600	2.60991800
C	-0.82405100	-0.68330300	3.30871000	C	-0.27124900	-0.68245400	3.91031700

H	0.22306200	-0.70286900	3.59301700	H	0.77629100	-0.71201000	4.19252600
C	-1.78446500	-0.22709400	4.20103000	C	-1.23059800	-0.20163800	4.79183500
H	-1.49377100	0.08069100	5.19868800	H	-0.94180400	0.11169300	5.78838900
C	-3.11143500	-0.13261700	3.78549300	C	-2.55385900	-0.08842100	4.36853600
H	-3.86831600	0.25976300	4.45620000	H	-3.30679800	0.32252100	5.03248900
C	-3.47401800	-0.55159700	2.51239600	C	-2.91827100	-0.51039800	3.09627500
H	-4.49695200	-0.47483300	2.17525000	H	-3.93829900	-0.41681900	2.75397500
C	-2.51940100	-1.05930800	1.62177100	C	-1.96583200	-1.04030700	2.21761100
C	-3.36806100	-2.97770700	0.29190100	C	-2.84737800	-2.94711100	0.89001700
C	-3.75616000	-3.29604100	-1.15597000	C	-3.17476500	-3.28260600	-0.56845000
H	-2.91772700	-3.11118300	-1.82515400	H	-2.30361900	-3.12304800	-1.20232000
H	-4.59136000	-2.67910100	-1.48260100	H	-3.98181600	-2.65804400	-0.94755800
H	-4.04109000	-4.34935700	-1.23263800	H	-3.47628200	-4.33142100	-0.64226100
C	-2.21299300	-3.89409800	0.70982700	C	-1.74219700	-3.88995000	1.37978200
H	-1.38465700	-3.83079700	0.00227800	H	-0.88023400	-3.87046400	0.71099400
H	-2.56735200	-4.92799700	0.71259400	H	-2.13138000	-4.91112700	1.38685300
H	-1.84730300	-3.66545400	1.71250300	H	-1.41468500	-3.65103300	2.39307900
C	-4.57940700	-3.21181100	1.20981300	C	-4.10570700	-3.12524200	1.75531700
H	-4.95768000	-4.22752500	1.06538400	H	-4.51083500	-4.13016100	1.60879300
H	-5.37575700	-2.50885300	0.96254000	H	-4.86633700	-2.40088000	1.46208900
H	-4.31725100	-3.09537900	2.26338300	H	-3.88652800	-3.00104000	2.81780200
C	0.07541900	1.16919100	0.90939400	C	0.56844300	1.13156100	1.43026000
H	0.50548900	1.10410700	1.90554200	H	0.84989300	1.10605800	2.47834500
H	-1.00278900	1.20730100	0.96711000	H	-0.50772200	1.16772100	1.32915700
C	0.63168600	2.35347600	0.17126300	C	1.22824500	2.29168200	0.73914300
C	1.96637700	2.71766600	0.37275500	C	2.56456600	2.58428800	1.02964700
H	2.55313600	2.16097500	1.09652400	H	3.07328200	1.98562400	1.77909800
C	2.53877200	3.74924700	-0.36180800	C	3.23228900	3.59416200	0.34754800
H	3.57872000	4.01064300	-0.20516100	H	4.27258900	3.79962300	0.57103100
C	1.77651800	4.41473700	-1.32029400	C	2.56547900	4.31191200	-0.64414500
H	2.22288900	5.19827200	-1.92335600	H	3.08691900	5.08073400	-1.20439300
C	0.43896500	4.08451800	-1.50485600	C	1.22753200	4.05348000	-0.91607000
H	-0.15749500	4.57872700	-2.25794800	H	0.70403700	4.58955900	-1.69438400
C	-0.15845900	3.07891900	-0.73709700	C	0.53502600	3.06638100	-0.20550800
C	-2.52961200	3.55969800	-0.11846500	C	-1.84419800	3.63934500	0.30231400
C	-2.56146500	5.01128400	-0.62509500	C	-1.79243900	5.10443800	-0.16221800
H	-2.72976400	5.02465200	-1.70206300	H	-1.91991400	5.15799400	-1.24331400
H	-1.62612200	5.53160800	-0.40469500	H	-0.84253900	5.57310300	0.10671800
H	-3.37434400	5.55604800	-0.13696000	H	-2.59659900	5.67211600	0.31397900
C	-3.89810600	2.89722700	-0.31244300	C	-3.22523500	3.03625700	0.02356400
H	-3.86830900	1.85668400	0.01379000	H	-3.25378800	1.99141500	0.33689300
H	-4.19151900	2.90985900	-1.36141300	H	-3.46007200	3.07438100	-1.03939900
H	-4.65358300	3.43184900	0.27139700	H	-3.99086700	3.59198300	0.57323600
C	-2.17535700	3.54629400	1.37432700	C	-1.56494400	3.57354900	1.80955700
H	-1.16800200	3.92242000	1.56336300	H	-0.55772500	3.91337200	2.05791800
H	-2.26914800	2.54771500	1.80346100	H	-1.70937700	2.56788700	2.20626600
H	-2.87817400	4.19513700	1.90295100	H	-2.27390000	4.22997600	2.32017200
C	-0.08363700	-0.19867600	-1.19045700	C	0.66073100	-0.30427300	-0.61202900
H	0.24750000	0.71434000	-1.67582400	H	1.06359800	0.58259800	-1.09301600
H	-1.16965100	-0.19021400	-1.17209300	H	-0.42246700	-0.27221700	-0.70584300
C	0.42063700	-1.43543900	-1.89010600	C	1.20314100	-1.58276700	-1.19809000
C	-0.49877700	-2.17472200	-2.64167900	C	0.33417400	-2.38369400	-1.94591700
H	-1.49709000	-1.77095000	-2.76688300	H	-0.65688400	-2.00369400	-2.16620200
C	-0.13900600	-3.38810000	-3.21439400	C	0.73019900	-3.63612500	-2.39821600
H	-0.86857100	-3.94778400	-3.78838700	H	0.03957700	-4.24198500	-2.97336800
C	1.14392800	-3.89374400	-3.01363300	C	1.99766400	-4.11703700	-2.07515200
H	1.42196600	-4.86082000	-3.41847300	H	2.30187300	-5.11088400	-2.38538500
C	2.07773300	-3.15211700	-2.30154000	C	2.88109900	-3.31914700	-1.35914600
H	3.07288400	-3.53339200	-2.12616100	H	3.85997500	-3.68316500	-1.08345600
C	1.74047300	-1.90108900	-1.77681900	C	2.51087600	-2.03295800	-0.95584600
C	3.60756500	-0.26003600	-1.98324200	C	4.40308000	-0.41472400	-1.10697100
C	2.73666800	0.73344900	-2.75867500	C	3.61698100	0.53612200	-2.01554200
H	2.23206500	1.42758400	-2.08781300	H	3.07082400	1.27747700	-1.43266600
H	1.99522000	0.22827800	-3.37991600	H	2.91925500	-0.00111200	-2.66056000
H	3.37790500	1.32287500	-3.41827300	H	4.31822500	1.07341100	-2.65866600
C	4.40944500	-1.13047900	-2.96267300	C	5.27739000	-1.35176400	-1.95485700



H	3.76396900	-1.60741000	-3.70243500	H	4.69484300	-1.86846200	-2.71993200
H	4.95942300	-1.90028800	-2.41960400	H	5.76254700	-2.09134300	-1.31598400
H	5.12980700	-0.50393500	-3.49545000	H	6.05409900	-0.76852600	-2.45707100
C	4.57221300	0.50464900	-1.07108400	C	5.29575900	0.39651400	-0.16123100
H	5.26916700	-0.17508400	-0.58307200	H	5.94687300	-0.25953900	0.41452500
H	4.02962400	1.03905800	-0.29372800	H	4.69300100	0.96774800	0.54157400
H	5.13936900	1.22599900	-1.66571200	H	5.91207400	1.08606400	-0.74486700
Cl	-3.21346900	0.14552600	-2.92705700	Cl	3.36936700	-0.30783000	3.09434400
I	3.22317300	-0.32970600	2.71222500	I	-2.65732200	0.04823300	-2.87619100
<b>[L(HClI)]<sup>-</sup>, 2a, E<sub>0</sub>=-9111.375069 au</b>				<b>[L(HClI)]<sup>-</sup>, 2b, E<sub>0</sub>=-9111.373435 au</b>			
N	0.40740200	-0.42961800	-0.02407100	N	-0.70673300	-0.88208300	0.58100100
C	0.02122900	0.26391300	1.26594700	C	-1.19659300	-0.58943400	-0.82760100
H	-0.08705600	-0.50615100	2.02314000	H	-1.53427600	-1.54929700	-1.20177500
H	-0.96326700	0.70367700	1.13838200	H	-0.31550800	-0.27607900	-1.39143500
C	-0.10894600	0.29978100	-1.24126000	C	0.10418100	0.22930400	1.19340100
H	-1.18156000	0.17720800	-1.20988700	H	0.95427600	0.41227000	0.53846200
H	0.30967400	-0.22305700	-2.09987000	H	0.46881700	-0.16362400	2.13805800
C	0.06076600	-1.91889100	-0.06755000	C	0.08842300	-2.19802300	0.50193100
H	0.03445200	-2.24353600	0.96356700	H	0.47993000	-2.23749300	-0.50727200
H	0.90950300	-2.37758600	-0.57458800	H	-0.65600200	-2.97569200	0.66678300
C	1.03270200	1.31362200	1.66939400	C	-2.28695700	0.43938900	-0.93981300
C	0.54561800	2.54821000	2.10961100	C	-1.96705300	1.71962800	-1.40103900
C	2.42207200	1.11660500	1.61063200	C	-3.61094800	0.14306700	-0.58648700
C	1.41254100	3.57723400	2.44984200	C	-2.93414700	2.71377300	-1.45231900
H	-0.52530800	2.69476000	2.16137900	H	-0.94497400	1.93521100	-1.68783900
C	3.28797700	2.16934200	1.91298300	C	-4.57122300	1.15755700	-0.60740200
C	2.78790400	3.39361300	2.33403100	C	-4.23389700	2.43554300	-1.03440400
H	1.00901800	4.53012000	2.77154500	H	-2.66239400	3.70870600	-1.78338100
H	4.34900800	2.02098900	1.77592900	H	-5.56649300	0.93835400	-0.24826200
H	3.47098800	4.20511900	2.56033000	H	-4.98526700	3.21811000	-1.03496500
C	-1.20076300	-2.25289100	-0.81470700	C	1.23056300	-2.29492800	1.47503300
C	-1.07415700	-2.65057300	-2.15148700	C	0.99307100	-2.55345700	2.82974000
C	-2.48120800	-2.11214600	-0.25663000	C	2.54068400	-2.02880700	1.04030000
C	-2.19371400	-2.85845200	-2.94660100	C	2.02832400	-2.47883900	3.75372700
H	-0.07805900	-2.74841400	-2.57041500	H	-0.02373500	-2.74676300	3.15319500
C	-3.60340800	-2.28874400	-1.07476600	C	3.56587200	-1.91101200	1.98407400
C	-3.46233500	-2.65483500	-2.40711800	C	3.31044100	-2.12794900	3.33238700
H	-2.07459200	-3.14768400	-3.98418100	H	1.82634900	-2.66173400	4.80277000
H	-4.57990100	-2.10095300	-0.65344300	H	4.55115200	-1.62276100	1.64635500
H	-4.34515900	-2.77926300	-3.02485700	H	4.11356400	-2.02699500	4.05447800
C	0.25475600	1.75548200	-1.26128700	C	-0.63400500	1.51829200	1.42802400
C	1.58170100	2.12668500	-1.49801900	C	-1.91987000	1.54396100	1.97768700
C	-0.71007200	2.74403300	-1.00748000	C	-0.00103700	2.72557900	1.09592000
C	1.96812100	3.45744400	-1.43865400	C	-2.60065200	2.74381900	2.11980600
H	2.31464800	1.35332700	-1.69830400	H	-2.40284800	0.61743300	2.26449700
C	-0.30939000	4.08312100	-0.94709100	C	-0.70539700	3.92827400	1.21957700
C	1.01701600	4.43520900	-1.15254300	C	-1.99847900	3.93709000	1.72082600
H	3.00660200	3.72492300	-1.59269000	H	-3.60990700	2.74108400	2.51351200
H	-1.04640300	4.82690900	-0.68225200	H	-0.23252800	4.83968600	0.88205400
H	1.31184700	5.47675600	-1.08116200	H	-2.53993300	4.87374600	1.80036700
N	2.93400600	-0.15690900	1.15378400	N	-3.91204600	-1.18831100	-0.13829400
N	-2.06172300	2.35633800	-0.71337000	N	1.33313800	2.67701100	0.57823000
N	-2.61382900	-1.72664500	1.11869600	N	2.77357500	-1.85182300	-0.36255000
O	4.06296100	0.10099600	0.30499100	O	-4.71682500	-1.09000300	1.04580200
H	3.83819700	-0.37661600	-0.52702300	H	-4.10330000	-1.42933500	1.73885600
O	-3.73840700	-0.84147900	1.19632700	O	3.63132700	-0.71680500	-0.53792300
H	-3.40693800	-0.05218000	1.69817400	H	3.12588700	-0.15070100	-1.16589000
O	-2.57234900	3.26159700	0.27345200	O	1.42769200	3.59003800	-0.52207800
H	-2.72085600	2.69548700	1.07002100	H	1.55825900	2.98229400	-1.28216300
C	3.38562000	-1.11364700	2.23201500	C	-4.62953000	-2.08477500	-1.09974900
C	-2.85926700	-2.84946500	2.09797700	C	3.37288400	-3.02415300	-1.08573100
C	-3.04300700	2.35372000	-1.85495700	C	2.45185900	2.96663000	1.53078400
H	1.44742800	-0.43596000	-0.01969000	H	-1.50795800	-1.10838100	1.21816100
C	2.22578000	-1.37391200	3.19812700	C	-3.85120300	-2.14563500	-2.41929200
H	1.85343400	-0.45337200	3.65000600	H	-3.71620700	-1.15589500	-2.85872800
H	1.39977300	-1.88227200	2.69967600	H	-2.87067600	-2.60607100	-2.28593000

H	2.57577600	-2.02720100	4.00065000	H	-4.40813100	-2.75916500	-3.13184700
C	4.58899700	-0.56261600	3.01257700	C	-6.06835100	-1.61429000	-1.37978400
H	4.31419700	0.31395600	3.60220800	H	-6.07759900	-0.67987400	-1.94463200
H	4.96168200	-1.32931900	3.69716300	H	-6.59784300	-2.36931300	-1.96802900
H	5.39010800	-0.29204900	2.32470100	H	-6.60098900	-1.46694400	-0.44004600
C	3.76917400	-2.42216200	1.53300000	C	-4.65151100	-3.47613400	-0.45462100
H	4.02601900	-3.17796400	2.28046200	H	-5.09227400	-4.20513500	-1.14098300
H	2.94335600	-2.79371300	0.92431300	H	-3.63565500	-3.78834100	-0.20398900
H	4.62249900	-2.27737500	0.87227300	H	-5.23205000	-3.46008200	0.46695300
C	-4.35123100	1.78093800	-1.29553400	C	3.75703200	2.66250700	0.78567400
H	-4.16779000	0.81449300	-0.82255900	H	3.77395400	1.62052400	0.46383100
H	-4.77304900	2.44853500	-0.54504600	H	3.85336100	3.29757600	-0.09428600
H	-5.07776800	1.65323800	-2.10376400	H	4.61164800	2.84208700	1.44512800
C	-3.26614300	3.77341300	-2.40323700	C	2.43583100	4.43001800	2.00521900
H	-2.36078600	4.16050700	-2.87748500	H	1.55195700	4.64007000	2.61185500
H	-4.06347000	3.76179900	-3.15182600	H	3.32125500	4.63509700	2.61372300
H	-3.55576400	4.44464800	-1.59474600	H	2.44148700	5.10086400	1.14518300
C	-2.54387900	1.44619000	-2.98673400	C	2.33721800	2.02716700	2.73745100
H	-1.55277300	1.73665000	-3.34055100	H	1.39526100	2.16193900	3.27276600
H	-2.52414300	0.39732300	-2.68917800	H	2.43055300	0.98358300	2.43529600
H	-3.23535600	1.53227200	-3.82869500	H	3.15271200	2.24484700	3.43186800
C	-2.84407700	-2.21514100	3.49351800	C	3.34730000	-2.67902200	-2.57895500
H	-3.65422900	-1.49650200	3.60637900	H	3.98649100	-1.82314200	-2.79231700
H	-2.94836900	-2.99190800	4.25679000	H	3.69679500	-3.53418600	-3.16488300
H	-1.90751600	-1.67889200	3.65833100	H	2.33650800	-2.41556300	-2.89407500
C	-1.73325100	-3.88545300	2.00383100	C	2.49840400	-4.25901300	-0.83392200
H	-1.96348500	-4.71505900	2.67662600	H	2.91438700	-5.10529000	-1.38603700
H	-1.62808000	-4.29101500	0.99594800	H	2.46493800	-4.52789900	0.22325200
H	-0.77606300	-3.46753800	2.32063200	H	1.47717300	-4.10100000	-1.18621600
C	-4.20913500	-3.54275800	1.84807500	C	4.81623500	-3.31266400	-0.63950300
H	-4.41031100	-4.25861000	2.64983800	H	5.25619600	-4.07967900	-1.28296100
H	-5.00882400	-2.80268300	1.83210000	H	5.41699200	-2.40612400	-0.71948200
H	-4.20886600	-4.08745800	0.90105200	H	4.85290600	-3.67539200	0.38996000
I	3.00093900	-1.65078300	-2.46914000	Cl	-2.46787400	-2.03378000	2.86152100
Cl	-2.89404700	1.57299100	2.80506600	I	1.81131500	1.07695400	-2.89823700
<b>[L(HCII)]<sup>-</sup>, 3a, E<sub>0</sub> = -9111.374096 au</b>				<b>[L(HCII)]<sup>-</sup>, 3b, E<sub>0</sub> = -9111.363292 au</b>			
N	-0.63992000	-0.00033500	0.00078600	N	1.60094700	0.00174500	0.00139500
C	-1.12241300	0.08232200	1.43807100	C	2.08584200	-0.68019300	-1.26621200
H	-0.64298200	-0.73964700	1.94678400	H	1.58937800	-1.63822000	-1.28195700
H	-2.19817900	-0.09246600	1.39023800	H	3.15866200	-0.81402900	-1.12018400
C	-1.12328500	-1.28595400	-0.64638300	C	2.08436700	-0.75432500	1.22675700
H	-0.64398000	-1.31558500	-1.61265700	H	1.58573200	-0.28939400	2.06326600
H	-2.19901400	-1.15639200	-0.77358000	H	3.15685400	-0.55959000	1.27184700
C	-1.12206700	1.20343800	-0.78913800	C	2.08211900	1.44168700	0.04448600
H	-0.64143200	2.05456400	-0.33215500	H	1.58419800	1.93292200	-0.77729500
H	-2.19764600	1.25029000	-0.61288400	H	3.15505800	1.38492900	-0.14465300
C	-0.83466200	1.41070500	2.07227200	C	1.82332400	0.13460500	-2.49768000
C	-1.87522100	2.34262700	2.15880100	C	2.88229300	0.87505400	-3.03560400
C	0.45168700	1.76173200	2.51100100	C	0.54745100	0.22619900	-3.07471900
C	-1.64053100	3.62907800	2.62817300	C	2.67512700	1.73761600	-4.10502000
H	-2.86304300	2.05027700	1.81618500	H	3.85936800	0.78907000	-2.57028600
C	0.68673400	3.07037800	2.94755900	C	0.33992400	1.12358000	-4.12821800
C	-0.34888000	3.99550800	3.00190800	C	1.39361100	1.87477000	-4.63530400
H	-2.45313700	4.34446500	2.67619400	H	3.50094200	2.31618800	-4.50234100
H	1.69467000	3.35056200	3.21509500	H	-0.65972900	1.23799400	-4.52018600
H	-0.14517500	5.00577000	3.34037300	H	1.21164100	2.56758200	-5.44988400
C	-0.83557600	1.08862500	-2.25690100	C	1.81789800	2.09991300	1.36595500
C	-1.87673900	0.69769900	-3.10656000	C	2.87626600	2.19714200	2.27669000
C	0.45020500	1.29393000	-2.78123900	C	0.54094800	2.55107900	1.73347000
C	-1.64310100	0.46189500	-4.45568300	C	2.66751300	2.69084600	3.55859100
H	-2.86422300	0.54682300	-2.68140900	H	3.85417800	1.83924300	1.96978800
C	0.68422900	1.01860800	-4.13323700	C	0.33185300	3.01346400	3.03757100
C	-0.35194400	0.60322400	-4.96093700	C	1.38500500	3.07858200	3.94218200
H	-2.45613800	0.14594100	-5.09876700	H	3.49290300	2.74698100	4.25870600
H	1.69179400	1.11081100	-4.51050100	H	-0.66855400	3.29329100	3.33239600
H	-0.14908500	0.39194900	-6.00539700	H	1.20184200	3.43658000	4.94962100

C	-0.83600700	-2.49975500	0.18654400	C	1.82370700	-2.22848900	1.13604300
C	-1.87662900	-3.04034300	0.95048600	C	2.88424900	-3.06321300	0.76521100
C	0.44992900	-3.05623300	0.27016000	C	0.54797200	-2.77547300	1.34233600
C	-1.64226600	-4.09079100	1.82910100	C	2.67889300	-4.42068300	0.55144600
H	-2.86424900	-2.59690100	0.86913900	H	3.86110300	-2.61607000	0.60900800
C	0.68471300	-4.08937800	1.18442300	C	0.34235800	-4.13654400	1.09056000
C	-0.35091100	-4.59869700	1.95862600	C	1.39762900	-4.94990300	0.69489600
H	-2.45488400	-4.48995200	2.42470000	H	3.50593800	-5.05297200	0.25013300
H	1.69241600	-4.46202900	1.29255400	H	-0.65710400	-4.53427100	1.18508500
H	-0.14747800	-5.39756600	2.66368300	H	1.21707400	-6.00176800	0.50093600
N	1.50573200	0.78809000	2.44395300	N	-0.52473500	-0.56447600	-2.53402500
N	1.50369800	-2.51176800	-0.54011200	N	-0.52601100	-1.91324000	1.75491400
N	1.50470000	1.72283400	-1.90519700	N	-0.53055200	2.47662300	0.77777700
O	2.71143500	1.51018100	2.15371000	O	-1.71873700	0.22302500	-2.68092300
H	3.14156900	0.99805700	1.42776600	H	-2.19770800	0.12836800	-1.82963700
O	2.71022300	1.11098600	-2.38651400	O	-1.72455400	2.20758700	1.53226000
H	3.14069400	0.73784900	-1.58046500	H	-2.20146900	1.51617600	1.02477500
O	2.70978000	-2.62214800	0.22962000	O	-1.71817300	-2.43524700	1.14364000
H	3.14026100	-1.73758200	0.14915000	H	-2.19707800	-1.65121700	0.79866100
C	1.75993600	0.00778700	3.72221100	C	-0.78039200	-1.88577000	-3.24165000
C	1.75844100	3.22005600	-1.86836200	C	-0.78819600	3.74976200	-0.01243700
C	1.75676200	-3.22854400	-1.85523400	C	-0.78476800	-1.86616100	3.25245700
H	0.38855600	-0.00096700	0.00077300	H	0.57374400	0.00034600	0.00085200
C	2.19259700	0.93806000	4.86691300	Cl	5.25815400	0.00594800	0.00404400
H	1.37877700	1.59833900	5.17612500	C	-1.19490600	-1.66576200	-4.70527300
H	2.48993600	0.33939000	5.73206700	H	-0.37215300	-1.25927600	-5.29820000
H	3.04287500	1.54444000	4.55546500	H	-1.49100800	-2.62076300	-5.14731900
C	0.50456600	-0.76548300	4.14247600	H	-2.04197400	-0.98222700	-4.75741100
H	-0.36525400	-0.11676900	4.26159700	C	0.47042000	-2.77138000	-3.19528400
H	0.26981000	-1.56474000	3.43778200	H	1.34738800	-2.27866700	-3.61894500
H	0.69986300	-1.23644900	5.10897600	H	0.69311200	-3.10069200	-2.17930300
C	2.87029900	-0.99973000	3.40536000	H	0.27586800	-3.66806400	-3.78864400
H	3.03474400	-1.64587600	4.27272200	C	-1.90247500	-2.58674000	-2.46913000
H	2.59184600	-1.62018500	2.55257400	H	-2.06603600	-3.58393300	-2.88796800
H	3.80505200	-0.49519900	3.16488900	H	-1.63562300	-2.68939800	-1.41624600
C	2.18975800	-4.68499300	-1.62241100	H	-2.83655200	-2.02972900	-2.52768600
H	1.37633000	-5.28294400	-1.20448300	C	-1.19787500	-3.24453600	3.79266600
H	2.48622800	-5.13484200	-2.57375200	H	-0.37362700	-3.95966500	3.73868200
H	3.04065300	-4.71844300	-0.94232600	H	-1.49631100	-3.15060300	4.84015000
C	0.50063000	-3.20600800	-2.73399400	H	-2.04304800	-3.63295000	3.22497100
H	-0.36878600	-3.63333100	-2.23087200	C	0.46379900	-1.38128800	3.99875700
H	0.26555700	-2.19622500	-3.07394300	H	1.34213000	-1.99314500	3.78541100
H	0.69513100	-3.80779000	-3.62511700	H	0.68532000	-0.33640500	3.77651200
C	2.86651700	-2.45015200	-2.57002700	H	0.26728000	-1.44729800	5.07159500
H	3.03034200	-2.87799800	-3.56349400	C	-1.90912900	-0.84870400	3.47123000
H	2.58789500	-1.40138700	-2.68050700	H	-2.07502900	-0.71331600	4.54394300
H	3.80166200	-2.49415900	-2.01348500	H	-1.64332800	0.11508400	3.03438600
C	2.86978900	3.44927600	-0.83842400	H	-2.84171500	-1.17961500	3.01627900
H	3.03414900	4.52349100	-0.71227500	C	-1.90862200	3.42880300	-1.00688600
H	2.59231900	3.02050400	0.12535700	H	-2.07374400	4.28986400	-1.66101400
H	3.80431000	2.98903400	-1.15621300	H	-1.63924900	2.56903100	-1.62219800
C	2.18965200	3.74682700	-3.24658900	H	-2.84256500	3.19864600	-0.49599900
H	1.37513100	3.68461100	-3.97223900	C	-1.20616000	4.90606400	0.90989400
H	2.48689500	4.79542600	-3.16058600	H	-0.38471300	5.21766400	1.55939400
H	3.03965500	3.17419300	-3.61706400	H	-1.50329900	5.76603700	0.30387100
C	0.50337200	3.97027600	-1.40731000	H	-2.05330600	4.60751300	1.52686400
H	-0.36703700	3.74936000	-2.02795100	C	0.46251600	4.15568300	-0.80107500
H	0.26958400	3.75923200	-0.36264600	H	1.33858400	4.27750000	-0.16153400
H	0.69851900	5.04282400	-1.48241100	H	0.68761000	3.44165000	-1.59461300
I	-4.75544000	0.00122400	0.00098200	H	0.26636400	5.11786500	-1.28033700
Cl	4.22143200	-0.00103100	-0.00150200	I	-3.87258800	-0.00433900	-0.00250000
<b>[L(HCl)]<sup>-</sup>, 4a, E<sub>0</sub>=-9111.368500 au</b>				<b>[L(HCl)]<sup>-</sup>, 4b, E<sub>0</sub>=-9111.360880 au</b>			
N	-0.76540900	0.01983400	-0.22034900	N	-1.46337500	0.41180800	1.04984000
C	-0.82727200	-1.49230400	-0.04352900	C	-0.92515000	1.78363700	1.44001000
H	0.00155300	-1.86765900	-0.62457900	H	0.09587500	1.60255100	1.73975700
H	-1.77706800	-1.79682100	-0.48831600	H	-1.53324300	2.09272200	2.29367400

C	-0.89258500	0.35845900	-1.69999100	C	-1.35192400	-0.53673100	2.23802100
H	-0.80550300	1.43874000	-1.76264800	H	-1.71394000	-1.49497600	1.88158500
H	-1.89126300	0.02882500	-1.99177200	H	-2.01804400	-0.12110600	2.99710800
C	-1.84280300	0.71420600	0.57828700	C	-2.89643800	0.49410500	0.57828700
H	-1.72347500	0.36560200	1.59327500	H	-2.90709700	1.24228800	-0.20085200
H	-2.79050100	0.34493900	0.18134800	H	-3.46337200	0.86012000	1.43779200
C	-0.71938300	-1.93050600	1.38663200	C	-0.98510000	2.77705600	0.31839100
C	-1.87734400	-2.01652100	2.17006700	C	-2.13809500	3.55505100	0.15314300
C	0.52418500	-2.25013400	1.95662700	C	0.08760000	2.93736900	-0.57406800
C	-1.80056700	-2.31535800	3.52465200	C	-2.27110700	4.41003800	-0.93377500
H	-2.83794400	-1.83447300	1.69953200	H	-2.93191600	3.46431400	0.88705400
C	0.59837700	-2.50030400	3.33219500	C	-0.07473800	3.76024200	-1.69473500
C	-0.55186200	-2.52189800	4.11028300	C	-1.24725700	4.48214500	-1.87776600
H	-2.70441000	-2.36799100	4.12028700	H	-3.17349200	4.99797000	-1.05439000
H	1.57116000	-2.66445700	3.77224300	H	0.72725900	3.81331600	-2.41646100
H	-0.47520100	-2.71958800	5.17400500	H	-1.35458300	5.11656300	-2.75082600
C	-1.76667800	2.21065100	0.50280700	C	-3.42213500	-0.82069600	0.08224700
C	-2.71476300	2.89772600	-0.26154900	C	-4.39484700	-1.47983300	0.84066100
C	-0.76259300	2.92868000	1.17148800	C	-2.95140300	-1.41023500	-1.10220100
C	-2.65749900	4.28081300	-0.38939000	C	-4.88594700	-2.71980000	0.44907100
H	-3.48483000	2.32614100	-0.76900400	H	-4.73960000	-1.01131400	1.75617600
C	-0.69371400	4.31567900	1.01402300	C	-3.42845600	-2.67073600	-1.47388800
C	-1.63465500	4.98654500	0.24194000	C	-4.38927300	-3.31884300	-0.70702000
H	-3.39282800	4.80040900	-0.99263700	H	-5.63239800	-3.22324700	1.05241500
H	0.12749500	4.84831200	1.47106200	H	-3.00523200	-3.14566200	-2.34674900
H	-1.56528500	6.06299100	0.12855900	H	-4.74560400	-4.29727300	-1.01037600
C	0.18144300	-0.30766400	-2.50478700	C	0.06815100	-0.62438100	2.71067400
C	-0.09515000	-1.46842000	-3.23007600	C	0.47661200	0.08483300	3.84302700
C	1.48677100	0.21150500	-2.48469500	C	1.01088100	-1.34191900	1.95995300
C	0.92317100	-2.12901500	-3.90986000	C	1.82018600	0.11563300	4.20223100
H	-1.11049700	-1.85034800	-3.24297200	H	-0.26560700	0.63291600	4.41338100
C	2.51204200	-0.48384600	-3.12967700	C	2.36589100	-1.25855200	2.29047200
C	2.22777600	-1.64443100	-3.84314800	C	2.76479400	-0.53395700	3.40976700
H	0.70287500	-3.03074300	-4.46950200	H	2.13265600	0.67217800	5.07840500
H	3.53186400	-0.14312600	-3.03453000	H	3.10766600	-1.71554600	1.65065900
H	3.03332000	-2.18031200	-4.33214800	H	3.81913700	-0.46746400	3.65241400
N	1.67820500	-2.31702400	1.11230800	N	1.32415800	2.26485000	-0.29996400
N	1.66302300	1.43089000	-1.75670400	N	0.49409100	-2.10336700	0.85627400
N	0.22550800	2.19138300	1.91515500	N	-1.91231800	-0.74209400	-1.84606000
O	2.79201500	-1.84045700	1.87923100	O	1.87665700	1.87195200	-1.56810300
C	3.30491900	-1.28068900	1.25051300	H	2.25088800	0.98208100	-1.41730300
O	1.50707400	2.78639000	1.64888300	O	-1.00221800	-1.75004300	-2.31407400
H	1.83949400	2.21334100	0.92656400	H	-0.25136800	-1.66015100	-1.68962800
O	2.01559400	1.12924300	-0.40066600	O	0.82763500	-1.46381000	-0.37836000
H	2.90115100	0.64256300	-0.37114800	H	1.81122800	-1.45040800	-0.53954400
C	2.01825300	-3.70932100	0.61180800	C	2.35735500	3.12040300	0.41294300
C	0.08625400	2.14571500	3.41000100	C	-2.32918200	0.03604200	-3.06715600
C	2.39568000	2.58917800	-2.33089300	C	0.69902500	-3.58072300	0.84601100
H	0.15806900	0.35208300	0.10496100	H	-0.89552100	0.04331400	0.27324000
C	0.81616900	-4.32158300	-0.11862700	C	1.77502800	3.65437000	1.72777200
H	0.56149800	-3.76129600	-1.01919100	H	1.54096500	2.84678600	2.42271200
H	1.08425200	-5.33382300	-0.43103400	H	2.52821100	4.28659000	2.20419000
H	-0.06746600	-4.39362100	0.51735800	H	0.88125700	4.26078300	1.57314900
C	3.16956500	-3.54470100	-0.38520400	C	3.53960700	2.20218700	0.73328300
H	2.89007200	-2.84593200	-1.17488900	H	3.20199900	1.33585400	1.30302400
H	4.06337100	-3.15243900	0.09670700	H	4.02500700	1.83568000	-0.16974600
H	3.40686800	-4.51348200	-0.83520900	H	4.27822800	2.74725000	1.32828800
C	2.44040300	-4.63650500	1.76316000	C	2.82470300	4.29841700	-0.45670000
H	2.80428000	-5.58369900	1.35583600	H	3.66031500	4.80362600	0.03491900
H	3.24103800	-4.17391800	2.33980800	H	3.16198800	3.93636900	-1.42776800
H	1.60235800	-4.85584200	2.42892600	H	2.02842000	5.03130900	-0.60467700
C	3.92928000	2.47035500	-2.33102200	C	2.16017400	-4.03927800	0.69607700
H	4.28548500	1.73495300	-3.05298200	H	2.74294000	-3.83690300	1.59578700
H	4.36617400	3.43646300	-2.60137100	H	2.18335900	-5.11934500	0.52454500
H	4.30721900	2.18191400	-1.35041100	H	2.65079800	-3.55314200	-0.14932200
C	1.86985200	2.76840800	-3.76322700	C	0.11977500	-4.09526500	2.17253600

H	2.15717000	1.93877200	-4.41042300	H	0.66697900	-3.70194600	3.03106100
H	0.78000000	2.84697300	-3.76718200	H	-0.93122100	-3.81454200	2.27154100
H	2.28404500	3.68807700	-4.18303300	H	0.18894400	-5.18540000	2.19627500
C	1.98530000	3.81908200	-1.50504600	C	-0.13177500	-4.14691500	-0.31197500
H	2.38632200	4.72402000	-1.96997500	H	-0.13031300	-5.23884100	-0.25673100
H	0.89821400	3.89845000	-1.45383000	H	-1.16047800	-3.79045400	-0.25821400
H	2.36489100	3.76529600	-0.48649800	H	0.28044100	-3.85544500	-1.27699600
C	1.20334900	1.22762500	3.92160100	C	-1.05392700	0.67261900	-3.63324700
H	1.07022900	1.04398400	4.99163500	H	-1.31566000	1.37507200	-4.42975900
H	1.18243400	0.27125900	3.39821900	H	-0.51407900	1.21350100	-2.85601400
H	2.18056600	1.67977500	3.75967800	H	-0.38820800	-0.08726800	-4.03925200
C	0.21828000	3.54377500	4.03907400	C	-2.98004400	-0.87177200	-4.12458900
H	-0.62567500	4.18377400	3.77102000	H	-3.94387500	-1.25738800	-3.78397200
H	0.24097400	3.45427800	5.12851300	H	-3.15009000	-0.29969900	-5.04062800
H	1.14318600	4.01965800	3.71247100	H	-2.32383400	-1.71009800	-4.35922300
C	-1.27304800	1.54557000	3.78302400	C	-3.31183200	1.14017600	-2.66864400
H	-2.10117600	2.08450800	3.31739500	H	-4.18219700	0.74419200	-2.14043400
H	-1.33044100	0.49037700	3.51689100	H	-2.82882600	1.90143900	-2.05747000
H	-1.39930300	1.61437600	4.86620500	H	-3.67075700	1.63177400	-3.57607800
Cl	4.59984000	-0.25090000	-0.07696000	I	3.98923800	-1.08327200	-1.43742400
I	-4.44473800	-1.24888800	-1.49799200	Cl	-3.54970700	1.73230400	3.72514900
<b>[L(HCII)]-, 5a, E<sub>0</sub>=-9111.365803 au</b>				<b>[L(HCII)]-, 5b, E<sub>0</sub>=-9111.361302 au</b>			
N	-0.90554000	-0.05741800	-0.24036800	N	-1.68002500	0.10563300	1.10065600
C	-0.87745900	0.50353400	-1.64811600	C	-1.16410800	-0.68600600	2.28575500
H	-0.70811500	1.56659600	-1.53839400	H	-1.16329900	-1.72111600	1.97027100
H	-1.87516300	0.33148000	-2.05624000	H	-1.90432300	-0.54124700	3.07568500
C	-1.86480100	0.71405000	0.63760800	C	-2.98148500	-0.46952400	0.58693800
H	-1.84864100	0.21636600	1.59657200	H	-3.29064700	0.18183800	-0.21796800
H	-2.84960800	0.58499200	0.18400100	H	-3.68389100	-0.37881800	1.41961300
C	-1.26484300	-1.53342300	-0.26574400	C	-1.85239200	1.56774500	1.47742100
H	-0.55807100	-1.99164300	-0.94496400	H	-0.89625200	1.87777800	1.87810600
H	-2.27361500	-1.58171100	-0.68078300	H	-2.61554000	1.57304000	2.25940900
C	0.19498300	-0.15919100	-2.45894200	C	0.20473100	-0.21762900	2.67996000
C	-0.16315400	-1.09462600	-3.43440700	C	0.35650400	0.55980000	3.83219900
C	1.55113700	0.09420600	-2.20070000	C	1.32223700	-0.49080000	1.87577600
C	0.81404700	-1.79801300	-4.12933100	C	1.59690000	1.08889200	4.17032900
H	-1.21570200	-1.27706300	-3.62246400	H	-0.51661300	0.76054200	4.44333100
C	2.52777700	-0.64669400	-2.87181300	C	2.55734700	0.07691300	2.19861700
C	2.15783400	-1.58402300	-3.83033000	C	2.69151300	0.85985300	3.33973500
H	0.52733000	-2.52311900	-4.88236200	H	1.70280800	1.69348400	5.06380400
H	3.57287300	-0.50911100	-2.61917000	H	3.40740700	-0.06704400	1.54169900
C	2.92835800	-2.15258000	-4.33856500	H	3.65642600	1.29635800	3.57067600
C	-1.19063200	-2.13212100	1.10656900	C	-2.24871900	2.38669200	0.28552100
C	-2.36413400	-2.31826100	1.84468500	C	-3.58980100	2.74152500	0.10641000
C	0.05044400	-2.43987000	1.68228600	C	-1.30142300	2.73851500	-0.68693800
C	-2.30628900	-2.75552500	3.16304900	C	-3.99987300	3.39327500	-1.05108500
C	-3.31618000	-2.08884800	1.37737700	H	-4.30541800	2.47139900	0.87564100
C	0.10321600	-2.83026600	3.02336200	C	-1.72881300	3.34887800	-1.86954900
C	-1.06668100	-2.98494200	3.75841400	C	-3.06880400	3.67192600	-2.05064400
H	-3.22016100	-2.88956200	3.72986200	H	-5.04262900	3.65674300	-1.18446500
H	1.06621800	-2.99084800	3.48555400	H	-1.00672400	3.54820500	-2.64784600
H	-1.01010200	-3.28700600	4.79829700	H	-3.38615200	4.14386300	-2.97388100
C	-1.49857700	2.16453400	0.74426500	C	-2.83654900	-1.89348200	0.13789700
C	-2.29708600	3.09829200	0.07453900	C	-3.40207900	-2.89515800	0.93495800
C	-0.36562700	2.60015700	1.44999000	C	-2.12383300	-2.24983600	-1.01836200
C	-1.96891200	4.44840400	0.07470400	C	-3.24642100	-4.23795200	0.61352300
H	-3.16466800	2.73972200	-0.46957700	H	-3.94108100	-2.59739300	1.82810200
C	-0.02772500	3.95657000	1.42096200	C	-1.94932600	-3.60413700	-1.31941700
C	-0.82070200	4.87218800	0.74046400	C	-2.50463300	-4.58925000	-0.51231800
H	-2.59011600	5.15787000	-0.45909600	H	-3.67963500	-5.00203000	1.24822500
H	0.87844700	4.27478100	1.91445600	H	-1.34920100	-3.87064100	-2.17664000
H	-0.53685400	5.91867500	0.72684700	H	-2.35215100	-5.63346300	-0.76187000
N	1.86584200	1.11580600	-1.23084400	N	1.12829700	-1.34724200	0.73017200
N	0.45867000	1.62585800	2.12841400	N	-1.52892000	-1.21039700	-1.82816900
N	1.22033900	-2.30865600	0.85748300	N	0.07642400	2.42494800	-0.42252100
O	2.71263200	0.57800700	-0.19956900	O	1.56887400	-0.67747900	-0.46627200

H	3.67048700	0.40279900	-0.51984700	H	2.57009600	-0.62053200	-0.53433300
O	2.20532900	-1.57525400	1.60437800	O	0.62095600	1.80950900	-1.60300000
H	2.42451200	-0.84706900	0.99281800	H	0.99406000	0.98206200	-1.25021900
O	1.82770800	2.04092900	1.98528400	O	-0.26598000	-1.70498700	-2.30803100
H	2.18178800	1.47156900	1.27095000	H	0.39683000	-1.27662800	-1.73166700
C	2.39384200	2.41327200	-1.81845200	C	1.69403900	-2.74884800	0.86828600
C	1.83948300	-3.60286100	0.39427900	C	0.95016600	3.59797500	-0.05324300
C	0.22860900	1.49882600	3.61787800	C	-2.30447600	-0.81881900	-3.06613900
C	2.99996700	-3.23305600	-0.53245200	C	2.33605900	3.03537100	0.26929000
H	3.44353600	-4.14218600	-0.94760600	H	2.99000600	3.84052200	0.61492400
H	2.64139800	-2.61866200	-1.35488200	H	2.26356400	2.28948300	1.05760600
H	3.77949700	-2.67762000	-0.01270300	H	2.80160600	2.56794300	-0.59739800
C	2.36159000	-4.46175300	1.55777700	C	1.06370100	4.63234700	-1.18496700
H	1.54930000	-4.87049800	2.16209300	H	0.12439700	5.16397800	-1.34993700
H	2.93594800	-5.30133600	1.15791500	H	1.82518600	5.37146600	-0.92338400
H	3.02178000	-3.86899500	2.19239700	H	1.36933200	4.14196800	-2.11010600
C	0.78288800	-4.38016200	-0.39982300	C	0.36462200	4.25547400	1.20214500
H	-0.09524200	-4.61687000	0.20454100	H	-0.65238100	4.61888800	1.04124800
H	0.46551400	-3.82231600	-1.28295500	H	0.36449500	3.56274800	2.04580300
H	1.21924600	-5.32175400	-0.74150000	H	0.98767800	5.11040100	1.47526000
C	1.23948200	0.47169800	4.14029700	C	-1.47289600	0.24106000	-3.79749300
H	0.98282600	0.20032200	5.16844200	H	-2.07698300	0.69407000	-4.58891500
H	1.23013800	-0.42212200	3.52006900	H	-1.14934400	1.01625200	-3.10592200
H	2.24910700	0.87928000	4.12549700	H	-0.58446600	-0.20279400	-4.24402800
C	-1.19022700	0.98272000	3.87256500	C	-3.64717700	-0.20917900	-2.65442300
H	-1.94962300	1.63078600	3.43005900	H	-4.23829600	-0.89277400	-2.04146300
H	-1.31463300	-0.03401500	3.50000600	H	-3.50847500	0.73191300	-2.12255100
H	-1.36482900	0.95980500	4.95093500	H	-4.22361900	0.00649500	-3.55726000
C	0.42846700	2.83757200	4.34808700	C	-2.54748000	-2.01849800	-3.99738400
H	0.38300300	2.66954700	5.42740700	H	-2.99199800	-1.66490900	-4.93149800
H	1.40606700	3.25769500	4.10926300	H	-1.60465800	-2.51271100	-4.23421600
H	-0.34483900	3.56281900	4.08648800	H	-3.22974700	-2.74620400	-3.55306500
C	3.44589000	2.23740200	-2.92784500	C	3.10596500	-2.81434100	1.47574200
H	3.03251100	1.73982300	-3.80680100	H	3.12487900	-2.45480300	2.50580100
H	3.78804800	3.22914200	-3.23769600	H	3.43071600	-3.85861900	1.48080400
H	4.31208200	1.67753400	-2.57191300	H	3.82705900	-2.24619200	0.88530000
C	3.00679800	3.25604800	-0.69671400	C	1.72353100	-3.41408700	-0.51060200
H	3.25328500	4.24037600	-1.10332200	H	1.99177500	-4.46529800	-0.37792300
H	2.31209700	3.38320200	0.12892200	H	0.75385400	-3.35948000	-0.99768200
H	3.92433400	2.80309300	-0.32088200	H	2.47090000	-2.95327100	-1.15718800
C	1.16911100	3.14508900	-2.38654400	C	0.71221400	-3.50762900	1.77271100
H	0.67210900	2.55478700	-3.16007300	H	0.62263400	-3.03488800	2.75355900
H	0.45350400	3.37949000	-1.59675700	H	-0.27435100	-3.56950600	1.31096800
H	1.49020400	4.08353700	-2.84550400	H	1.08024400	-4.52446900	1.93007400
H	0.03542300	0.04929800	0.15950500	I	4.83293300	-0.18009700	-1.05349400
Cl	5.46514800	-0.06536600	-0.92190900	H	-0.98767800	0.03573000	0.34503800
I	-4.70028600	-0.39691400	-1.69133400	Cl	-4.22720900	0.30526400	3.67642700
<b>[L(HClI)]<sup>-</sup>, 6a, E<sub>0</sub>=-9111.361241 au</b>				<b>[L(HClI)]<sup>-</sup>, 6b, E<sub>0</sub>=-9111.360872 au</b>			
O	-2.11743400	-0.02760400	0.69318300	O	1.24227500	-0.80275700	0.91446700
O	-0.87547500	3.73702000	-1.62904700	O	-2.91017200	-1.97251300	-1.24313300
O	-2.96764500	-2.07801600	-0.88228300	O	3.24624000	-0.47457800	-0.93450900
N	-2.24481400	0.12486700	2.10621800	N	1.34153800	-0.82796300	2.34199300
N	-0.02679500	3.23584600	-0.59290600	N	-2.83294300	-0.94145700	-0.25092200
N	-1.66426500	-2.31032700	-1.46617500	N	2.67875900	0.71524500	-1.53045800
N	1.15607300	-0.69767000	0.04862100	N	-0.14033000	2.24904100	0.07926200
C	0.25888000	-1.47551000	1.02078000	C	1.05542800	2.00955900	1.00058300
C	0.13557700	-0.76413800	2.34543600	C	0.61299400	1.61548600	2.38900100
C	1.26879700	-0.80660400	3.17103000	C	-0.00097400	2.61927700	3.15276200
C	1.35149800	-0.07992500	4.35024700	C	-0.56841400	2.35544700	4.39170300
C	0.28927000	0.74372300	4.71157500	C	-0.55500400	1.05285800	4.88225300
C	-0.84416000	0.79355400	3.91318300	C	0.05432800	0.04821500	4.14425200
C	-0.97282200	0.01656900	2.75150300	C	0.68319400	0.30672900	2.91771200
C	-3.33172700	-0.78755300	2.61597200	C	2.77460000	-1.04782300	2.74793300
C	-2.94706900	-2.27209200	2.49442800	C	3.68236200	0.13429000	2.36736700
C	-3.61271000	-0.45969000	4.08930300	C	2.82670300	-1.25401800	4.26855300
C	-4.60020900	-0.47589300	1.80940400	C	3.24509700	-2.34295800	2.07232500

C	0.97981400	0.78664500	0.19877300	C	-1.24171700	1.26287400	0.32761900
C	1.80312000	1.64505500	-0.71555500	C	-2.48059400	1.45105400	-0.50038200
C	3.07966700	1.28945600	-1.15770500	C	-2.90761300	2.70063700	-0.95844200
C	3.72636400	2.05400800	-2.12332600	C	-3.96761100	2.79545300	-1.85435300
C	3.09684700	3.17926200	-2.65542400	C	-4.60628600	1.63947300	-2.30203300
C	1.85661900	3.57815800	-2.17005300	C	-4.23579900	0.39996400	-1.79347600
C	1.22190900	2.84398200	-1.16500500	C	-3.20620200	0.30045400	-0.85433200
C	0.03953400	4.25288600	0.51335700	C	-3.65736400	-1.36213900	0.93908800
C	0.53173500	5.61636700	-0.00075300	C	-5.11919300	-1.63818100	0.54913500
C	-1.37635600	4.38373100	1.08530600	C	-3.01560200	-2.63292200	1.50404200
C	0.97291200	3.74527500	1.61899700	C	-3.60170800	-0.26568400	2.00946900
C	1.06738300	-1.26701300	-1.36362000	C	0.30444900	2.42578300	-1.36613400
C	-0.00386400	-0.68746700	-2.25110100	C	0.36547600	1.17365700	-2.20390200
C	0.33263700	0.37654600	-3.09568700	C	-0.75564000	0.82842000	-2.96741100
C	-0.62708000	1.02318200	-3.86255700	C	-0.80995900	-0.36415900	-3.67665800
C	-1.94993400	0.60185000	-3.80179800	C	0.27364300	-1.23355100	-3.63784600
C	-2.29054900	-0.49945200	-3.02956100	C	1.42338800	-0.87606100	-2.94725300
C	-1.32372300	-1.17148600	-2.28028600	C	1.49363700	0.33556600	-2.25795400
C	-1.76347400	-3.63298100	-2.16000500	C	3.78846600	1.33111900	-2.32594400
C	-0.44173700	-3.92713700	-2.87830000	C	3.25712200	2.56373900	-3.06591500
C	-2.91616500	-3.67640900	-3.17941200	C	4.39466200	0.34969400	-3.34513900
C	-1.98906800	-4.68431000	-1.06505700	C	4.85833000	1.76949000	-1.31692100
H	2.13475500	-0.96069600	0.33881400	H	-0.46712400	3.23421700	0.33921700
H	-0.67674500	-1.64622300	0.51519000	H	1.69242900	1.28763000	0.51688900
H	0.78190500	-2.42397700	1.15182500	H	1.55946000	2.97653200	1.03070500
H	2.11694900	-1.40194600	2.84663500	H	-0.06326800	3.61844000	2.73188400
H	2.24784600	-0.13310000	4.95652100	H	-1.04216900	3.15478000	4.94913400
H	0.34792700	1.36386400	5.59921300	H	-1.03359200	0.81234500	5.82509500
H	-1.65828000	1.45996400	4.16061500	H	0.04388200	-0.97494500	4.49355000
H	-2.05098200	-2.49111500	3.08057900	H	3.35056200	1.05423000	2.85519900
H	-2.77136700	-2.55729900	1.45821700	H	3.70594800	0.28977600	1.29019100
H	-3.75976000	-2.89723300	2.87540400	H	4.70665400	-0.06769000	2.69338400
H	-2.76507500	-0.69359800	4.73392200	H	2.53474500	-0.35750300	4.81632100
H	-4.46366600	-1.05899500	4.42209800	H	3.85237700	-1.50330200	4.55088300
H	-3.86790300	0.59510800	4.20929100	H	2.17747800	-2.07833600	4.57005900
H	-4.79179800	0.59840000	1.80687400	H	2.53830700	-3.15065700	2.26975900
H	-5.45090100	-0.99202700	2.26257600	H	4.22577900	-2.62096000	2.46765800
H	-4.52724600	-0.79650400	0.77225800	H	3.33548500	-2.24350600	0.99250600
H	1.22381800	0.99358300	1.23628000	H	-1.47424100	1.35908700	1.38333000
H	-0.07208100	1.01581500	0.05506900	H	-0.84818600	0.26213600	0.16988300
H	3.56177000	0.39619900	-0.77232300	H	-2.39582700	3.60195700	-0.63589100
H	4.70836100	1.75628500	-2.47232100	H	-4.27614300	3.76940500	-2.21653200
H	3.58170800	3.75702500	-3.43509200	H	-5.40735900	1.70554800	-3.03049600
H	1.35326500	4.44696200	-2.57056300	H	-4.72178000	-0.50686300	-2.12476400
H	-0.07812300	5.93303400	-0.84766500	H	-5.15501500	-2.35345200	-0.27350600
H	1.57787900	5.57091400	-0.31287800	H	-5.63285700	-0.72257100	0.24723600
H	0.44677500	6.36639200	0.79068900	H	-5.65625600	-2.06256800	1.40197600
H	-1.36442400	5.06417800	1.94250100	H	-3.53696900	-2.93163500	2.41855300
H	-1.75131400	3.41005700	1.40292000	H	-1.96289000	-2.46220700	1.73158000
H	-2.06781400	4.76881100	0.33772000	H	-3.06405200	-3.45203200	0.78848000
H	0.58451600	2.83303900	2.07339000	H	-2.58502300	-0.12978300	2.38038400
H	1.03198700	4.50424500	2.40324500	H	-4.22284100	-0.57129600	2.85516700
H	1.98549400	3.56201700	1.25452600	H	-3.98182300	0.69019500	1.64442700
H	0.96037100	-2.33446000	-1.21405500	H	1.26029300	2.93058300	-1.29509300
H	2.04836900	-1.09763600	-1.80038800	H	-0.40364700	3.12831100	-1.79845900
H	1.35561300	0.72485300	-3.12218600	H	-1.61175200	1.48867300	-2.97330100
H	-0.34671300	1.88076400	-4.46088600	H	-1.71304600	-0.62974900	-4.21159200
H	-2.72374100	1.14002800	-4.33483900	H	0.22181400	-2.20104700	-4.12102100
H	-3.31994700	-0.81275500	-2.94659400	H	2.25432800	-1.56112300	-2.87862500
H	0.38619400	-4.03082500	-2.17533000	H	2.93138100	3.34117100	-2.37312200
H	-0.19385800	-3.15052800	-3.60352700	H	2.42780500	2.31171800	-3.72855200
H	-0.53801500	-4.87334900	-3.41602900	H	4.06236600	2.98065800	-3.67543100
H	-2.72963300	-2.99764200	-4.01371400	H	3.67336200	0.09545400	-4.12394900
H	-3.85600500	-3.39597800	-2.70450900	H	4.71119300	-0.56780800	-2.84987000
H	-3.01397200	-4.68916400	-3.58030100	H	5.26449700	0.80828200	-3.82375400
H	-1.98557300	-5.68720900	-1.50085600	H	5.65900300	2.30987000	-1.82940000

H	-2.94263200	-4.51999000	-0.56486200	H	5.28495300	0.90551700	-0.80909200
H	-1.19275700	-4.62458000	-0.31960500	H	4.41647900	2.42846600	-0.56592800
H	-2.54603400	0.78574600	0.27724300	H	0.81669400	-1.66331700	0.65470700
H	-1.69284100	3.19590700	-1.50890100	H	-2.02445100	-2.39170700	-1.18928500
H	-2.77451800	-1.35380100	-0.24889200	H	2.60092200	-0.67422800	-0.22563400
Cl	-3.42265600	2.12102000	-0.86023500	I	0.16109500	-3.64532700	-0.56442600
I	4.12707400	-2.21991800	0.69918900	Cl	-0.62982400	5.14470100	0.61693000
<b>[L(HClI)]<sup>-</sup>, 7a, E<sub>0</sub>=-9111.358638 au</b>				<b>[L(HClI)]<sup>-</sup>, 8a, E<sub>0</sub>=-9111.361402 au</b>			
N	0.16723600	0.18355600	0.17611600	N	-0.77314000	-0.48452700	-0.07869800
C	0.39106700	0.68346400	1.58018500	C	-0.98396300	-1.05831400	1.31049000
H	-0.49207700	0.40948600	2.14802100	H	-0.11416000	-1.67463000	1.50556900
H	0.41317300	1.76584300	1.56741400	H	-1.88061900	-1.67721200	1.23997200
C	1.09059100	0.78244700	-0.89173500	C	-0.55280100	-1.59358900	-1.08490500
H	0.44515000	1.02264700	-1.72780800	H	-0.49011800	-1.10700900	-2.04904300
H	1.76004900	-0.01739300	-1.20901100	H	-1.45532500	-2.20653100	-1.05009100
C	-1.28360100	0.28089600	-0.19748400	C	-1.94562400	0.39549400	-0.48042100
H	-1.43538200	1.28557500	-0.58043100	H	-2.07833800	1.09129100	0.33647900
H	-1.86197200	0.22503900	0.72085000	H	-2.80660100	-0.27334200	-0.54474200
C	1.64714300	0.11752000	2.18267800	C	-1.13575100	0.03500100	2.32591600
C	2.48553600	0.99438900	2.87657400	C	-2.40343800	0.34557900	2.82578000
C	2.01317900	-1.23620800	2.07732400	C	-0.02138500	0.78111400	2.73608600
C	3.66866700	0.55585700	3.45321900	C	-2.57107900	1.40985400	3.70554900
H	2.21212300	2.04196600	2.92441500	H	-3.25326100	-0.24535500	2.50001500
C	3.22703400	-1.66356900	2.62291800	C	-0.20510800	1.87758700	3.58067300
C	4.04375900	-0.77867800	3.31326000	C	-1.47189700	2.18628800	4.06658600
H	4.30995000	1.25692200	3.97437300	H	-3.55687900	1.64383400	4.09024000
H	3.52915200	-2.68627600	2.45540800	H	0.64368500	2.49394000	3.83748800
H	4.98190600	-1.12947000	3.72856000	H	-1.60088100	3.03970700	4.72305100
C	-1.74980900	-0.80255300	-1.12508100	C	-1.67750400	1.11383800	-1.76802900
C	-0.90040000	-1.49426100	-1.98446600	C	-2.17977400	0.60183900	-2.96893100
C	-3.12112500	-1.15802200	-1.05481000	C	-0.88844100	2.27364600	-1.78646500
C	-1.36825300	-2.54282800	-2.77344200	C	-1.84887000	1.19244200	-4.18281400
H	0.15855800	-1.27450900	-2.03676800	H	-2.81666100	-0.27551300	-2.93563000
C	-3.57991400	-2.19193400	-1.87812500	C	-0.50599800	2.82202400	-3.01338700
C	-2.71092700	-2.88620900	-2.71769500	C	-0.98192100	2.28374400	-4.20340000
H	-0.67081800	-3.07570100	-3.40778400	H	-2.23761700	0.78389500	-5.10806200
H	-4.62209300	-2.46559800	-1.87047800	H	0.17563000	3.65994900	-3.02481200
H	-3.09763700	-3.69181100	-3.33254400	H	-0.67739300	2.71928200	-5.14830900
C	1.90394400	1.96493600	-0.45400600	C	0.67703100	-2.39858700	-0.78086500
C	3.28576900	1.79479700	-0.32701700	C	0.51257600	-3.71835000	-0.34811600
C	1.32621600	3.20546600	-0.14036200	C	1.97031300	-1.85806300	-0.88731600
C	4.08835500	2.82496500	0.14665900	C	1.61244300	-4.49514700	-0.00380200
H	3.71515400	0.83244800	-0.58303800	H	-0.49281400	-4.11697900	-0.26458800
C	2.13317700	4.22084300	0.38088700	C	3.07034700	-2.63709900	-0.51648400
C	3.50402900	4.03252200	0.52175600	C	2.88948600	-3.94448800	-0.07876000
H	5.15604700	2.67317700	0.25257800	H	1.47060800	-5.51431500	0.33706000
H	1.66607400	5.14035700	0.70216100	H	4.06718800	-2.20988500	-0.53575400
H	4.11536900	4.83178900	0.92705700	H	3.75630000	-4.52810400	0.20992400
N	1.18453400	-2.14853700	1.30945100	N	1.26177700	0.34379000	2.26374300
N	-0.10025200	3.35754300	-0.26752800	N	2.10732400	-0.48444700	-1.31764900
N	-3.91336800	-0.47584000	-0.09886800	N	-0.51461400	2.84812300	-0.52144300
O	2.03932800	-3.11083500	0.68526300	O	1.91664200	1.45825600	1.61178000
H	2.24034500	-2.75578500	-0.21602500	H	2.38092200	1.00072500	0.86034000
O	-4.01280400	0.90899900	-0.45628700	O	0.89243400	3.14198100	-0.55008300
H	-3.69807000	1.39605900	0.34660700	H	1.22631500	2.61919000	0.20200200
O	-0.55181700	4.04257500	0.91261200	O	2.97761800	0.21775000	-0.42925500
H	-1.28861000	3.47814200	1.25987300	H	3.94619300	-0.08391000	-0.46186900
C	0.16779600	-2.96757800	2.08007200	C	2.17057600	-0.23545700	3.32090400
C	-5.21557500	-0.97441000	0.41033800	C	-1.25459300	4.10462400	-0.14862600
C	-0.58809100	4.12088300	-1.47077900	C	2.54745400	-0.26795900	-2.74923600
H	0.41609200	-0.83142600	0.25460100	C	-0.77368000	4.50245200	1.24950900
Cl	-2.83446200	2.32963100	2.04034700	H	-1.34615900	5.36259700	1.60719700
C	-0.78465300	-2.05149300	2.85233200	H	-0.91394900	3.67558400	1.94220000
H	-0.25602700	-1.39312400	3.54365200	H	0.28295500	4.76910800	1.23508600
H	-1.40819700	-1.45500500	2.18596400	C	-1.00072200	5.26586000	-1.12481400
H	-1.45799000	-2.67635400	3.44312300	H	-1.46203200	5.08875200	-2.09757700



C	0.86668400	-3.91997800	3.06281200	H	-1.42763800	6.18519500	-0.71509800
H	1.38866700	-3.36621500	3.84654800	H	0.07166900	5.41604700	-1.25862500
H	0.12024800	-4.56004700	3.54009000	C	-2.75259700	3.78181500	-0.09415100
H	1.58344400	-4.55076000	2.53835800	H	-3.13247400	3.44075200	-1.05867000
C	-0.63433100	-3.76078000	1.04148600	H	-2.96454100	3.01890800	0.65718900
H	-1.40459800	-4.34919800	1.54727700	H	-3.30125700	4.68539400	0.18247700
H	-1.12458000	-3.08905100	0.33526000	C	2.81257200	1.23371500	-2.91254200
H	0.01616200	-4.43037500	0.48225700	H	2.88986100	1.46826600	-3.97813400
C	-2.12030700	4.04662600	-1.45153200	H	2.00373500	1.81729400	-2.47546700
H	-2.46773900	3.01209400	-1.47776500	H	3.74291400	1.52073400	-2.42451300
H	-2.52147500	4.51106100	-0.55161600	C	1.38707100	-0.68252400	-3.65940200
H	-2.52373600	4.56640100	-2.32513000	H	1.11629700	-1.73130200	-3.51560600
C	-0.13724100	5.59084900	-1.44529400	H	0.51330000	-0.05386800	-3.49587200
H	0.94370700	5.68027400	-1.57294000	H	1.69370300	-0.56359900	-4.70131500
H	-0.61879000	6.13786800	-2.26031700	C	3.80331900	-1.06380700	-3.13902100
H	-0.42427100	6.05202000	-0.49988200	H	4.09384500	-0.78130300	-4.15531300
C	-0.06502600	3.44315900	-2.74217400	H	4.64456300	-0.85177300	-2.47710100
H	1.02484600	3.38235800	-2.75710000	H	3.61348000	-2.13955200	-3.13322400
H	-0.47794500	2.43990700	-2.85794200	C	2.67019000	0.81000300	4.33177700
H	-0.38050100	4.02801900	-3.60948200	H	1.88423600	1.12705500	5.01958400
C	-5.56718100	-0.10024500	1.62845200	H	3.47784300	0.37774700	4.92753400
H	-5.77129500	0.92777200	1.33288900	H	3.06413700	1.67945200	3.80400600
H	-6.45653600	-0.50410500	2.12023800	C	3.36837400	-0.86476300	2.60466500
H	-4.73951400	-0.07729600	2.33824400	H	3.99796200	-1.38133400	3.33370700
C	-5.02985600	-2.41352400	0.91568800	H	3.03322200	-1.58895800	1.86441900
H	-5.93814300	-2.72788600	1.43583900	H	3.99252700	-0.13108100	2.09717300
H	-4.82966000	-3.13048200	0.12157900	C	1.38960400	-1.34029200	4.04563800
H	-4.19800700	-2.45163000	1.62276300	H	0.51796100	-0.95262400	4.57604600
C	-6.35636900	-0.85090100	-0.61856800	H	1.06097100	-2.11199000	3.34645600
H	-7.32144200	-1.00780700	-0.12841500	H	2.04888400	-1.81315000	4.77701800
H	-6.34160600	0.15440900	-1.04191600	Cl	5.85090400	-0.42419900	-0.20990800
H	-6.27821900	-1.56923300	-1.43524200	H	0.08638900	0.08007400	-0.07290600
I	3.07830500	-2.07416000	-2.39833100	I	-4.19196600	-2.69425300	-0.14104200
<b>[L(HClI)]<sup>-</sup>, 8b, E<sub>0</sub> = -9111.357238 au</b>				<b>[L(HBrI)]<sup>-</sup>, 1a, E<sub>0</sub> = -11225.303798 au</b>			
N	-1.48158400	0.01907400	1.31921000	O	-3.80274000	-0.78312800	0.59504600
C	-1.52597400	1.45994800	1.79363000	H	-3.69926600	-0.45476900	-0.33246600
H	-0.50497800	1.71166200	2.05546000	O	-1.98543600	2.95003800	-1.72954900
H	-2.16016900	1.45059400	2.68326400	H	-2.42542300	2.09254400	-1.94298800
C	-0.85572600	-0.86884200	2.37337800	O	3.65737900	-1.91488900	-0.83619900
H	-0.93969600	-1.87824600	1.99360300	H	3.75482500	-1.58170200	0.08456900
H	-1.49061600	-0.75893000	3.25532200	N	-2.64398700	-1.60233000	0.81263600
C	-2.87676700	-0.46580600	0.95682000	N	-1.47330400	2.75923900	-0.40539500
H	-3.27083500	0.27446600	0.27412100	N	2.70379500	-1.00907700	-1.41163900
H	-3.43719200	-0.45139500	1.89539600	N	0.60819400	-0.16240100	0.28089600
C	-2.06487500	2.35735800	0.71914800	H	1.62224400	-0.22573600	0.05303500
C	-3.37529200	2.83481400	0.80892500	C	0.29141300	-1.42861300	1.09388300
C	-1.28319000	2.67647800	-0.40065900	H	-0.07552100	-2.14800900	0.37539400
C	-3.91886800	3.59950000	-0.21800600	H	1.25231600	-1.75766600	1.48516600
H	-3.96357400	2.57934000	1.68384800	C	-0.66961700	-1.19025800	2.22612400
C	-1.85067500	3.40396100	-1.44865800	C	-0.12865800	-0.86991400	3.47840900
C	-3.15943300	3.86699900	-1.35510100	H	0.95013000	-0.88997100	3.59468600
H	-4.93567600	3.96652500	-0.14019200	C	-0.94014400	-0.47177700	4.53183300
H	-1.26892100	3.58645000	-2.34010600	H	-0.49853700	-0.21046800	5.48641700
H	-3.58826600	4.43150800	-2.17563800	C	-2.31625600	-0.37504900	4.33401800
C	-2.83595600	-1.82294200	0.32174300	H	-2.96119600	-0.02748600	5.13394600
C	-3.10056700	-2.95902000	1.09392000	C	-2.87122500	-0.73507400	3.11326300
C	-2.49000100	-1.97195200	-1.02971500	H	-3.93493100	-0.65670200	2.94508300
C	-2.96170400	-4.23170500	0.55259300	C	-2.06473500	-1.18382200	2.05952800
H	-3.39530600	-2.82595200	2.12908300	C	-3.09836900	-3.04724200	0.78229000
C	-2.28914700	-3.25370700	-1.54876000	C	-3.70767900	-3.30020500	-0.60074300
C	-2.52235500	-4.37594200	-0.76233500	H	-2.98880400	-3.06532600	-1.38373900
H	-3.16207300	-5.10498100	1.16210300	H	-4.59166000	-2.68534700	-0.76012300
H	-1.93554300	-3.36018400	-2.56387500	H	-3.98854900	-4.35389200	-0.68637100
H	-2.36246200	-5.36440300	-1.17789400	C	-1.88461800	-3.96491200	0.96505700
C	0.57069600	-0.49607800	2.65772200	H	-1.18016700	-3.85519800	0.13894100
C	0.86681500	0.08258600	3.89624600	H	-2.22682600	-5.00282700	0.97192300

C	1.59996700	-0.68499600	1.71926200	H	-1.36568100	-3.77991200	1.90728300
C	2.16032400	0.48978500	4.20151500	C	-4.14683300	-3.34551300	1.86674100
H	0.05944200	0.22795900	4.60570600	H	-4.53557300	-4.35842500	1.73103700
C	2.89402000	-0.25487100	2.02505500	H	-4.97785900	-2.64389400	1.78568700
C	3.17014700	0.32855900	3.25627700	H	-3.72154800	-3.27837400	2.87017500
H	2.37287000	0.94456800	5.16224000	C	0.37287200	1.11000600	1.06126400
H	3.68594800	-0.34177400	1.28919200	H	0.93729500	0.99830700	1.98341400
H	4.17992300	0.66176400	3.46676300	H	-0.68679400	1.13679000	1.27130600
N	0.08480300	2.24008900	-0.38469200	C	0.82280200	2.33446800	0.31579300
N	1.26510400	-1.26356100	0.43711300	C	2.17399300	2.69246100	0.34766700
N	-2.36117200	-0.77865700	-1.82378200	H	2.85466000	2.09837500	0.94922000
O	0.34072300	1.49207700	-1.59909800	C	2.64169600	3.76595700	-0.40060700
H	0.95930000	0.79245400	-1.27196300	H	3.69443200	4.02188000	-0.37720500
O	-1.14002600	-0.86390100	-2.57929600	C	1.75489500	4.48198500	-1.20263500
O	-0.66605600	-0.06243100	-2.29323500	H	2.11487200	5.30048400	-1.81687400
O	1.82125900	-0.46627900	-0.61221200	C	0.40341600	4.15765600	-1.21507500
H	2.81771500	-0.50186900	-0.65841000	H	-0.29112600	4.69227100	-1.84666100
C	1.10515300	3.34478700	-0.24388100	C	-0.08398300	3.10724200	-0.42961300
C	-3.49427300	-0.52469500	-2.78193700	C	-2.34075000	3.54253800	0.54884500
C	1.63310800	-2.71612100	0.23096200	C	-2.44189300	5.02038700	0.13610400
C	-3.19994700	0.81018800	-3.47183300	H	-2.76785200	5.09514500	-0.90133000
H	-4.04241300	1.09041800	-4.10999300	H	-1.48212000	5.53139300	0.24510400
H	-3.04939700	1.58974100	-2.72833000	H	-3.17114300	5.53225700	0.77005100
H	-2.30451400	0.73951800	-4.08903400	C	-3.72396300	2.88319700	0.51807800
C	-3.64364000	-1.62570900	-3.84543700	H	-3.64938800	1.82758700	0.78339500
H	-4.00135700	-2.56249300	-3.41537600	H	-4.16485300	2.94662700	-0.47597900
H	-4.36776200	-1.30626900	-4.59971900	H	-4.38763700	3.38260600	1.23043800
H	-2.68772600	-1.80089200	-4.34147800	C	-1.77358300	3.44764100	1.97129600
C	-4.78918400	-0.39828500	-1.97058200	H	-0.74934400	3.82037600	2.03361400
H	-5.01073500	-1.30847700	-1.41070000	H	-1.80493200	2.42622900	2.35295200
H	-4.73692800	0.44009600	-1.27366100	H	-2.39216700	4.06054200	2.63159300
H	-5.62096600	-0.21390900	-2.65485100	C	-0.09111600	-0.16057500	-1.05536300
C	1.36880200	-3.04065400	-1.24464300	H	0.15405500	0.78002300	-1.53931400
H	1.37737100	-4.12616900	-1.37735000	H	-1.16226100	-0.17187200	-0.87312100
H	0.40217000	-2.64904400	-1.55758200	C	0.31585200	-1.35638800	-1.87951100
H	2.13647200	-2.60777900	-1.88492900	C	-0.69751900	-2.08178800	-2.51454800
C	0.70481700	-3.55674200	1.11298300	H	-1.70879200	-1.69301900	-2.47153500
H	0.81058500	-3.30008800	2.16971100	C	-0.41461400	-3.26239600	-3.18941600
H	-0.33501000	-3.44276200	0.81167300	H	-1.21656400	-3.81045800	-3.67051000
H	0.97132900	-4.61055300	1.00344600	C	0.89020800	-3.75088500	-3.20952100
C	3.09317000	-3.04125000	0.58295100	H	1.11570800	-4.69394600	-3.69552500
H	3.28986800	-4.08620500	0.32659000	C	1.91191700	-3.02248500	-2.61416700
H	3.80060800	-2.42656700	0.02324700	H	2.92673600	-3.39190200	-2.60864800
H	3.28725600	-2.91591200	1.65034700	C	1.64316600	-1.80205600	-1.98760600
C	1.17801000	4.26559600	-1.47304200	C	3.44057900	-0.11912900	-2.39133000
H	0.30764900	4.91956000	-1.55070900	C	2.45355000	0.89845800	-2.97163500
H	2.06429400	4.89985900	-1.39470500	H	2.05332200	1.55088400	-2.19664800
H	1.26692500	3.66881900	-2.38168000	H	1.62894300	0.41345300	-3.49672900
C	2.46826600	2.68576900	-0.02128200	H	2.98094300	1.52937000	-3.69095800
H	3.21670200	3.45407400	0.18761900	C	4.08888900	-0.92713100	-3.52554100
H	2.42958700	2.00334300	0.82585900	H	3.34121900	-1.37613400	-4.18182200
H	2.81332600	2.12785100	-0.89040400	H	4.72126800	-1.71470400	-3.11346300
C	0.73665100	4.15817800	1.00425700	H	4.71451400	-0.26383200	-4.12880900
H	-0.23471000	4.64677100	0.90885500	C	4.52855700	0.61221300	-1.59831300
H	0.72772500	3.52770000	1.89562200	H	5.30012100	-0.08029200	-1.26510700
H	1.49250500	4.93267700	1.15238300	H	4.10922400	1.09238300	-0.71642000
H	-0.87904000	-0.03353900	0.48860700	H	4.98813900	1.37612200	-2.23136100
Cl	-3.61664800	0.17005000	4.24277500	Br	-3.58322900	0.23566700	-2.43711400
I	5.14651800	-0.12797500	-1.25291700	I	3.76714200	-0.44623200	2.30813200
<b>[L(HBrI)]<sup>-</sup>, 1b, E<sub>0</sub>=-11225.302611 au</b>				<b>[L(HBrI)]<sup>-</sup>, 2a, E<sub>0</sub>=-11225.300322 au</b>			
O	-3.45464500	-0.74134600	0.86386600	N	0.60933800	-0.44686800	-0.00851600
H	-3.35629300	-0.46687500	-0.07656800	C	-0.01240200	0.41147900	1.07406000
O	-1.55561800	3.00531800	-1.61270800	H	-0.15248100	-0.22096000	1.94495000
H	-1.99755600	2.15964600	-1.84909900	H	-1.00630900	0.70557200	0.74979800
O	4.04261800	-1.97412400	-0.36041200	C	0.19840300	-0.00494300	-1.39247300
H	4.07423100	-1.58363400	0.54632000	H	-0.85086800	-0.24899400	-1.46701000

N	-2.31226400	-1.57747300	1.11343900	H	0.78061000	-0.61331600	-2.08281300
N	-1.07576400	2.78868200	-0.28000200	C	0.41261300	-1.95200900	0.18914500
N	3.12180600	-1.10861700	-1.03957900	H	0.26066200	-2.08973300	1.25068500
N	0.96134800	-0.19797300	0.54982500	H	1.36611100	-2.38914000	-0.10629200
H	1.98763600	-0.25928000	0.38785000	C	0.83461900	1.62505400	1.38773400
C	0.61247200	-1.43909300	1.38951500	C	0.18287900	2.85424200	1.52611900
H	0.21979000	-2.16173700	0.68866300	C	2.23124500	1.58106800	1.53001200
H	1.56658300	-1.78264900	1.78350200	C	0.89798900	4.01925700	1.76507900
C	-0.33831100	-1.15178100	2.51776500	H	-0.89408400	2.88505700	1.42602100
C	0.20938500	-0.80197700	3.75888200	C	2.94873100	2.76245400	1.72805000
H	1.28886900	-0.82769000	3.86911700	C	2.28717200	3.97646200	1.84873600
C	-0.59754000	-0.36433500	4.80051900	H	0.36914600	4.96110600	1.85183100
H	-0.15311100	-0.08015900	5.74730000	H	4.02753500	2.71415500	1.74748600
C	-1.97276900	-0.25711400	4.60113000	H	2.85660400	4.88757500	1.99696600
H	-2.61242000	0.12056100	5.39157200	C	-0.68780800	-2.55829100	-0.63703000
C	-2.53394500	-0.64395800	3.39112100	C	-0.33469000	-3.14132500	-1.86045000
H	-3.59692600	-0.55650500	3.22221600	C	-2.04101900	-2.49666100	-0.26923500
C	-1.73265900	-1.13100200	2.35105800	C	-1.30450900	-3.60819900	-2.73798700
C	-2.79454500	-3.01406900	1.12584400	H	0.71508800	-3.17906800	-2.13225400
C	-3.38121800	-3.30562400	-0.25903700	C	-3.01369900	-2.93629300	-1.17506300
H	-2.64483400	-3.10769100	-1.03638000	C	-2.65042200	-3.48263600	-2.39923000
H	-4.25359300	-2.68573600	-0.45849500	H	-1.01202900	-4.03863900	-3.68854900
H	-3.67593600	-4.35744300	-0.31490100	H	-4.05368500	-2.81082600	-0.91245400
C	-1.60171900	-3.94639300	1.36549500	H	-3.42042200	-3.81018900	-3.08932900
H	-0.87881400	-3.88040600	0.55080400	C	0.41984400	1.45806700	-1.64212300
H	-1.96448100	-4.97661700	1.40235100	C	1.72498400	1.93464500	-1.79783000
H	-1.09763800	-3.73694400	2.31059000	C	-0.65897300	2.35620200	-1.68578600
C	-3.86810200	-3.25386100	2.19997800	C	1.97250100	3.29102800	-1.94864100
H	-4.27420500	-4.26316000	2.09139000	H	2.54750300	1.22893000	-1.76780600
H	-4.68355700	-2.53982500	2.07965200	C	-0.39839200	3.72235900	-1.83683000
H	-3.45948100	-3.16079600	3.20822900	C	0.90396600	4.18562800	-1.95876200
C	0.67619100	1.10167100	1.26300100	H	2.99203800	3.64691700	-2.03580300
H	1.17352000	1.02574500	2.22540400	H	-1.23013100	4.41033600	-1.80015600
H	-0.39613400	1.13989500	1.39481900	H	1.08669900	5.25068100	-2.05380700
C	1.18566100	2.29541700	0.50524900	N	2.91519400	0.31474900	1.38376500
C	2.54745300	2.60752700	0.56693900	N	-1.99503200	1.87197700	-1.47050400
H	3.18994700	1.99643200	1.19366100	N	-2.40238400	-1.93041800	0.99818500
C	3.06967700	3.65305500	-0.18468400	O	4.12163900	0.54936900	0.64160900
H	4.12982400	3.87306300	-0.13930200	H	4.05661600	-0.08576100	-0.10887400
C	2.22811500	4.38814300	-1.01784900	O	-3.61651800	-1.19581400	0.79371900
H	2.63090700	5.18559600	-1.63320000	H	-3.44701400	-0.30815800	1.19795800
C	0.86721900	4.11015000	-1.05994100	O	-2.70856900	2.87601700	-0.73607900
H	0.20714200	4.66015300	-1.71483500	H	-2.92167300	2.44661500	0.12627700
C	0.32534300	3.08648600	-0.27443200	C	3.30038900	-0.38146200	2.66788800
C	-1.93611000	3.60037900	0.65802400	C	-2.65837200	-2.91896000	2.11131900
C	-1.98263000	5.07939700	0.23982200	C	-2.82005000	1.55436600	-2.68986400
H	-2.29311000	5.16328600	-0.80152200	H	1.63520800	-0.33083300	0.11944800
H	-1.00715100	5.55727600	0.35933000	C	2.04782700	-0.60136900	3.52176600
H	-2.70147200	5.61729300	0.86396600	H	1.53380800	0.33447500	3.74578500
C	-3.33766000	2.98297400	0.60278500	H	1.34821000	-1.28090600	3.03392600
H	-3.29941200	1.92741500	0.87669600	H	2.34308700	-1.05979800	4.46830600
H	-3.75703200	3.05363500	-0.40006300	C	4.32958600	0.43206400	3.46777600
H	-4.00086100	3.50548700	1.29867800	H	3.89729300	1.36056600	3.84529600
C	-1.39963900	3.49389900	2.09156400	H	4.67323200	-0.15525600	4.32354100
H	-0.36659700	3.83728700	2.17277000	H	5.18942400	0.66866000	2.84100900
H	-1.46807900	2.47583100	2.47694000	C	3.89485000	-1.73845100	2.27664100
H	-2.01330500	4.12756400	2.73661300	H	4.11583200	-2.31771700	3.17745400
C	0.32843900	-0.24650800	-0.81748200	H	3.19757200	-2.30335700	1.65598800
H	0.61109300	0.66972000	-1.32793400	H	4.81333300	-1.61323400	1.70532800
H	-0.75049000	-0.23524500	-0.68378800	C	-4.12952400	0.94355000	-2.17545000
C	0.75358700	-1.48450900	-1.56630800	H	-3.91931800	0.10028400	-1.51505500
C	-0.24144900	-2.25076100	-2.18133500	H	-4.70196600	1.67900400	-1.61126600
H	-1.25588200	-1.86934500	-2.18650200	H	-4.73461000	0.59619000	-3.01834300
C	0.06041600	-3.46849500	-2.77745400	C	-3.10297100	2.81922700	-3.51802000
H	-0.72797500	-4.04638400	-3.24570600	H	-2.18451400	3.21840500	-3.95554200
C	1.36656200	-3.95206700	-2.73461200	H	-3.79281200	2.58284300	-4.33310200

H	1.60652500	-4.92122600	-3.15840000	H	-3.55592100	3.58501500	-2.88839900
C	2.37049800	-3.18706100	-2.15477400	C	-2.09966500	0.52394900	-3.56890900
H	3.38489000	-3.55344200	-2.09722300	H	-1.10261800	0.85808500	-3.86231400
C	2.08384300	-1.93240000	-1.60902200	H	-2.02195200	-0.44679900	-3.07849800
C	3.90364200	-0.27849900	-2.03264200	H	-2.68358900	0.38078000	-4.48155900
C	2.94834000	0.71504200	-2.70145400	C	-2.90879900	-2.09040500	3.37635600
H	2.52812100	1.41026200	-1.97539700	H	-3.80504500	-1.48034400	3.27568100
H	2.13729900	0.20887300	-3.22804200	H	-3.02556300	-2.75391200	4.23827600
H	3.50545300	1.30252600	-3.43515400	H	-2.07310800	-1.41250800	3.56009700
C	4.58882100	-1.14801400	-3.09795300	C	-1.42273000	-3.80095900	2.32448900
H	3.86357300	-1.62494600	-3.75983000	H	-1.65223000	-4.54490300	3.09112000
H	5.19626400	-1.91815500	-2.62021200	H	-1.13329300	-4.33366800	1.41692300
H	5.24492500	-0.52234300	-3.70916400	H	-0.57127100	-3.21927700	2.68206700
C	4.96762200	0.48475800	-1.23616500	C	-3.87513400	-3.81194900	1.81622600
H	5.72518500	-0.19558400	-0.84995000	H	-4.10720000	-4.42048400	2.69456800
H	4.52004200	0.99966000	-0.38863400	H	-4.74140000	-3.19373100	1.58185300
H	5.44951600	1.22084500	-1.88557900	H	-3.68204000	-4.48696200	0.97922100
Br	3.83732600	-0.40467100	2.44704800	I	3.61315900	-1.75848400	-1.86705700
I	-3.34407700	0.16113000	-2.47966500	Br	-3.31139300	1.65088800	2.18270400
<b>[L(HBrI)]<sup>-</sup>, 2b, E<sub>0</sub>=-11225.298454 au</b>				<b>[L(HBrI)]<sup>-</sup>, 3a, E<sub>0</sub>=-11225.297838 au</b>			
N	-0.73137000	-0.79429000	0.24479200	N	0.85374500	0.00009100	-0.00054800
C	-0.94894700	-0.11778900	-1.09832600	C	1.33667600	1.41058600	0.28726700
H	-1.28860800	-0.91115700	-1.75419600	H	0.85340600	2.03271500	-0.45012300
H	0.03519300	0.21397500	-1.43509800	H	2.41156500	1.38901000	0.10233800
C	0.08738500	0.02296400	1.21079900	C	1.33640700	-0.45613100	-1.36588700
H	1.05544600	0.19221500	0.74489900	H	0.85320400	-1.40583200	-1.53573800
H	0.21772500	-0.60676500	2.08632800	H	2.41134400	-0.60540900	-1.25506800
C	-0.09779200	-2.17532400	-0.03297600	C	1.33516700	-0.95466500	1.07754600
H	0.32571800	-2.09873300	-1.02570200	H	0.85124900	-0.62683300	1.98456200
H	-0.93765300	-2.86804300	-0.01509000	H	2.41010700	-0.78444500	1.15227200
C	-1.92477000	1.02648000	-1.10257000	C	1.05629600	1.84560100	1.69497200
C	-1.44099600	2.32698600	-1.26922600	C	2.10219600	1.79597100	2.62364500
C	-3.30248700	0.81765600	-0.94660800	C	-0.22715800	2.23035300	2.11308500
C	-2.30386700	3.41333800	-1.22671900	C	1.87556200	2.07498800	3.96566400
H	-0.37707600	2.47860300	-1.40328500	H	3.08790000	1.49859600	2.27922200
C	-4.16052400	1.91724400	-0.87147700	C	-0.45406900	2.47426000	3.47229400
C	-3.66419600	3.20722300	-1.00904600	C	0.58676000	2.39333700	4.38961200
H	-1.90726300	4.41611200	-1.32976000	H	2.69231500	2.01864700	4.67568300
H	-5.20689300	1.74609600	-0.66397900	H	-1.45956700	2.70061000	3.79426600
H	-4.33929600	4.05341500	-0.93775000	H	0.38923500	2.58295800	5.43921300
C	0.97927400	-2.58124600	0.93490100	C	1.05411500	-2.39108300	0.75008500
C	0.64481500	-3.10420300	2.18889000	C	2.09971000	-3.17081500	0.24256000
C	2.33020700	-2.35889100	0.61743200	C	-0.22959000	-2.94503700	0.87406900
C	1.62748300	-3.33686400	3.14328000	C	1.87254400	-4.47229500	-0.18726100
H	-0.40187000	-3.26332700	2.42342700	H	3.08562600	-2.72425200	0.15755300
C	3.30655600	-2.55283800	1.59977500	C	-0.45702100	-4.24384000	0.40520100
C	2.95734700	-3.03202700	2.85615800	C	0.58349100	-4.99804600	-0.12379900
H	1.35035700	-3.72346000	4.11715800	H	2.68907000	-5.05927100	-0.59115700
H	4.33092000	-2.29744900	1.36942400	H	-1.46267200	-4.63548300	0.44005200
H	3.72449300	-3.17131900	3.61025800	H	0.38554100	-6.00163500	-0.48471300
C	-0.51370700	1.34203800	1.60765900	C	1.05551800	0.54529400	-2.44650000
C	-1.84733000	1.44336400	2.01679600	C	2.10129000	1.37410200	-2.86867400
C	0.28923200	2.49222500	1.57600100	C	-0.22825500	0.71503800	-2.98803000
C	-2.40070000	2.67888500	2.31641100	C	1.87429900	2.39648900	-3.78160100
H	-2.46223100	0.55236000	2.06980800	H	3.08719700	1.22452800	-2.43938100
C	-0.28350700	3.73685700	1.86140800	C	-0.45547300	1.76984900	-3.87918200
C	-1.61959100	3.83056700	2.22080700	C	0.58526400	2.60441800	-4.26867700
H	-3.44530000	2.74295300	2.59607800	H	2.69096500	3.03932600	-4.08852900
H	0.32830100	4.62133700	1.75542200	H	-1.46113300	1.93551900	-4.23573600
H	-2.05557700	4.80266500	2.42513600	H	0.38747800	3.41830400	-4.95795500
N	-3.77466600	-0.53045500	-0.77923000	N	-1.28676700	2.30781600	1.14573200
N	1.66130600	2.36338300	1.18513100	N	-1.28787800	-0.16098400	-2.57034800
N	2.66081600	-1.90414600	-0.70127600	N	-1.28882600	-2.14579500	1.42526900
O	-4.72765000	-0.53085100	0.29502300	O	-2.48875200	1.92278800	1.83025800
H	-4.28016600	-1.08964400	0.97152200	H	-2.94291900	1.29758200	1.21873700
O	3.65067900	-0.87403400	-0.58015200	O	-2.49107900	-2.54495000	0.74937500

H	3.26782900	-0.12692900	-1.09593000	H	-2.94473000	-1.70228500	0.51430000
O	1.99468600	3.46776600	0.33550900	O	-2.48958500	0.62481900	-2.57852500
H	2.13735500	3.03180800	-0.53301700	H	-2.94349200	0.40785900	-1.73116200
C	-4.43673100	-1.17178800	-1.96310100	C	-1.53894100	3.68811700	0.56121900
C	3.18059000	-2.95384900	-1.64594600	C	-1.54103600	-2.33044900	2.91274900
C	2.68409200	2.29286700	2.27935500	C	-1.54105800	-1.35750300	-3.47298100
H	-1.64470900	-1.02101700	0.69499200	H	-0.17452000	0.00048100	-0.00106800
C	-3.48511700	-1.13621200	-3.16435700	C	-1.96340200	4.68622600	1.65035800
H	-3.15861900	-0.12119800	-3.39741700	H	-1.14612900	4.89225400	2.34566300
H	-2.60575900	-1.76031600	-2.99573300	H	-2.25800000	5.63064300	1.18508200
H	-4.00467600	-1.53265000	-4.04014700	H	-2.81355200	4.29394800	2.20793000
C	-5.75794700	-0.47852500	-2.34027900	C	-2.65356500	3.52589500	-0.47760800
H	-5.58233700	0.52430200	-2.73498800	H	-2.81685800	4.47920500	-0.98880500
H	-6.27374100	-1.05930400	-3.11029600	H	-2.37979200	2.77296800	-1.21791400
H	-6.40462100	-0.40819000	-1.46541600	H	-3.58826300	3.21641000	-0.01216600
C	-4.70483100	-2.62990900	-1.57029900	C	-0.28450900	4.21260100	-0.14729900
H	-5.09678800	-3.18477000	-2.42775200	H	0.58798400	4.23373100	0.50832800
H	-3.78180500	-3.10228200	-1.22843000	H	-0.05486000	3.63160800	-1.04183100
H	-5.42557900	-2.68219500	-0.75535000	H	-0.47848300	5.23788700	-0.47157200
C	4.02504200	1.97255100	1.60825700	C	-2.65588300	-2.17535000	-2.81257000
H	3.95781200	1.03283800	1.05807100	H	-2.81993700	-3.09462500	-3.38248900
H	4.30210800	2.76160000	0.90995800	H	-2.38188000	-2.44025100	-1.79049900
H	4.80825100	1.88312500	2.36727800	H	-3.59026100	-1.61701900	-2.77690900
C	2.77645200	3.61636300	3.05782600	C	-1.96577500	-0.91360000	-4.88195300
H	1.85303300	3.81808600	3.60572200	H	-1.14845100	-0.41513800	-5.40859000
H	3.59603400	3.56774700	3.78044400	H	-2.26112700	-1.78879000	-5.46676800
H	2.96637200	4.44155200	2.37056800	H	-2.81553600	-0.23410400	-4.82089800
C	2.32149000	1.15254500	3.23851000	C	-0.28708100	-2.23398800	-3.57296200
H	1.34325900	1.30131100	3.69989200	H	0.58561800	-1.67725600	-3.91936000
H	2.33463400	0.18741900	2.73145500	H	-0.05753900	-2.71805300	-2.62244100
C	3.06673800	1.11573600	4.03712600	H	-0.48154600	-3.02754700	-4.29852100
C	3.28315900	-2.29114200	-3.02403900	C	-2.65529000	-1.34948500	3.29227500
H	4.01501500	-1.48445300	-3.01671900	H	-2.81854700	-1.38396400	4.37345100
H	3.58233300	-3.03147800	-3.77180000	H	-2.38121700	-0.33184400	3.01093700
H	2.32481500	-1.85642900	-3.31243300	H	-3.59008800	-1.59723300	2.79141900
C	2.17465700	-4.11003100	-1.71171800	C	-0.28632600	-1.98001000	3.72119400
H	2.54588400	-4.85992400	-2.41443800	H	0.58590400	-2.55839700	3.41099300
H	2.04049500	-4.59253900	-0.74211400	H	-0.05635200	-0.91486100	3.66587300
H	1.20090800	-3.77234300	-2.07165200	H	-0.48004300	-2.21246100	4.77115900
C	4.55644000	-3.49305100	-1.21972000	C	-1.96616400	-3.77268500	3.23184300
H	4.95376300	-4.14814500	-1.99995900	H	-1.14918400	-4.47819000	3.06262400
H	5.25071100	-2.66507400	-1.07450500	H	-2.26115200	-3.84229000	4.28224200
H	4.49190200	-4.07114600	-0.29538400	H	-2.81626900	-4.05872900	2.61294100
Br	-2.89160600	-2.26948600	2.23251700	I	4.96839900	-0.00142800	0.00046200
I	2.34788600	1.63044800	-2.59228000	Br	-4.26575900	0.00168800	0.00070100
<b>[L(HBrI)]<sup>-</sup>, 3b, E<sub>0</sub>=-11225.290918</b>				<b>[L(HBrI)]<sup>-</sup>, 4a, E<sub>0</sub>=-11225.293278 au</b>			
N	-1.34812300	0.00065700	-0.00006300	N	-1.01456700	0.01818400	-0.21103400
C	-1.82962200	1.20882100	0.78410400	C	-1.03153800	-1.49870100	-0.06111800
H	-1.33457300	1.14284800	1.74068900	H	-0.19307500	-1.83981100	-0.64938300
H	-2.90329300	1.05683900	0.90696000	H	-1.97272400	-1.82291000	-0.51008300
C	-1.82961900	-1.28227800	0.65469200	C	-1.16243900	0.38243000	-1.68358700
H	-1.33487300	-2.07786300	0.11919300	H	-1.09917100	1.46489000	-1.72589200
H	-2.90334900	-1.31235100	0.46206600	H	-2.15680800	0.03717100	-1.97199100
C	-1.83200200	0.07526700	-1.43763000	C	-2.10558200	0.66820200	0.60649000
H	-1.33806700	0.93681000	-1.85979900	H	-1.97544200	0.30043700	1.61337700
H	-2.90562900	0.25716600	-1.36576600	H	-3.04540200	0.28467600	0.20458500
C	-1.56226800	2.50292200	0.07478600	C	-0.90942200	-1.95776000	1.36112300
C	-2.61846400	3.10509800	-0.61867200	C	-2.06476400	-2.09612400	2.14104300
C	-0.28397600	3.08051100	0.03238800	C	0.34329700	-2.24709800	1.92685500
C	-2.40631800	4.24160100	-1.38927600	C	-1.97934700	-2.41771800	3.48977700
H	-3.59813300	2.63927100	-0.57188400	H	-3.03023600	-1.93656800	1.67223700
C	-0.07163500	4.20410000	-0.77424400	C	0.42462000	-2.51945700	3.29773900
C	-1.12255700	4.77607300	-1.48139700	C	-0.72504200	-2.59344100	4.07350600
H	-3.23023700	4.68901800	-1.93291400	H	-2.88145700	-2.51123500	4.08295400
H	0.92964500	4.60020100	-0.85501900	H	1.40153300	-2.66040300	3.73664600
H	-0.93662000	5.64457300	-2.10410500	H	-0.64281800	-2.80801000	5.13349100

C	-1.56534700	-1.18599100	-2.20404400	C	-2.06306500	2.16695800	0.56189700
C	-2.62183500	-2.08736700	-2.37842700	C	-3.04248900	2.84817100	-0.16739500
C	-0.28741800	-1.51153100	-2.68407500	C	-1.05818100	2.89295400	1.22083000
C	-2.41035100	-3.32259900	-2.97838300	C	-3.01738800	4.23428300	-0.26958600
H	-3.60115200	-1.81407700	-1.99737700	H	-3.81092300	2.26994600	-0.66969300
C	-0.07577000	-2.77153800	-3.25486400	C	-1.02217600	4.28397900	1.08848700
C	-1.12702900	-3.66955700	-3.39654200	C	-1.99486400	4.94925800	0.35163100
H	-3.23446600	-4.01691800	-3.09379200	H	-3.77692600	4.74937900	-0.84606300
H	0.92524800	-3.03962600	-3.55833300	H	-0.20130000	4.82459700	1.53648000
H	-0.94166000	-4.64281000	-3.83818200	H	-1.95044000	6.02887700	0.25780600
C	-1.56187800	-1.31509000	2.13001500	C	-0.08207400	-0.25372300	-2.50410300
C	-2.61757900	-1.01460900	2.99853000	C	-0.34478100	-1.40591800	-3.24831400
C	-0.28365000	-1.56818800	2.65107000	C	1.21946400	0.27051000	-2.46080700
C	-2.40486100	-0.91539200	4.36797200	C	0.68701100	-2.05553600	-3.91825500
H	-3.59726000	-0.82155600	2.57202700	H	-1.35754000	-1.79388300	-3.27698100
C	-0.07069600	-1.43121300	4.02734800	C	2.25993900	-0.41811200	-3.08898400
C	-1.12107000	-1.10371200	4.87651200	C	1.99030900	-1.57276100	-3.81810100
H	-3.22836100	-0.66751700	5.02749000	H	0.47874800	-2.95126300	-4.49201400
H	0.93061300	-1.55998400	4.41047400	H	3.27831800	-0.08157700	-2.96472500
H	-0.93469600	-0.99856300	5.93991900	H	2.80606500	-2.10470400	-4.29420800
N	0.78568900	2.47198300	0.77578100	N	1.49906800	-2.26654700	1.08128200
N	0.78537600	-1.90912700	1.75218100	N	1.37946600	1.48796100	-1.72081800
N	0.78268300	-0.56395400	-2.52854500	N	-0.03499400	2.16509500	1.92624300
O	1.98084600	2.68293400	0.00490800	O	2.59646900	-1.76464300	1.85793100
H	2.45941400	1.82645100	0.02770700	H	3.10321100	-1.19177700	1.24013400
O	1.97755400	-1.33759000	-2.32592200	O	1.22083900	2.80841100	1.65445900
H	2.45664900	-0.88931100	-1.59609300	H	1.57811100	2.24776200	0.93400400
O	1.98131000	-1.34788000	2.31952500	O	1.83011900	1.18716700	-0.39509300
H	2.45898600	-0.93888600	1.56609500	H	2.74090400	0.76237000	-0.41225800
C	1.04149800	3.06464100	2.15269600	C	1.88164900	-3.64392800	0.56798600
C	1.03888900	0.33202500	-3.73029000	C	-0.14533200	2.08021700	3.42341000
C	1.03965700	-3.39825100	1.57746600	C	2.03741700	2.67024600	-2.33840100
H	-0.32079000	0.00081100	-0.00118000	H	-0.10207700	0.36925600	0.12172900
Br	-5.16671900	0.00057600	0.00296300	C	0.69675700	-4.28341600	-0.16718300
C	1.45650100	4.54146400	2.05782800	H	0.42077700	-3.71821400	-1.05838100
H	0.63394800	5.16696100	1.70305500	H	0.99601900	-5.28170600	-0.49559200
H	1.75257800	4.90073600	3.04694800	H	-0.18159400	-4.39316300	0.47068100
H	2.30371200	4.65123300	1.38134900	C	3.02577700	-3.43552600	-0.42839700
C	2.16334300	2.23485300	2.78532300	H	2.72246100	-2.74132000	-1.21320000
H	2.32614400	2.56650100	3.81491600	H	3.90848900	-3.01869300	0.05349900
H	1.89694700	1.17687200	2.79698500	H	3.29310500	-4.39262800	-0.88627600
H	3.09774500	2.34150800	2.23603700	C	2.33313800	-4.56957100	1.70916500
C	-0.20930700	2.94378400	3.03117100	H	2.72416900	-5.50090900	1.29078500
H	-1.08609100	3.40813400	2.57620500	H	3.12132600	-4.09023500	2.28925100
H	-0.43229800	1.90364100	3.27336400	H	1.50351800	-4.82122200	2.37389700
H	-0.01458000	3.45898700	3.97488200	C	3.55601000	2.55078300	-2.55784400
C	2.16037600	-3.53271700	0.54153800	H	3.79671300	1.87301100	-3.37797300
H	2.32198000	-4.59043500	0.31419100	H	3.96233300	3.53352400	-2.81508700
H	1.89351700	-3.01388400	-0.38037200	H	4.06349800	2.19294100	-1.66093200
H	3.09553900	-3.11106200	0.90741600	C	1.32169500	2.89697900	-3.67888200
C	1.45534000	-4.05440500	2.90373400	H	1.48410000	2.06770200	-4.36931000
H	0.63359300	-4.05859300	3.62374600	H	0.24620400	3.01555300	-3.52741500
H	1.74990700	-5.09109100	2.72040500	H	1.70852600	3.80714700	-4.14331100
H	2.30368200	-3.52433100	3.33590100	C	1.75361900	3.86812000	-1.42073900
C	-0.21225900	-4.09782700	1.03502100	H	2.07139500	4.78885000	-1.91754600
H	-1.08821300	-3.93568600	1.66571000	H	0.68844700	3.93612100	-1.19615000
H	-0.43639100	-3.78723800	0.01344200	H	2.29429100	3.78866500	-0.47916400
H	-0.01809600	-5.17279800	1.00892600	C	1.01639000	1.19652100	3.89443900
C	2.16005300	1.29536600	-3.32764400	H	0.90629400	0.97959600	4.96084500
H	2.32306200	2.02094900	-4.12983600	H	1.02869700	0.25400500	3.34647800
H	1.89285900	1.83468400	-2.41769100	H	1.97162400	1.69322100	3.73221300
H	3.09459200	0.76689200	-3.14450100	C	-0.05587000	3.46842000	4.08058700
C	-0.21195500	1.15278300	-4.06588200	H	-0.92808100	4.08132100	3.84108300
H	-1.08841900	0.52636700	-4.24131700	H	-0.01049900	3.35618400	5.16717800
H	-0.43579000	1.88261000	-3.28640200	H	0.84455000	3.98630700	3.74955800
H	-0.01659600	1.71250500	-4.98375300	C	-1.47236600	1.41890700	3.80769900

C	1.45517500	-0.48860200	-4.96137900	H	-2.33021800	1.93550400	3.37129400
H	0.63316700	-1.10885900	-5.32648700	H	-1.49359500	0.36866700	3.51820700
H	1.75180100	0.18840600	-5.76683900	H	-1.57964100	1.45790600	4.89437800
H	2.30234300	-1.12908700	-4.71737800	Br	4.65480600	-0.08682100	-0.08337600
I	4.13716700	-0.00086600	-0.00152800	I	-4.65936100	-1.33407200	-1.48933800
<b>[L(HBrI)]<sup>-</sup>, 4b, E<sub>0</sub>=-11225.288500 au</b>				<b>[L(HBrI)]<sup>-</sup>, 5a, E<sub>0</sub>=-11225.291457 au</b>			
N	-1.48359400	0.21302300	0.51279900	N	-1.15964700	-0.06341700	-0.26999300
C	-1.27032700	1.71648800	0.64819400	C	-1.04994700	0.48300200	-1.67959400
H	-0.32331100	1.81376600	1.15677300	H	-0.89880900	1.54899100	-1.57134700
H	-2.08977900	2.06386100	1.28249000	H	-2.01868700	0.29581200	-2.14653200
C	-1.48982100	-0.42853900	1.89572300	C	-2.18076400	0.70628600	0.53710100
H	-1.59953500	-1.49366500	1.72331300	H	-2.21984200	0.21870600	1.50055400
H	-2.36883300	-0.01883500	2.39821900	H	-3.13361700	0.56145800	0.02379300
C	-2.76778800	-0.10128100	-0.21791700	C	-1.49970500	-1.54407500	-0.30058400
H	-2.72090300	0.45043900	-1.14539700	H	-0.74601700	-2.00116200	-0.92812200
H	-3.56648900	0.30944600	0.40460600	H	-2.47927500	-1.60910900	-0.77847400
C	-1.24381500	2.42731900	-0.67159300	C	0.07727500	-0.17598900	-2.41575600
C	-2.44355000	2.89468000	-1.22327000	C	-0.20990200	-1.12653700	-3.40003800
C	-0.04075400	2.62760200	-1.36845400	C	1.41221900	0.09639500	-2.07879100
C	-2.47050200	3.46436000	-2.49005400	C	0.81601200	-1.82575900	-4.02553800
H	-3.35450600	2.79035800	-0.64310100	H	-1.24688800	-1.32385900	-3.64948700
C	-0.08325000	3.15357900	-2.66492500	C	2.43648200	-0.63980200	-2.68004600
C	-1.28858300	3.55854600	-3.22413400	C	2.13656600	-1.59227300	-3.64798400
H	-3.40774000	3.81201300	-2.90864000	H	0.58412500	-2.56283000	-4.78578500
H	0.83939400	3.22872800	-3.22170600	H	3.46349000	-0.48883100	-2.36623000
H	-1.30231300	3.96599300	-4.22914300	H	2.94323100	-2.15740800	-4.10087200
C	-2.95360400	-1.56966900	-0.46228400	C	-1.50616000	-2.12695100	1.08060200
C	-3.95194500	-2.24471800	0.24710300	C	-2.72199000	-2.31681000	1.74561000
C	-2.14245900	-2.27977400	-1.36215600	C	-0.30109200	-2.41708800	1.73649000
C	-4.13751400	-3.61318300	0.08887900	C	-2.74324900	-2.74000100	3.06962100
H	-4.56264500	-1.67929500	0.94291400	H	-3.64476000	-2.10184500	1.21681400
C	-2.31601700	-3.66066900	-1.49404300	C	-0.32913100	-2.79340700	3.08231300
C	-3.30648800	-4.32137200	-0.77713100	C	-1.54152700	-2.95159200	3.74405700
H	-4.90863800	-4.12513600	0.65272000	H	-3.68971000	-2.87716700	3.57931200
H	-1.63862100	-4.20722100	-2.13358100	H	0.60440400	-2.94058500	3.60544200
H	-3.42453400	-5.39349900	-0.89081900	H	-1.54782000	-3.24274700	4.78855500
C	-0.21901200	-0.11575900	2.62669800	C	-1.83714000	2.16185500	0.65064200
C	-0.19819300	0.88042600	3.60603000	C	-2.60143200	3.07962300	-0.07845200
C	0.97288400	-0.75620500	2.25721800	C	-0.75566900	2.61761600	1.42149100
C	1.00672500	1.26739700	4.18369700	C	-2.28821400	4.43326600	-0.07260200
H	-1.12944000	1.36435100	3.88079800	H	-3.42905100	2.70573600	-0.67222800
C	2.18642600	-0.32217900	2.79671200	C	-0.43100500	3.97735700	1.39892800
C	2.19880600	0.68411200	3.75819000	C	-1.18900900	4.87688300	0.65960600
H	1.01860600	2.04488200	4.93895300	H	-2.88184600	5.13007600	-0.65243400
H	3.11777100	-0.73312000	2.43318900	H	0.43870800	4.31082700	1.94512500
H	3.14598200	1.02058900	4.16386800	H	-0.91596700	5.92629100	0.65233700
N	1.19715700	2.30261400	-0.72201000	N	1.65524200	1.13193400	-1.10306200
N	0.84828300	-1.81846700	1.29772000	N	0.03477200	1.65969000	2.16090300
N	-1.08465300	-1.57775200	-2.04577600	N	0.91688200	-2.28447400	0.98491900
O	2.07797800	1.79146000	-1.73684700	O	2.44026800	0.61260900	-0.01438700
H	2.55083500	1.04901300	-1.31216300	H	3.41166700	0.45105600	-0.26922200
O	0.05713000	-2.44855400	-2.08024000	O	1.84954100	-1.53993200	1.78640200
H	0.62477200	-2.07627100	-1.37254200	H	2.10399100	-0.81634500	1.18445500
O	1.33263500	-1.38643200	0.02346000	O	1.40562600	2.08956700	2.09990200
H	2.31114000	-1.19652500	0.03966700	H	1.81028400	1.51568600	1.41777900
C	1.88637400	3.48268900	-0.05861000	C	2.20634700	2.42954100	-1.66876900
C	-1.33603000	-1.17019100	-3.47440100	C	1.57150500	-3.57878400	0.57190700
C	1.29416400	-3.18888200	1.68142200	C	-0.28698400	1.54488000	3.63449400
H	-0.70465600	-0.18139000	-0.03441400	C	2.78063800	-3.20879300	-0.28999100
C	0.94413100	4.13092300	0.96363200	H	3.25518200	-4.11807300	-0.66893300
H	0.69969000	3.44702500	1.77754100	H	2.46517900	-2.60627200	-1.13864600
H	1.45515500	4.99101300	1.40298200	H	3.52514400	-2.64141900	0.26703700
C	0.01876400	4.48994400	0.51056100	C	2.03137900	-4.42057400	1.77348800
C	3.10330800	2.91908000	0.67966400	H	1.18832300	-4.82841900	2.33475300
H	2.79635400	2.13003900	1.36699700	H	2.63330200	-5.26041500	1.41716100
H	3.83320400	2.49396700	-0.00728900	H	2.64994200	-3.81593100	2.43802800

H	3.58748900	3.71522400	1.25272400	C	0.56903000	-4.37366300	-0.27323100
C	2.33244300	4.53614400	-1.08499400	H	-0.34036300	-4.61246700	0.28198200
H	2.93886700	5.29632900	-0.58544900	H	0.29832200	-3.82827000	-1.17933600
H	2.93531400	4.06881100	-1.86343200	H	1.03282900	-5.31442800	-0.57904100
H	1.47800600	5.03666300	-1.54602500	C	0.69975200	0.53404100	4.22969400
C	2.80772200	-3.34720600	1.90829700	H	0.38211200	0.26987500	5.24254000
H	3.13517000	-2.84811500	2.82138300	H	0.73820800	-0.36602900	3.61967300
H	3.04815200	-4.40952700	2.00919900	H	1.70411600	0.95234500	4.27390600
H	3.38464700	-2.94901500	1.07146800	C	-1.71356500	1.01578300	3.80518600
C	0.53004900	-3.53466600	2.96857700	H	-2.45034100	1.65102900	3.30909900
H	0.80040400	-2.86824700	3.78956400	H	-1.80379700	-0.00600100	3.43661700
H	-0.54853800	-3.46950500	2.80844700	H	-1.95522100	1.00187300	4.87067300
H	0.77301700	-4.55712400	3.26736600	C	-0.14714900	2.89300100	4.36131600
C	0.84581400	-4.14140700	0.56628600	H	-0.25815600	2.73516800	5.43739300
H	1.01343000	-5.17378500	0.88474100	H	0.83897900	3.32170300	4.17964500
H	-0.21316400	-4.00533900	0.34653600	H	-0.91023300	3.60691200	4.04433800
H	1.40905800	-3.97370700	-0.35068800	C	3.32393900	2.25332300	-2.71155100
C	-0.08515200	-0.41262400	-3.93631900	H	2.96824200	1.74399300	-3.60874900
H	-0.27027500	0.04220800	-4.91365300	H	3.67601500	3.24519600	-3.00936600
H	0.17231600	0.37579500	-3.22894600	H	4.17313800	1.70498000	-2.29973000
H	0.76774700	-1.08455800	-4.01704300	C	2.74385600	3.28705700	-0.51972900
C	-1.57848400	-2.39069900	-4.37854200	H	3.00351700	4.27080500	-0.91932600
H	-2.51907700	-2.89010800	-4.13441800	H	2.00094400	3.41322000	0.26307600
H	-1.62893900	-2.06699900	-5.42159700	H	3.64312000	2.84741600	-0.08767500
H	-0.76022600	-3.10411900	-4.27874600	C	1.01063300	3.14408400	-2.31498500
C	-2.54709500	-0.23613700	-3.54293500	H	0.56624000	2.54229900	-3.11131900
H	-3.43845100	-0.68600700	-3.09973200	H	0.24734800	3.37754900	-1.57095200
H	-2.34152400	0.71872700	-3.06077500	H	1.34939200	4.08183800	-2.76243100
H	-2.76828000	-0.02854400	-4.59264600	H	-0.24718800	0.05889100	0.18725300
I	4.54335300	-0.57331700	-0.52073200	Br	5.41087500	-0.05171900	-0.52740400
Br	-4.41644700	1.65569800	2.44703600	I	-4.84620300	-0.46746000	-1.95577600
<b>[L(HBrI)]-, 5b, E<sub>g</sub>=-11225.288762 au</b>				<b>[L(HBrI)]-, 6a, E<sub>g</sub>=-11225.287098 au</b>			
N	1.61428600	0.09553400	-0.63314300	O	-1.66895900	-0.95878500	0.87194500
C	1.30555900	-0.62203300	-1.93182000	O	-2.24595800	3.14155500	-1.30903600
H	1.22672100	-1.67060300	-1.67673000	O	-1.74166800	-3.09626800	-0.82763300
H	2.17841800	-0.46180000	-2.56883000	N	-1.70817800	-0.95373400	2.29976000
C	2.79123400	-0.53863000	0.07461100	N	-1.19309600	2.96496900	-0.35639400
H	2.95606200	0.05991900	0.95891900	N	-0.50346000	-2.75357700	-1.49321800
H	3.63794300	-0.42077700	-0.60669000	N	1.52862500	-0.18054900	-0.04454600
C	1.87388000	1.57039400	-0.89137200	C	1.11785300	-1.29347900	0.92760700
H	1.00758200	1.92591400	-1.43348400	C	0.83441700	-0.74546900	2.30447200
H	2.76170500	1.59942200	-1.52798800	C	1.95219000	-0.32896800	3.04242800
C	0.04104100	-0.09456300	-2.54057800	C	1.83059500	0.32060500	4.26260600
C	0.11691800	0.74464000	-3.65631000	C	0.55954400	0.59570100	4.75861300
C	-1.20880100	-0.37574400	-1.96710400	C	-0.55885700	0.18391700	4.04832700
C	-1.03099500	1.32653900	-4.18227000	C	-0.45517400	-0.52843400	2.84397400
H	1.09049300	0.95061500	-4.08764600	C	-2.23915000	-2.27420400	2.79596800
C	-2.35338100	0.24387200	-2.47499400	C	-1.27453900	-3.43639000	2.50431700
C	-2.26241300	1.08785600	-3.57630700	C	-2.47095000	-2.17982700	4.31072400
H	-0.96119200	1.97877900	-5.04524800	C	-3.59807200	-2.49974700	2.11880100
H	-3.31131800	0.09142000	-1.99130400	C	0.76065700	1.08579400	0.20342500
H	-3.16053500	1.56389300	-3.95272600	C	1.10273600	2.24480300	-0.68663400
C	2.06983300	2.31413700	0.39549700	C	2.37844800	2.45293400	-1.21670600
C	3.36469000	2.62019600	0.82686800	C	2.59320900	3.45323400	-2.15917000
C	0.97192900	2.64123100	1.20447300	C	1.52963400	4.25076900	-2.58077000
C	3.57522500	3.19775300	2.07382900	C	0.27348100	4.09636400	-2.00547000
H	4.20003000	2.37098200	0.18093500	C	0.06106100	3.12760600	-1.02144500
C	1.19447100	3.17536800	2.47675300	C	-1.44304500	3.87950400	0.81310700
C	2.48727700	3.44962100	2.90854000	C	-1.54458900	5.34930100	0.37175600
H	4.58261500	3.42397700	2.40324900	C	-2.75824700	3.43132400	1.45898900
H	0.34992600	3.35365100	3.12623900	C	-0.31238600	3.71977300	1.83647000
H	2.64515100	3.86259600	3.89865600	C	1.57118800	-0.69022600	-1.48226200
C	2.54634800	-1.98112300	0.40445000	C	0.29172700	-0.56831500	-2.26856000
C	3.22996900	-2.95137900	-0.33690600	C	0.10102500	0.57010900	-3.06006200
C	1.63046100	-2.38117300	1.39072900	C	-1.09479400	0.79433900	-3.72889500
C	2.99592700	-4.30516500	-0.12921800	C	-2.12394500	-0.13319300	-3.62090400



H	3.92619400	-2.61917000	-1.09989100	C	-1.92805800	-1.30399000	-2.90212700
C	1.38188700	-3.74482400	1.57454800	C	-0.71707300	-1.54794800	-2.25291300
C	2.05722600	-4.69807500	0.82245900	C	-0.10887300	-3.97617400	-2.26228700
H	3.52359100	-5.04433600	-0.72040600	C	1.15904700	-3.67788300	-3.07027100
H	0.63266200	-4.04250500	2.29292200	C	-1.21875900	-4.45261900	-3.21661200
H	1.84465400	-5.75002500	0.97777100	C	0.19678800	-5.06476800	-1.22472500
N	-1.24136600	-1.29592100	-0.85546900	H	2.54740900	-0.01878400	0.16956200
N	0.91711800	-1.37158600	2.14027100	H	0.29186400	-1.81580600	0.47425500
N	-0.34230500	2.38199700	0.68287600	H	1.99115800	-1.94687300	0.95645300
O	-1.87534700	-0.67707200	0.28008900	H	2.93793100	-0.49440200	2.61803000
H	-2.87101200	-0.59175300	0.17151000	H	2.71847700	0.63403400	4.79858100
O	-1.09926700	1.71554200	1.70826300	H	0.43479300	1.14711200	5.68393300
H	-1.41790400	0.92035700	1.24494400	H	-1.55168300	0.42397800	4.40198400
O	-0.41981400	-1.85687900	2.35664600	H	-0.31197600	-3.27677600	2.99674400
H	-0.96085800	-1.37852000	1.69836900	H	-1.11064800	-3.56211500	1.43519100
C	-1.80030300	-2.67100400	-1.17170300	H	-1.69614500	-4.37097900	2.88521600
C	-1.11543200	3.59760700	0.23568500	H	-1.53990400	-2.05450700	4.86414400
C	1.46366100	-1.06901400	3.51777200	H	-2.94129200	-3.10642400	4.64857200
C	-2.42717500	3.09138800	-0.36796900	H	-3.13829400	-1.34927800	4.54924500
H	-2.99483400	3.93194800	-0.77606700	H	-4.23012100	-1.61808400	2.23732900
H	-2.22278300	2.39087700	-1.17462900	H	-4.09152300	-3.36021800	2.57863200
H	-3.05065200	2.58653900	0.36880700	H	-3.50800400	-2.69537700	1.05224500
C	-1.41850600	4.56586000	1.39077000	H	0.95487000	1.33292500	1.24244500
H	-0.51747200	5.06258300	1.75624800	H	-0.29803100	0.85983200	0.11173100
H	-2.10854000	5.33865000	1.04256700	H	3.20521400	1.81534100	-0.91903900
H	-1.89498100	4.02971500	2.21251400	H	3.58388000	3.59071800	-2.57674100
C	-0.29960600	4.31235200	-0.84813200	H	1.68404400	5.00675600	-3.34322200
H	0.67474900	4.64122600	-0.48114600	H	-0.56264100	4.70578700	-2.31841800
H	-0.15226300	3.67004600	-1.71839700	H	-2.28629900	5.44625800	-0.42196600
H	-0.85041400	5.19632700	-1.17807300	H	-0.58471800	5.72522500	0.00978100
C	0.53198200	-0.02834900	4.14921100	H	-1.85484900	5.97082000	1.21643500
H	0.99062300	0.36339300	5.06171600	H	-2.94240200	4.02080700	2.36250900
H	0.35274200	0.79242600	3.45774100	H	-2.71451600	2.37368400	1.72119000
H	-0.43021100	-0.47117900	4.40172500	H	-3.59619300	3.56065900	0.77606200
C	2.86840700	-0.47377200	3.38930700	H	-0.29353500	2.70935200	2.24674900
H	3.54894100	-1.13753800	2.85199800	H	-0.49128100	4.40848600	2.66601600
H	2.84284000	4.09914200	2.89864700	H	0.66607200	3.95433200	1.41305100
H	3.27669700	-0.32436900	4.39174700	H	1.91732900	-1.71267300	-1.39321300
C	1.51478800	-2.32399900	4.40527800	H	2.36279300	-0.12070000	-1.96265400
H	1.78861100	-2.03431000	5.42324000	H	0.88935900	1.30728200	-3.12112300
H	0.53679200	-2.80525700	4.43924800	H	-1.23371200	1.71202700	-4.28627500
H	2.25431400	-3.04399900	4.04865900	H	-3.08868200	0.06005400	-4.07281700
C	-3.08391300	-2.66275800	-2.01961100	H	-2.73315800	-2.01205800	-2.77981100
H	-2.91378700	-2.24849300	-3.01462300	H	2.00918100	-3.45812200	-2.42269100
H	-3.42316200	-3.69523400	-2.14158000	H	1.01370700	-2.84310900	-3.75768000
H	-3.88649000	-2.10580600	-1.53273900	H	1.41424900	-4.56111900	-3.66056600
C	-2.08511600	-3.40834800	0.13964800	H	-1.38870400	-3.72840200	-4.01547900
H	-2.34594400	-4.44264900	-0.09862600	H	-2.15207300	-4.59885600	-2.67355500
H	-1.21565200	-3.40817000	0.79117700	H	-0.92664000	-5.40175300	-3.67454400
H	-2.92571300	-2.96128900	0.67111700	H	0.57576200	-5.96181100	-1.72208100
C	-0.68896000	-3.40846300	-1.93285100	H	-0.70024900	-5.32457300	-0.66408600
H	-0.41709100	-2.88560500	-2.85275300	H	0.95338700	-4.70924800	-0.52149000
H	0.19877500	-3.52625000	-1.30947700	H	-2.43633700	-0.38843800	0.56721600
H	-1.04393900	-4.40336500	-2.21272000	H	-2.77947500	2.32083100	-1.19054400
I	-5.17985800	-0.10645000	0.30152200	H	-1.80936500	-2.38724500	-0.15387900
H	0.79652600	0.00518200	-0.01800100	Br	-4.04882500	0.52200900	-0.50349500
Br	4.71075600	0.37657100	-2.79294100	I	4.90816500	-0.37428900	0.31733800
<b>[L(HBr)]<sup>-</sup>, 6b, E<sub>0</sub>=-11225.286581 au</b>				<b>[L(HBr)]<sup>-</sup>, 7a, E<sub>0</sub>=-11225.284597 au</b>			
O	-1.39723900	-0.76998500	0.96810100	N	0.27410800	0.11168000	0.10705400
O	-1.00322100	3.56176300	-1.10046700	C	0.34473900	0.77594200	1.45766600
O	-2.02054900	-2.69963800	-0.88299700	H	-0.50462700	0.41157000	2.02693600
N	-1.35891600	-0.88449800	2.39422700	H	0.18320600	1.83904300	1.33283600
N	-0.01505800	3.05879800	-0.19285600	C	1.12635700	0.76214500	-0.99051000
N	-0.75087400	-2.62772900	-1.57263200	H	0.48080400	0.82188100	-1.85792500
N	1.87709000	-0.67674900	-0.10332000	H	1.92746800	0.05935700	-1.22030200
C	1.25754100	-1.70901100	0.84036600	C	-1.15219900	-0.08312500	-0.31676900

C	1.16961600	-1.18358000	2.25252100	H	-1.46743600	0.85356100	-0.76760600
C	2.38600500	-1.03752200	2.93575700	H	-1.75240500	-0.19408600	0.58377100
C	2.45831300	-0.44444200	4.18852300	C	1.65123400	0.50125600	2.14970700
C	1.29584200	0.04642200	4.77609300	C	2.28739000	1.57374700	2.78087000
C	0.08204600	-0.09620400	4.11906600	C	2.25613500	-0.76764400	2.18688900
C	-0.01855300	-0.74406700	2.87930400	C	3.50147500	1.40987500	3.43176100
C	-2.10083900	-2.12203900	2.82539100	H	1.83050700	2.55453100	2.71950500
C	-1.40456500	-3.41483400	2.36740900	C	3.49981800	-0.91809100	2.80670900
C	-2.20584400	-2.12141000	4.35719300	C	4.11382900	0.15833800	3.43200700
C	-3.51957300	-2.02619700	2.24818700	H	3.98318800	2.25923000	3.90171900
C	1.42307700	0.71649100	0.21613400	H	3.98562000	-1.88033500	2.74810600
C	2.02071000	1.80382900	-0.63011100	H	5.07917800	0.02193600	3.90648600
C	3.29904100	1.71877700	-1.18858100	C	-1.37443100	-1.28091000	-1.19469500
C	3.73565000	2.68054700	-2.09381000	C	-0.36282100	-1.88679600	-1.93526300
C	2.89388100	3.73354600	-2.45032800	C	-2.67941300	-1.83731100	-1.20437500
C	1.65041000	3.86506200	-1.84304400	C	-0.60216000	-3.03641300	-2.68480700
C	1.22476500	2.93180000	-0.89446100	H	0.65341000	-1.51442800	-1.92412000
C	0.01187000	3.94883900	1.02369800	C	-2.90920000	-2.97207500	-1.98973300
C	0.30196800	5.41240400	0.65099300	C	-1.88018600	-3.57352700	-2.71150000
C	-1.36241700	3.83918500	1.69102000	H	0.21852000	-3.49082800	-3.22590900
C	1.07603300	3.43983600	2.00319800	H	-3.89686700	-3.39871600	-2.04434300
C	1.75927100	-1.11833700	-1.55724200	H	-2.09196300	-4.46008800	-3.29945100
C	0.52568500	-0.66191500	-2.29302900	C	1.72563800	2.09375100	-0.64560800
C	0.59225000	0.52445100	-3.03278200	C	3.11083500	2.15749500	-0.46675200
C	-0.53276200	1.05926000	-3.64640200	C	0.95050600	3.25143800	-0.47336900
C	-1.75163200	0.40089600	-3.53448700	C	3.72394300	3.34189200	-0.07850900
C	-1.82320300	-0.81493300	-2.86868500	H	3.69466200	1.25581100	-0.61573400
C	-0.68874100	-1.37095800	-2.27556900	C	1.56853700	4.42721300	-0.03808800
C	-0.67812800	-3.87030000	-2.40601000	C	2.94490500	4.47231900	0.15672100
C	0.60632700	-3.84494200	-3.24199900	H	4.79695900	3.37152600	0.06961700
C	-1.89044100	-4.01978100	-3.34260800	H	0.95225600	5.28826100	0.17560000
C	-0.62065000	-5.05039400	-1.42670900	H	3.40781200	5.39348100	0.49435900
H	2.92171600	-0.76604500	0.07600400	N	1.63734000	-1.87979200	1.48835600
H	0.31209400	-2.00168500	0.41438300	N	-0.47644000	3.16411800	-0.65046900
H	1.95251600	-2.54887100	0.79735300	N	-3.64483800	-1.23713100	-0.35792700
H	3.29511400	-1.36758400	2.44111000	O	2.67445800	-2.72658800	0.98520600
H	3.41749600	-0.34126000	4.68189700	H	2.85224500	-2.42434500	0.06009500
H	1.33268000	0.55666700	5.73219000	O	-3.91520600	0.09729500	-0.80883200
H	-0.82507500	0.30960500	4.54493600	H	-3.75792200	0.66384900	-0.01404100
H	-0.39710100	-3.48477800	2.78508100	O	-1.07342600	3.89185700	0.43662200
H	-1.34619400	-3.47480200	1.28202100	H	-1.71721800	3.25680600	0.83614600
H	-1.97274600	-4.28239400	2.71485900	C	0.74558500	-2.79358500	2.30556000
H	-1.23188000	-2.22083900	4.83731000	C	-4.90335700	-1.90276400	0.06694600
H	-2.82166400	-2.97024600	4.66389500	C	-1.02808200	3.71504400	-1.93959000
H	-2.68216400	-1.20548000	4.71225200	H	0.69323100	-0.83071400	0.29562000
H	-3.96533700	-1.06199600	2.49814700	C	-0.37754500	-1.99405500	2.97030000
H	-4.13547400	-2.82519400	2.66955100	H	0.00443600	-1.19612800	3.60909300
H	-3.53916200	-2.12480500	1.16469400	H	-1.06969400	-1.57421300	2.24019000
H	1.67908700	0.86433200	1.26043600	H	-0.95500500	-2.67310300	3.60132300
H	0.33959000	0.74828200	0.13792800	C	1.55783300	-3.52353500	3.38664900
H	3.94866700	0.88506600	-0.93943000	H	1.94808300	-2.82244400	4.12799100
H	4.72203100	2.59133800	-2.53423600	H	0.91285400	-4.23864300	3.90360700
H	3.21466600	4.46408800	-3.18524300	H	2.39059600	-4.06422100	2.93872000
H	0.98555000	4.67653300	-2.10328900	C	0.13245400	-3.79820900	1.32266000
H	-0.40158600	5.74724100	-0.11220600	H	-0.54523100	-4.46769100	1.85919800
H	1.32023300	5.53583800	0.27512500	H	-0.43686000	-3.28306400	0.54699600
H	0.18689200	6.04892900	1.53272700	H	0.90969900	-4.38854800	0.84115400
H	-1.36320400	4.40946700	2.62489500	C	-2.52947100	3.40057200	-1.94911300
H	-1.60135000	2.79743500	1.90737100	H	-2.70926400	2.32596800	-1.88132200
H	-2.14831500	4.22447600	1.04353200	H	-3.03342200	3.87875400	-1.11007600
H	0.82989200	2.44158300	2.36737100	H	-2.97462100	3.76447900	-2.87944400
H	1.10345400	4.10818400	2.86744000	C	-0.81088500	5.23272500	-2.05857400
H	2.07377100	3.42531200	1.56080300	H	0.24790900	5.47808700	-2.16573800
H	1.85316100	-2.19668400	-1.51929700	H	-1.33501300	5.61126800	-2.94021200
H	2.65076200	-0.73219200	-2.04489900	H	-1.20616600	5.73672200	-1.17624700
H	1.53289000	1.05384300	-3.09453600	C	-0.35636500	3.00495000	-3.12019500

H	-0.46227300	2.00799400	-4.16330300	H	0.72967800	3.11366800	-3.10186400
H	-2.65426300	0.83932000	-3.94094700	H	-0.60699600	1.94338500	-3.14234200
H	-2.77171800	-1.31406200	-2.74326700	H	-0.72197500	3.44561000	-4.05072900
H	1.49801400	-3.86646400	-2.61361000	C	-5.49470200	-1.03588000	1.19382000
H	0.65123200	-2.96722200	-3.88853200	H	-5.81979000	-0.06608500	0.81999500
H	0.62852700	-4.73379500	-3.87694800	H	-6.35785300	-1.54715900	1.62894800
H	-1.89894500	-3.23694300	-4.10325100	H	-4.75195200	-0.85405900	1.97126700
H	-2.81961800	-3.96581000	-2.77602900	C	-4.55774000	-3.27049100	0.67616700
H	-1.84478100	-4.98717000	-3.85054200	H	-5.45507700	-3.69088100	1.13699700
H	-0.47578600	-5.98580600	-1.97415500	H	-4.18279900	-3.98883700	-0.05034900
H	-1.54292600	-5.11799900	-0.85117200	H	-3.79877100	-3.14674500	1.45207400
H	0.21191300	-4.91953700	-0.73161600	C	-5.94832700	-2.00239500	-1.06169100
H	-2.03890400	-0.03609400	0.77057900	H	-6.92127000	-2.28002900	-0.64642700
H	-1.73213900	2.91079500	-1.00993700	H	-6.04221000	-1.02758100	-1.54234600
H	-1.89860300	-2.04495900	-0.16512500	H	-5.69110300	-2.73806600	-1.82417000
I	-3.69126300	1.37531600	-0.28709300	I	3.66060000	-1.81570700	-2.15394700
Br	4.90316800	-1.49731700	0.16070300	Br	-3.19298200	1.89430600	1.82876400
<b>[L(HBrI)]<sup>-</sup>, 8a, E<sub>0</sub> = -11225.287185 au</b>				<b>[L(HBrI)]<sup>-</sup>, 8b, E<sub>0</sub> = -11225.284774 au</b>			
N	-1.04794400	-0.49679500	-0.08539200	N	1.46408000	-0.34828300	0.81634300
C	-1.25942800	-1.08351500	1.29826500	C	1.59097300	-1.85467900	0.68339000
H	-0.37501200	-1.67612600	1.50089200	H	0.62524600	-2.25438100	0.96952000
H	-2.13728500	-1.72718200	1.21366600	H	2.35617100	-2.14665000	1.40677400
C	-0.78132200	-1.59376400	-1.09371200	C	1.00934200	0.02735600	2.21016500
H	-0.72285100	-1.10095800	-2.05496300	H	1.02278800	1.10845200	2.24104600
H	-1.66474700	-2.23455700	-1.07201400	H	1.77801700	-0.36342000	2.88087800
C	-2.24103000	0.34965400	-0.49870300	C	2.77934300	0.33102400	0.46859100
H	-2.40551200	1.03698500	0.31958300	H	3.05832400	-0.05987900	-0.50016900
H	-3.08051000	-0.34446400	-0.57758800	H	3.48819400	-0.00533700	1.22995300
C	-1.45431300	-0.00003100	2.31688800	C	1.96090500	-2.23423700	-0.71973000
C	-2.73618300	0.27206300	2.80273600	C	3.27280300	-2.61839100	-1.01041000
C	-0.36667600	0.77525400	2.74429300	C	1.01473500	-2.15050800	-1.75147900
C	-2.94453500	1.32691700	3.68518500	C	3.65341600	-2.88923700	-2.32063400
H	-3.56487000	-0.34118000	2.46404600	H	3.98981800	-2.67891000	-0.19839600
C	-0.59133800	1.86166800	3.59187900	C	1.41540600	-2.37760300	-3.06947000
C	-1.87224400	2.13224500	4.06333800	C	2.72631100	-2.74940000	-3.35132900
H	-3.94116500	1.53106200	4.05877500	H	4.67260100	-3.18699500	-2.53795200
C	0.23666100	2.50012800	3.86229100	H	0.70162000	-2.24267300	-3.86863800
H	-2.03324400	2.97834700	4.72217500	H	3.02485900	-2.92341400	-4.37915600
C	-1.97803100	1.08188100	-1.77952400	C	2.63205900	1.82198400	0.43085800
C	-2.45284600	0.56270600	-2.98848900	C	3.01300600	2.58573500	1.53921400
C	-1.22110600	2.26304800	-1.78332700	C	2.07280200	2.45773900	-0.68767600
C	-2.12567300	1.16907800	-4.19559300	C	2.78377500	3.95638000	1.56661300
H	-3.06535100	-0.33219600	-2.96669100	H	3.47115400	2.08259000	2.38383800
C	-0.84098200	2.82862600	-3.00314400	C	1.78651400	3.82412500	-0.62748400
C	-1.28930500	2.28415400	-4.20104800	C	2.13857500	4.56790200	0.49289400
H	-2.49305800	0.75509700	-5.12712500	H	3.07607600	4.53769700	2.43313600
H	-0.18287100	3.68521100	-3.00290600	H	1.27468000	4.29114000	-1.45623700
H	-0.98711300	2.73335800	-5.14028200	H	1.91043200	5.62721400	0.52634100
C	0.46940500	-2.36174300	-0.77883600	C	-0.34895800	-0.52471200	2.53270800
C	0.34148600	-3.68714800	-0.35092000	C	-0.43679200	-1.55253600	3.47725000
C	1.74663800	-1.78209800	-0.87085400	C	-1.51688400	-0.06340700	1.90122100
C	1.46128500	-4.43051500	0.00302000	C	-1.66117700	-2.13497200	3.78363100
H	-0.65187700	-4.11691400	-0.27884500	H	0.47542000	-1.90154700	3.94907300
C	2.86632400	-2.52773800	-0.49109000	C	-2.74136100	-0.66765900	2.19891500
C	2.72160000	-3.84097700	-0.05775100	C	-2.81099800	-1.69564400	3.13224500
H	1.34738300	-5.45436100	0.34027000	H	-1.71301900	-2.93632600	4.51171300
H	3.85097300	-2.07162300	-0.49866500	H	-3.64181600	-0.36131000	1.67779500
H	3.60315700	-4.39793600	0.23871600	H	-3.77091300	-2.15415600	3.34034000
N	0.93415400	0.37684100	2.28606800	N	-0.33657900	-1.84805200	-1.37142700
N	1.84613000	-0.40403400	-1.29699300	N	-1.39607900	0.98428700	0.91211900
N	-0.87646900	2.84053300	-0.51134000	N	1.82255800	1.65721000	-1.85706600
O	1.56800000	1.51580300	1.65520900	O	-0.78678500	-0.71028000	-2.14776300
H	2.05658400	1.07983200	0.90886600	H	-1.35072000	-0.23405000	-1.48883600
O	0.52218500	3.17388900	-0.52466500	O	0.49518100	1.94493600	-2.33057400
H	0.86230000	2.66076800	0.23098600	H	0.07780700	1.06513500	-2.31559900
O	2.68498700	0.32164700	-0.39620000	O	-2.10543400	0.61297400	-0.27309900

H	3.65657200	0.05282000	-0.42706200	H	-3.09698900	0.59520300	-0.15876000
C	1.84320500	-0.18738700	3.35167900	C	-1.31385600	-2.98895200	-1.52819100
C	-1.65504900	4.07421700	-0.14001500	C	2.78709300	1.86755900	-2.99341100
C	2.29563000	-0.16982100	-2.72296400	C	-1.80494200	2.37522200	1.34441400
C	-1.19700500	4.48055200	1.26335500	C	2.38864700	0.88690900	-4.09990200
H	-1.79821600	5.32132100	1.61991600	H	3.11940300	0.92900000	-4.91212900
H	-1.31740100	3.64702900	1.95175500	H	2.35910700	-0.12719700	-3.70760200
H	-0.14897100	4.77952100	1.25833300	H	1.40644500	1.13347500	-4.50263100
C	-1.42671100	5.24600800	-1.10981100	C	2.76079200	3.30118400	-3.54993700
H	-1.87506000	5.05981400	-2.08691300	H	3.18023500	4.02019500	-2.84457000
H	-1.88296200	6.15108300	-0.69998500	H	3.35536400	3.34606800	-4.46632400
H	-0.35804000	5.42743300	-1.23438700	H	1.73716700	3.59152200	-3.79169700
C	-3.14356600	3.70843900	-0.09885400	C	4.19598000	1.52226700	-2.49652500
H	-3.50549700	3.35914400	-1.06732900	H	4.50230400	2.15746500	-1.66362700
H	-3.33985600	2.93798800	0.64904400	H	4.25882000	0.47808500	-2.18494100
H	-3.72018300	4.59525700	0.17512300	H	4.90741300	1.67180400	-3.31234300
C	2.52354500	1.33890200	-2.87786300	C	-1.78565400	3.25920800	0.09114600
H	2.60271600	1.57963500	-3.94186300	H	-1.82768400	4.30875400	0.39567100
H	1.69679600	1.89969500	-2.44450100	H	-0.87784300	3.08983600	-0.48574900
H	3.44302000	1.64774400	-2.38235300	H	-2.64175600	3.05054900	-0.54930400
C	1.15523800	-0.61105500	-3.64566400	C	-0.75339000	2.87681300	2.33890000
H	0.91153100	-1.66739500	-3.50903400	H	-0.68375000	2.22720100	3.21460700
H	0.26353900	-0.00681500	-3.48730100	H	0.22472500	2.96234600	1.86868200
H	1.46821900	-0.47911300	-4.68407300	H	-1.04371600	3.86983600	2.68981700
C	3.57529300	-0.93154700	-3.10244400	C	-3.19155000	2.43598900	2.00374200
H	3.86948400	-0.63689600	-4.11414600	H	-3.43601600	3.48250900	2.20706400
H	4.40527700	-0.70053100	-2.43193200	H	-3.97465100	2.03496100	1.35762800
H	3.41369100	-2.01183900	-3.10287600	H	-3.20952700	1.89706800	2.95341500
C	2.29851200	0.86192700	4.37922700	C	-1.57073000	-3.37245300	-2.99482700
H	1.49379200	1.15134600	5.05746600	H	-0.71821500	-3.88657400	-3.44225600
H	3.10825400	0.44594200	4.98362300	H	-2.42899600	-4.04686200	-3.04472300
H	2.67711800	1.74650100	3.86563200	H	-1.80518800	-2.48113000	-3.57817300
C	3.06797800	-0.77606300	2.64717400	C	-2.63034200	-2.55884400	-0.87724000
H	3.70151600	-1.28291600	3.37953400	H	-3.33045600	-3.39782400	-0.87714200
H	2.76350500	-1.50146200	1.89486400	H	-2.46442300	-2.24869400	0.15285300
H	3.67996400	-0.02057400	2.15684600	H	-3.11201000	-1.73728400	-1.40509600
C	1.08300800	-1.32015200	4.05497900	C	-0.74836900	-4.19065100	-0.75921500
H	0.19256200	-0.96202900	4.57479700	H	0.20062000	-4.53772300	-1.17197700
H	0.78777900	-2.09531100	3.34483200	H	-0.60651000	-3.95009800	0.29632800
H	1.74432200	-1.77993200	4.79279900	H	-1.46498800	-5.01279300	-0.81943500
H	-0.20655100	0.09391800	-0.06495700	H	0.73576200	-0.02395600	0.16801400
I	-4.39747400	-2.80568500	-0.19738300	I	-5.48581800	0.32457700	-0.51563500
Br	5.75040900	-0.21150400	-0.10843800	Br	4.15001500	-1.50285000	3.21424900
<b>[LCI], 10CI, E<sub>0</sub> = -2191.178656 au</b>				<b>[LCI], 11CI, E<sub>0</sub> = -2191.177840 au</b>			
O	-3.53548200	-1.23493400	-0.40098300	N	0.00021100	0.00034200	-1.58878400
H	-3.13322500	-0.79506700	-1.19405200	C	-1.39022300	0.00199000	-2.04187200
O	-2.34022300	2.90410500	-2.17108900	H	-1.84415900	-0.90313100	-1.66408800
H	-2.27234500	2.00158500	-2.56679800	H	-1.43333800	-0.05421000	-3.15059400
O	3.09377800	-0.34127900	1.53439500	C	0.69378200	-1.20485500	-2.04175900
H	2.14508400	-0.14780800	1.25948000	H	1.70470200	-1.14564600	-1.66423000
N	-2.50092300	-2.14079200	-0.00942600	H	0.76380100	-1.21409700	-3.15048800
N	-2.09869500	2.61342000	-0.79339000	C	0.69725800	1.20324600	-2.04250100
C	3.81260900	-0.00544000	0.32241400	H	0.14047300	2.04957700	-1.66602900
N	0.73656400	-0.16823900	0.31864500	H	0.67074400	1.26760400	-3.15129400
C	0.23185200	-1.56901500	0.46396400	C	-2.18207500	1.21571400	-1.61489500
H	-0.27148700	-1.86927500	-0.45557500	C	-2.37132400	2.24092800	-2.54952100
H	1.10130500	-2.21115500	0.62020100	C	-2.68304100	1.39455200	-0.31185700
C	-0.74168700	-1.69972000	1.60281700	C	-2.98769800	3.44118900	-2.21930600
C	-0.31725700	-1.51194700	2.92187400	H	-1.98534600	2.09398100	-3.55303900
H	0.74313000	-1.38864900	3.11650800	C	-3.27844300	2.62010000	0.02385200
C	-1.23594300	-1.42655000	3.96114600	C	-3.42750900	3.63378400	-0.91226100
H	-0.89383500	-1.26738000	4.97794800	H	-3.09971900	4.22201700	-2.96344000
C	-2.60120100	-1.50948000	3.68396900	H	-3.59285200	2.76621800	1.04635000
H	-3.32662400	-1.40325000	4.48357600	H	-3.88830300	4.57159200	-0.62018200
C	-3.03399900	-1.73522800	2.38255800	C	2.14423000	1.28208300	-1.61496600
H	-4.08952500	-1.78384800	2.15282100	C	3.12689100	0.93361200	-2.54949500

C	-2.11094800	-1.87258300	1.33993400	C	2.54945100	1.62599900	-0.31167600
C	-2.89731300	-3.53846700	-0.34007900	C	4.47441600	0.86648400	-2.21890800
C	-3.03616000	-3.60743600	-1.86643800	H	2.80686800	0.67342400	-3.55324000
H	-2.12764000	-3.24228200	-2.34709800	C	3.90835900	1.52804500	0.02438100
H	-3.85596600	-2.97648000	-2.20802500	C	4.86084600	1.15011700	-0.91158500
H	-3.22843600	-4.63896000	-2.17794700	H	5.20672800	0.57314400	-2.96298400
C	-1.76841800	-4.47484100	0.11070900	H	4.19189900	1.72669000	1.04705600
H	-0.82343900	-4.19937700	-0.36179100	H	5.90326200	1.07949300	-0.61917900
H	-2.01263800	-5.49927300	-0.18272900	C	0.03840300	-2.49744700	-1.61476600
H	-1.63224300	-4.45411100	1.19377500	C	-0.75462600	-3.17386900	-2.54960000
C	-4.22352800	-3.95269800	0.32311200	C	0.13362600	-3.02074900	-0.31167200
H	-4.55100100	-4.92295700	-0.06222600	C	-1.48634700	-4.30755200	-2.21951900
H	-4.99154300	-3.21140100	0.09666000	H	-0.81989400	-2.76619500	-3.55317100
H	-4.11970600	-4.03876100	1.40723800	C	-0.63049900	-4.14887800	0.02390500
C	-0.36969500	0.80671400	0.48851800	C	-1.43387500	-4.78454000	-0.91237500
H	-0.74991500	0.69018300	1.50345100	H	-2.10643200	-4.79490800	-2.96380300
H	-1.19060500	0.58779100	-0.19858800	H	-0.60019700	-4.49420800	1.04642700
C	0.04592900	2.23910100	0.27635900	H	-2.01606200	-5.65224400	-0.62036100
C	1.27780100	2.72355700	0.72899000	N	-2.53304800	0.36962900	0.67756400
H	1.93507900	2.05791700	1.27327100	N	0.94613000	-2.37858300	0.67788600
C	1.68487000	4.02054100	0.44201700	N	1.58686000	2.00857300	0.67770800
H	2.64693300	4.37538400	0.79566600	O	-2.37805100	1.03416700	1.93829600
C	0.86797100	4.84979100	-0.32856900	H	-1.55225300	0.66187300	2.32801100
H	1.19615300	5.85079100	-0.58884000	O	2.08447500	1.54171500	1.93844500
C	-0.37086500	4.39262000	-0.75766500	H	1.34887400	1.01292000	2.32784600
H	-1.00869800	5.01079500	-1.37444000	O	0.29331300	-2.57697200	1.93862300
C	-0.81066000	3.10645500	-0.42102100	H	0.20219200	-1.67567100	2.32812000
C	-3.26973300	3.04500200	0.01797100	C	-3.68042400	-0.59703600	0.84124100
C	-3.59155500	4.53900600	-0.17416000	C	1.32322700	3.48547700	0.84159400
H	-3.70586600	4.75684000	-1.23719200	C	2.35724400	-2.88811200	0.84133400
H	-2.79893100	5.17110600	0.23328800	Cl	-0.00054000	-0.00034900	3.53490800
H	-4.52444000	4.79362400	0.33786700	C	-4.96468600	0.12261900	1.28952500
C	-4.45996100	2.18723100	-0.43035400	H	-5.34335100	0.78569900	0.50711800
H	-4.24977600	1.13159700	-0.25544200	H	-5.74155000	-0.61290300	1.51781300
H	-4.64871700	2.32921800	-1.49390700	H	-4.76759300	0.71045900	2.18600500
H	-5.35674700	2.46964900	0.13058600	C	-3.23960400	-1.61218800	1.90350900
C	-2.97566000	2.75749600	1.49545200	H	-3.98908900	-2.40526200	1.98981000
H	-2.11339700	3.32245000	1.85587300	H	-2.28232000	-2.05632200	1.62745600
H	-2.79183700	1.69393300	1.65303100	H	-3.11924700	-1.13450400	2.87489300
H	-3.84455300	3.04420100	2.09420000	C	-3.94923300	-1.34746300	-0.46749900
C	1.32964600	-0.03139900	-1.04312600	H	-3.11959900	-2.00624200	-0.72511900
H	1.77022400	0.96320600	-1.10525600	H	-4.83491500	-1.97375600	-0.33015300
H	0.53358200	-0.11031500	-1.79320700	H	-4.14800500	-0.66818500	-1.29928700
C	2.39769500	-1.05848900	-1.32261300	C	0.22394500	3.61087300	1.90420900
C	2.16222700	-2.03401600	-2.29115700	H	-0.08937200	4.65615500	1.98984700
H	1.20850000	-2.02565000	-2.80738600	H	-0.63863600	3.00267600	1.62877100
C	3.12595100	-2.98789500	-2.60795400	H	0.57812900	3.26889900	2.87572600
H	2.92595400	-3.73037700	-3.37228800	C	2.58860100	4.23796800	1.28959500
C	4.34108800	-2.97781400	-1.93328700	H	3.35189400	4.23501300	0.50689000
H	5.09972300	-3.72025800	-2.15785700	H	2.33990400	5.27833400	1.51856900
C	4.58684200	-2.02085600	-0.95135400	H	2.99968800	3.77301600	2.18566300
H	5.52684100	-2.04616200	-0.42245700	C	0.80708200	4.09331600	-0.46690100
C	3.63603300	-1.04301000	-0.64135300	H	-0.17835700	3.70400600	-0.72385400
C	5.13407200	0.53429700	0.69958200	H	0.70750700	5.17349700	-0.32965700
C	5.92073800	0.85615700	-0.57857200	H	1.49431000	3.92575500	-1.29902700
H	5.30910800	1.46331200	-1.24980400	C	3.01524300	-1.99865500	1.90395100
H	6.23298400	-0.03622700	-1.11969100	H	4.07712300	-2.24997700	1.98983900
H	6.81576600	1.42570200	-0.31488100	H	2.91983100	-0.94755900	1.62835400
C	5.93680700	-0.38133200	1.64870400	H	2.54178100	-2.13429400	2.87537600
H	6.32999000	-1.26719700	1.14890100	C	2.37694500	-4.36032100	1.28892900
H	5.29228700	-0.70633200	2.46560700	H	1.99255800	-5.01966700	0.50615500
H	6.78642300	0.16602400	2.06743600	H	3.40250300	-4.66485700	1.51723300
C	4.85460000	1.86122000	1.42979400	H	1.76918700	-4.48438300	2.18521600
H	4.26604500	1.68153100	2.32873500	C	3.14165700	-2.74452000	-0.46721100
H	4.29509800	2.53161800	0.77593100	H	3.29674900	-1.69640000	-0.72417900
H	5.79561900	2.34210500	1.71200500	H	4.12716400	-3.19780700	-0.32992300

Cl	-2.07949400	-0.10601600	-2.89302900	H	2.65334100	-3.25610700	-1.29945500
<b>[LCI]<sup>-</sup>, 12Cl, E<sub>0</sub>=-2191.177087 au</b>				<b>[LCI]<sup>-</sup>, 13Cl, E<sub>0</sub>=-2191.176152 au</b>			
N	0.52794900	0.28026600	-1.75070500	N	-0.07538400	-0.04295200	1.25389100
C	-0.19587800	-0.80266600	-2.41437700	C	0.29541200	-1.35251500	1.87206900
H	0.26966600	-1.73321200	-2.10881100	H	-0.50092100	-2.05261000	1.61867200
H	-0.09742700	-0.72736300	-3.51713700	H	0.35080400	-1.23949200	2.96002200
C	1.97315200	0.14847700	-1.91009200	C	-1.42732500	0.38690100	1.71281800
H	2.43013600	0.99192900	-1.40582000	H	-1.57496600	1.38359400	1.31529700
H	2.25721900	0.22568800	-2.98074400	H	-1.42916100	0.43487900	2.80800700
C	0.06287900	1.59534100	-2.19440400	C	0.93263200	0.98209300	1.66870200
H	-1.01914700	1.59945200	-2.10450500	H	1.90526500	0.55997900	1.44225300
H	0.31750000	1.76656500	-3.26098200	H	0.85331200	1.13223400	2.75167000
C	-1.66037700	-0.82656900	-2.05511800	C	1.58852600	-1.88437000	1.31496400
C	-2.60133600	-0.33407900	-2.96449000	C	2.72385900	-1.93354200	2.12292000
C	-2.10242300	-1.28739300	-0.80393200	C	1.66221200	-2.35701300	-0.01404200
C	-3.95230800	-0.26102400	-2.64263500	C	3.92411600	-2.45687400	1.64742500
H	-2.25537400	0.01288600	-3.93321400	H	2.64495300	-1.56538400	3.14012200
C	-3.45532700	-1.17234100	-0.46652700	C	2.87986300	-2.85116900	-0.49076500
C	-4.37392000	-0.66728100	-1.37997900	C	3.99737400	-2.91815300	0.33784800
H	-4.66387600	0.12962700	-3.36228900	H	4.79342800	-2.49821900	2.29393100
H	-3.78122400	-1.44716700	0.52996700	H	2.96932200	-3.17694200	-1.51570300
H	-5.41660700	-0.58373000	-1.09433400	H	4.92994900	-3.30931900	-0.05436900
C	0.64786400	2.70940800	-1.36136200	C	0.76533200	2.28273700	0.92680700
C	1.74131200	3.44278000	-1.83124100	C	0.02792700	3.32350200	1.50368500
C	0.16508500	2.96577100	-0.06924800	C	1.31296500	2.47404200	-0.35166000
C	2.38974500	4.37442700	-1.02727300	C	-0.21785800	4.50348000	0.81022800
H	2.10388900	3.25014900	-2.83593200	H	-0.35996400	3.18557000	2.50698300
C	0.85287800	3.86267600	0.75486900	C	1.02296900	3.64107400	-1.06558500
C	1.95692200	4.56334400	0.28303900	C	0.26172900	4.65147300	-0.49013200
H	3.24366700	4.92346400	-1.40862100	H	-0.79827600	5.29361200	1.27343400
H	0.52440300	3.98745400	1.77632600	H	1.37874600	3.73327000	-2.08202400
H	2.47808100	5.25362100	0.93744600	H	0.04184700	5.55075700	-1.05542000
C	2.54000500	-1.14560100	-1.37373000	C	-2.52799200	-0.51870600	1.22532700
C	2.94247600	-2.12395800	-2.29024900	C	-3.03612100	-1.49795000	2.08633900
C	2.64116900	-1.43055600	-0.00022800	C	-3.04706400	-0.42638000	-0.07593600
C	3.40192900	-3.37114000	-1.88564000	C	-4.00207200	-2.40187900	1.65821300
H	2.85781100	-1.89987700	-3.34870500	H	-2.64266000	-1.54597800	3.09622000
C	3.08102000	-2.69893300	0.40107300	C	-3.99673900	-1.35526700	-0.51198400
C	3.45725200	-3.66176200	-0.52514400	C	-4.47066600	-2.33952100	0.34689000
H	3.68808900	-4.11367800	-2.62217700	H	-4.37394500	-3.16039600	2.33811200
H	3.09026600	-2.92436800	1.45722100	H	-4.33009700	-1.31735700	-1.53947900
H	3.78728700	-4.63714700	-0.18434800	H	-5.20469100	-3.05590300	-0.00695100
N	-1.13694000	-1.86105800	0.09722800	N	0.44757900	-2.31197900	-0.75986000
N	2.23045100	-0.45430200	0.97304900	N	-2.52428800	0.59841500	-0.94331200
N	-1.01363100	2.27158400	0.36219100	N	2.15241700	1.43623900	-0.88304300
O	-1.13284200	-1.13168800	1.33289600	O	0.17611600	-0.94539500	-1.17281800
H	-1.95481200	-1.31764100	1.89862700	H	0.00064000	-0.45966300	-0.25658100
O	-0.72508300	1.65405700	1.62309500	O	1.68734100	1.08358500	-2.19905900
H	-0.83644800	0.70284700	1.42573200	H	1.23534100	0.23700600	-2.00378700
O	1.55182300	-1.15495300	2.02824400	O	-2.21252500	0.00173800	-2.22278500
H	0.60214800	-1.05852200	1.80612100	H	-1.30374200	-0.31336500	-2.05610100
C	-1.21090900	-3.35495400	0.28555300	C	0.13415800	-3.24541500	-1.86091000
C	-2.25681500	3.09377100	0.50335700	C	3.61494800	1.71612400	-0.95248000
C	3.31521000	0.34313300	1.63211700	C	-3.39088800	1.78176000	-1.21487700
C	-3.39578900	2.11387000	0.79990800	C	4.29451400	0.39431700	-1.32762800
H	-4.34448600	2.65409800	0.87345700	H	5.38163000	0.51746400	-1.33725400
H	-3.47237400	1.38136400	-0.00070600	H	4.03292500	-0.37838700	-0.60612400
H	-3.23061600	1.57647900	1.73353500	H	3.97004200	0.06622400	-2.31548200
C	-2.17441500	4.14143800	1.62873500	C	3.97794800	2.79803200	-1.98714900
H	-1.48625900	4.95289600	1.38262700	H	3.63082900	3.78449300	-1.67475500
H	-3.16258300	4.57968300	1.79412300	H	5.06429500	2.84713900	-2.10607500
H	-1.85277400	3.66270600	2.55467700	H	3.53398200	2.55418000	-2.95358500
C	-2.51954600	3.78588000	-0.84001300	C	4.08884600	2.14887200	0.44053900
H	-1.71587100	4.47559400	-1.10751700	H	3.60296300	3.07064400	0.76470600
H	-2.63105000	3.04957000	-1.63855200	H	3.88968500	1.37327100	1.18147900
H	-3.44946700	4.35663300	-0.77287200	H	5.16758600	2.32380400	0.41233700

C	2.62614300	1.28384000	2.62916500	C	-2.54275100	2.76623800	-2.02893100
H	3.34057900	2.03373600	2.98300400	H	-3.08715500	3.70538000	-2.16650800
H	1.78425800	1.78138000	2.15128100	H	-1.61009300	2.97345600	-1.50596800
H	2.24393100	0.72733700	3.48370500	H	-2.30281000	2.34962500	-3.00675200
C	4.03590900	1.17798500	0.56937700	C	-3.77019500	2.42711700	0.12319200
H	4.45532800	0.55265500	-0.22228600	H	-4.28811500	1.72521100	0.77928800
H	3.36375100	1.91494300	0.13091100	H	-2.88912900	2.80821000	0.63987700
H	4.86137000	1.71685000	1.04230300	H	-4.43964500	3.26976400	-0.06848600
C	4.33444900	-0.54109600	2.37438700	C	-4.66985100	1.42132900	-1.99436200
H	5.02315700	0.09121900	2.94230000	H	-5.19471800	2.33649100	-2.28305300
H	3.81972500	-1.20111400	3.07394300	H	-4.41758900	0.86770300	-2.89991700
H	4.92355500	-1.14745200	1.68237700	H	-5.35048800	0.81968600	-1.38874100
C	-2.62456300	-3.92868900	0.49983700	C	0.79082000	-2.86391700	-3.20204400
H	-3.25819100	-3.78177500	-0.37714500	H	1.88020200	-2.89147200	-3.15731500
H	-2.54013700	-5.00615600	0.67390600	H	0.46667200	-3.55514200	-3.98523300
H	-3.10902400	-3.48129300	1.36934800	H	0.49337500	-1.85631100	-3.49417700
C	-0.34094200	-3.73783400	1.48716300	C	-1.39636600	-3.23945500	-2.02744500
H	-0.25043800	-4.82742200	1.51857400	H	-1.68933900	-3.97965500	-2.77821800
H	0.65204200	-3.30325400	1.40542500	H	-1.87324600	-3.48759300	-1.07805900
H	-0.79415000	-3.40357200	2.42057100	H	-1.77266900	-2.26949700	-2.33927500
C	-0.60326800	-3.96250400	-0.98861200	C	0.53057400	-4.66664200	-1.42587300
H	-1.15964600	-3.65481200	-1.87774100	H	1.60621800	-4.83119900	-1.40981800
H	0.43986000	-3.66282500	-1.09931500	H	0.14050000	-4.87295900	-0.42675700
H	-0.64702500	-5.05373400	-0.92986200	H	0.08709000	-5.38219900	-2.12220200
Cl	-3.49530600	-1.51423900	3.09142000	Cl	-0.10664300	0.18094000	5.04578400
<b>[LCI]<sup>-</sup>, 14Cl, E<sub>0</sub>=-2191.174212 au</b>				<b>[LCI]<sup>-</sup>, 15Cl, E<sub>0</sub>=-2191.174002 au</b>			
N	-0.51345800	-0.02554200	1.74635800	N	-0.41977200	-0.23913600	-1.66617900
C	-0.42647700	1.36013900	2.20361400	C	-0.40908600	1.10140200	-2.25622000
H	0.60804500	1.67113900	2.08608600	H	-1.30976700	1.60878600	-1.91769800
H	-0.68804000	1.44797600	3.27798000	H	-0.44226600	1.04618100	-3.36441700
C	0.52323400	-0.87318100	2.33684800	C	-1.64663700	-0.95768000	-1.98823000
H	0.37349100	-1.87254800	1.94535700	H	-1.56247800	-1.94686500	-1.55404300
H	0.39104200	-0.93069300	3.43735100	H	-1.75270900	-1.08787900	-3.08653900
C	-1.84619900	-0.58839200	1.97728300	C	0.78338800	-0.99247400	-2.02951700
H	-2.56846900	0.13030700	1.60319100	H	1.62334900	-0.34265300	-1.82448200
H	-2.03493800	-0.72985900	3.06132400	H	0.79170900	-1.22265700	-3.11596700
C	-1.31795600	2.27398400	1.39977500	C	0.80053000	1.89995100	-1.84339700
C	-2.51962200	2.74217300	1.93633100	C	1.85607500	2.08746700	-2.73927200
C	-0.97595600	2.63128200	0.08577700	C	0.91247400	2.41041800	-0.54040200
C	-3.39099300	3.52745300	1.18743100	C	3.02348600	2.73804200	-2.35335300
H	-2.77447200	2.47370700	2.95666700	H	1.76130000	1.69513600	-3.74685300
C	-1.88212900	3.36626800	-0.68280600	C	2.10920600	3.01280300	-0.13939200
C	-3.07653400	3.82390400	-0.13546400	C	3.15550800	3.18148700	-1.04099900
H	-4.31750200	3.88310700	1.62475100	H	3.83393300	2.86934600	-3.06231800
H	-1.64911900	3.56563800	-1.71805700	H	2.24252200	3.30144800	0.89282300
H	-3.76393200	4.39973600	-0.74559400	H	4.07774400	3.64402300	-0.70760900
C	-2.02692600	-1.90640500	1.26359100	C	0.96074100	-2.27796600	-1.25447000
C	-1.85304700	-3.11099000	1.95068200	C	0.34855800	-3.44943000	-1.71611000
C	-2.27926700	-1.94809200	-0.11584800	C	1.70791200	-2.33863500	-0.06404200
C	-1.85724400	-4.33291700	1.28614800	C	0.38456300	-4.63494000	-0.99149900
H	-1.67641000	-3.07869600	3.02086400	H	-0.18101400	-3.41678200	-2.66257600
C	-2.21235300	-3.16978800	-0.79161500	C	1.70170000	-3.52203200	0.68674500
C	-2.00356100	-4.35622100	-0.09839000	C	1.04226500	-4.65724600	0.23557800
H	-1.70533700	-5.25377200	1.83803700	H	-0.11337200	-5.52130000	-1.36886100
H	-2.30590100	-3.17386300	-1.86789200	H	2.21135300	-3.52147400	1.63883900
H	-1.95160200	-5.29480600	-0.63881400	H	1.05089600	-5.55968700	0.83737100
C	1.94165700	-0.43488700	2.05928700	C	-2.89477200	-0.28796200	-1.46336700
C	2.64967500	0.22446100	3.06993900	C	-3.72618200	0.41365900	-2.34135400
C	2.57920000	-0.66337500	0.82669200	C	-3.22145700	-0.31201400	-0.09780300
C	3.94833500	0.68041600	2.87408000	C	-4.84066700	1.11228000	-1.89005400
H	2.15577000	0.39324800	4.02185900	H	-3.46919000	0.42932100	-3.39579600
C	3.88131200	-0.18842800	0.62729300	C	-4.32285500	0.42133900	0.35751300
C	4.55970300	0.47917100	1.64013700	C	-5.12921700	1.12627900	-0.52724400
H	4.47022500	1.19881800	3.67144200	H	-5.46201000	1.65990500	-2.59023500
H	4.34876900	-0.29727400	-0.34511500	H	-4.50792900	0.46086200	1.42114900
H	5.56257400	0.84720300	1.45413100	H	-5.97628800	1.69106800	-0.15257700

N	0.31808200	2.24391400	-0.39687800	N	-0.23749700	2.29891400	0.31477700
N	1.85246700	-1.33457400	-0.21812700	N	-2.36729100	-1.02974700	0.80454000
N	-2.60824600	-0.71917200	-0.78382300	N	2.47899100	-1.20671400	0.36324200
O	0.13487600	1.45561000	-1.59017300	O	-0.01196800	1.36455400	1.36294100
H	0.79295000	0.72019200	-1.47279400	H	0.78252400	1.61127800	1.91300100
O	-1.80942500	-0.61295200	-1.97086200	O	2.43999500	-1.19517300	1.79744500
H	-1.20023300	0.12162800	-1.75718000	H	2.30778500	-0.25550200	2.04908200
O	1.85781000	-0.53614100	-1.40175900	O	-2.12559000	-0.18963200	1.94136700
H	2.76856500	-0.44775600	-1.82100000	H	-1.28313400	0.26564900	1.71332500
C	1.27727400	3.36609200	-0.67282100	C	-0.86411100	3.55733600	0.81090800
C	-4.04664400	-0.57021600	-1.17379800	C	3.93673400	-1.24593500	-0.04490200
C	2.22313200	-2.75165200	-0.53102300	C	-2.86029600	-2.33906400	1.32356700
C	-4.20661600	0.84847000	-1.72692900	C	4.55988700	0.06463300	0.44629100
H	-5.25295700	1.03498900	-1.98707700	H	5.59887700	0.12944000	0.10749800
H	-3.89165800	1.57566900	-0.98190600	H	4.00481700	0.91353100	0.04932300
H	-3.59318700	0.98157100	-2.61779700	H	4.53746500	0.13461200	1.53256400
C	-4.50333100	-1.58636400	-2.23747100	C	4.68170200	-2.44200100	0.57261700
H	-4.55146900	-2.60018700	-1.83670600	H	4.33540200	-3.39165900	0.15814600
H	-5.50208100	-1.31956600	-2.59508700	H	5.75239700	-2.35232900	0.36736200
H	-3.81736800	-1.57016300	-3.08561100	H	4.53493000	-2.45083500	1.65273400
C	-4.90526900	-0.71637900	0.08874300	C	4.05001500	-1.30593500	-1.57300700
H	-4.80498000	-1.70734600	0.53500300	H	3.55076000	-2.18338300	-1.98879300
H	-4.62961300	0.03255700	0.83365800	H	3.63832100	-0.40806000	-2.03546200
H	-5.95597100	-0.56562100	-0.17324200	H	5.10854800	-1.36369100	-1.84100700
C	1.36858000	-3.17147100	-1.73452500	C	-1.70773700	-2.93985600	2.13695600
H	1.41518500	-4.25840000	-1.85311800	H	-1.96213000	-3.95472300	2.45855400
H	0.33330100	-2.87024700	-1.57862100	H	-0.80430900	-2.97633200	1.52995400
H	1.72768400	-2.70189600	-2.64915200	H	-1.50152300	-2.32898000	3.01469000
C	1.83440600	-3.60082900	0.68628100	C	-3.17839400	-3.25821700	0.13859800
H	2.34422200	-3.25832400	1.59044900	H	-3.91890400	-2.81445400	-0.53085300
H	0.75757200	-3.57734100	0.84934100	H	-2.27644800	-3.49122200	-0.42757700
H	2.13058100	-4.63842400	0.50955400	H	-3.58735400	-4.19823200	0.51888000
C	3.71305900	-2.97306200	-0.84794000	C	-4.11045900	-2.19659800	2.21342400
H	3.86058900	-4.01367500	-1.15469200	H	-4.34072000	-3.15720400	2.68357900
H	4.05796900	-2.32724800	-1.65757700	H	-3.92733000	-1.46190000	2.99826200
H	4.33780900	-2.79226200	0.03022000	H	-4.98333900	-1.88796900	1.63331000
C	0.89369200	4.23815200	-1.88248900	C	-0.03043300	4.34059100	1.84331100
H	0.04952700	4.89634500	-1.66768200	H	0.82944500	4.82974900	1.38333000
H	1.74324900	4.86733300	-2.16079500	H	-0.65039300	5.11983900	2.29750400
H	0.65043200	3.59917300	-2.73254800	H	0.33390700	3.68702800	2.63762000
C	2.64864100	2.73204300	-0.92436600	C	-2.20582100	3.15757000	1.43929700
H	3.40312000	3.51558600	-1.03768400	H	-2.74860000	4.05402200	1.75450500
H	2.92989800	2.09882000	-0.08519000	H	-2.81057000	2.60974800	0.71707100
H	2.67081700	2.12329700	-1.82711300	H	-2.05542500	2.51596700	2.30595300
C	1.35329300	4.22473400	0.59733300	C	-1.13733300	4.43492100	-0.41916400
H	0.40014400	4.70602500	0.82650500	H	-0.21160200	4.75024900	-0.90411500
H	1.65525900	3.61840400	1.45413600	H	-1.74547000	3.89403400	-1.14811700
H	2.10422500	5.00571800	0.45374900	H	-1.68350200	5.33034500	-0.11044700
Cl	4.43492900	-0.04054600	-2.88321500	Cl	2.43432700	1.70763700	3.08207000
<b>[LCI]<sup>-</sup>, 16Cl, E<sub>0</sub>=-2191.173959 au</b>				<b>[LCI]<sup>-</sup>, 17Cl, E<sub>0</sub>=-2191.171325 au</b>			
N	-0.68465500	0.15930200	1.64853700	N	0.11521800	0.11600800	1.28311500
C	-0.13704600	-1.07543900	2.23924100	C	-1.08328100	-0.59543700	1.80394900
H	-0.70725700	-1.89856400	1.82236300	H	-1.94531900	-0.11166500	1.35882800
H	-0.32885600	-1.07435800	3.32841000	H	-1.13810400	-0.47466800	2.89214900
C	-2.11367200	0.26573400	1.99098000	C	-0.01293100	1.58725900	1.48680400
H	-2.47707800	1.20035600	1.56762600	H	0.86393000	2.03007400	1.02991500
H	-2.23182600	0.30726800	3.09011300	H	0.01414900	1.79307800	2.56259300
C	0.05383400	1.34993600	2.10682200	C	1.34023900	-0.34036000	2.00599400
H	1.10699000	1.12979400	1.97941900	H	1.39948400	-1.42121100	1.88077200
H	-0.13356800	1.52591900	3.18232800	H	1.24699200	-0.09334200	3.06941500
C	1.34255500	-1.29847300	2.03615800	C	-1.05714800	-2.05245000	1.42070900
C	2.18021900	-1.15288200	3.14902900	C	-0.62360000	-3.00379700	2.34996400
C	1.91834200	-1.63442900	0.79666600	C	-1.40354300	-2.48209100	0.12975900
C	3.55765200	-1.30743200	3.05538500	C	-0.47960400	-4.34201600	2.00018000
H	1.73148700	-0.89160500	4.10227000	H	-0.37943400	-2.66824500	3.35182800
C	3.30946200	-1.77371200	0.70448100	C	-1.21821300	-3.81953700	-0.23158100



C	4.12126800	-1.61155700	1.81964100	C	-0.75735400	-4.74617800	0.69608400
H	4.18215800	-1.17767800	3.93273700	H	-0.13165900	-5.06020700	2.73437700
H	3.76486000	-1.97417200	-0.25989300	H	-1.40901900	-4.11851900	-1.25207500
H	5.19511500	-1.71734000	1.71273500	H	-0.61580100	-5.78030800	0.40057400
C	-0.30187500	2.58754300	1.31952700	C	2.58138100	0.27820700	1.41964400
C	-1.30779200	3.44766700	1.77148500	C	3.26002500	1.27399100	2.12209500
C	0.33331100	2.87144100	0.09966000	C	3.05358300	-0.12207400	0.15105700
C	-1.72806500	4.53524500	1.01376300	C	4.39544700	1.88090700	1.59246700
H	-1.77602500	3.24585600	2.72950100	H	2.87603500	1.56949400	3.09247500
C	-0.12572600	3.93680700	-0.68144700	C	4.17933300	0.51293900	-0.38302500
C	-1.14698100	4.76396900	-0.23144400	C	4.85181700	1.49830200	0.33542900
H	-2.51519200	5.18437400	1.38134800	H	4.91210000	2.65139300	2.15361000
H	0.31477600	4.08849700	-1.65605500	H	4.53525500	0.24944000	-1.36676400
H	-1.48884900	5.58550600	-0.85179300	H	5.72424400	1.97443500	-0.09931200
C	-2.97076500	-0.85278500	1.45132100	C	-1.26629500	2.19636600	0.91400400
C	-3.47466300	-1.83748800	2.29947200	C	-2.27755100	2.55849800	1.81390600
C	-3.30138500	-0.88520000	0.08059600	C	-1.47061400	2.41486000	-0.45873900
C	-4.30584500	-2.84689700	1.82147600	C	-3.47872600	3.10039700	1.37105100
H	-3.21213300	-1.80552600	3.35180700	H	-2.10477500	2.37582500	2.87063000
C	-4.13207100	-1.90488200	-0.39213100	C	-2.68640700	2.95172000	-0.89856800
C	-4.63648100	-2.87402200	0.47093500	C	-3.68546100	3.28947900	0.00601900
H	-4.68766300	-3.60477900	2.49620200	H	-4.25214300	3.35827000	2.08600300
H	-4.37231700	-1.95673500	-1.44277000	H	-2.84969700	3.05974800	-1.96148800
H	-5.27438700	-3.65941500	0.08023900	H	-4.62405600	3.69598400	-0.35631400
N	1.07703900	-1.76788800	-0.36240000	N	-1.90836700	-1.49362000	-0.79356400
N	-2.70294900	0.13624800	-0.71157500	N	-0.45458800	2.00461000	-1.39450100
N	1.42753500	2.04303000	-0.31317000	N	2.30536700	-1.15843600	-0.48997600
O	1.60792000	-0.99161900	-1.43531700	O	-1.16888300	-1.60297600	-2.04638000
H	2.47112200	-1.35470200	-1.79825400	H	-0.26057200	-1.34225100	-1.76127600
O	1.20995900	1.68353800	-1.68414200	O	1.10787600	-0.56303600	-1.06089000
H	1.25820600	0.70128400	-1.64756400	H	0.58808300	-0.24904700	-0.22594600
O	-1.38470700	-0.30968300	-1.07458300	O	-1.11364600	1.40712200	-2.53317400
H	-0.83700800	-0.10602300	-0.28388200	H	-1.05597200	0.45506400	-2.35686900
C	0.74296700	-3.16365400	-0.81648800	C	-3.36334400	-1.59056900	-1.12216500
C	2.79696600	2.64920000	-0.18266500	C	2.89972000	-2.08451600	-1.47558900
C	-3.34194100	0.71279600	-1.91418500	C	0.45380800	3.05911700	-1.94659300
C	3.80571700	1.54605900	-0.51514700	C	-3.75224100	-2.90178700	-1.83198600
H	4.82445300	1.92552600	-0.39244500	H	-3.67524600	-3.76187300	-1.16534200
H	3.66851700	0.69704200	0.15143800	H	-4.78850400	-2.83477800	-2.17471200
H	3.69642400	1.18627000	-1.53686000	H	-3.11320600	-3.06659500	-2.70109800
C	3.01110500	3.84739600	-1.12451200	C	-4.13961100	-1.46203900	0.19507400
H	2.41268000	4.71194500	-0.82817200	H	-3.88460700	-2.25837500	0.89614800
H	4.06328300	4.14447200	-1.10513000	H	-3.94365400	-0.50034800	0.67110300
H	2.75284800	3.56340700	-2.14536400	H	-5.20984900	-1.52535600	-0.01731800
C	2.99632900	3.09092300	1.27299300	C	-3.72119000	-0.40381700	-2.02340600
H	2.27166900	3.85058300	1.57460800	H	-4.80238000	-0.38772400	-2.18821100
H	2.92108100	2.24047900	1.95330000	H	-3.42288700	0.53244100	-1.55678200
H	3.99753600	3.51633300	1.37950500	H	-3.22540400	-0.47972700	-2.99097000
C	-2.57802900	2.01810400	-2.18936300	C	-0.30754300	4.10445500	-2.78266000
H	-2.98005300	2.51347800	-3.07861700	H	-0.97642400	4.70085700	-2.15836200
H	-2.67097200	2.69023600	-1.33582900	H	0.40405600	4.78292000	-3.26206800
H	-1.51859400	1.81469800	-2.34118300	H	-0.89442900	3.61361800	-3.56008400
C	-4.79788100	1.05436300	-1.57343500	C	1.18310800	3.76076500	-0.79539700
H	-5.41752500	0.16747600	-1.43335800	H	0.48743800	4.17455300	-0.06323900
H	-4.84010700	1.64976100	-0.65784100	H	1.87179100	3.08271600	-0.29111200
H	-5.22748600	1.64430900	-2.38693800	H	1.77005100	4.58641900	-1.20634200
C	-3.25260600	-0.18337100	-3.16627100	C	1.49031800	2.33632200	-2.81766200
H	-3.58581400	0.37850300	-4.04349200	H	2.26379500	3.04113700	-3.13736000
H	-2.21954900	-0.49121700	-3.32426300	H	1.94641300	1.53060600	-2.24338100
H	-3.87283400	-1.07819500	-3.09476100	H	1.01918400	1.90567800	-3.70110500
C	1.96885100	-4.08078000	-0.97142000	C	1.92357900	-3.26845500	-1.60300600
H	2.45358400	-4.26536300	-0.00938700	H	2.37744000	-4.06018400	-2.20638700
H	1.64353900	-5.04554100	-1.37364200	H	1.68431300	-3.66300400	-0.61529300
H	2.70593800	-3.65814400	-1.65713400	H	0.99076800	-2.97464700	-2.08019600
C	0.01031300	-3.04561400	-2.15947200	C	3.11200300	-1.47335100	-2.87651300
H	-0.40302700	-4.02392600	-2.42440100	H	3.91991700	-0.74179300	-2.90339000

H	-0.79417900	-2.31604400	-2.07630700	H	3.35758700	-2.26452200	-3.59083500
H	0.69115400	-2.72944600	-2.94837100	H	2.19814600	-0.97974300	-3.20709700
C	-0.21835800	-3.76752400	0.21603800	C	4.21212400	-2.62890300	-0.89147100
H	0.23663400	-3.81620700	1.20859400	H	4.99402400	-1.87368300	-0.82638700
H	-1.14336300	-3.19101100	0.26686300	H	4.03780300	-3.02443200	0.11179200
H	-0.46759900	-4.78936100	-0.08227500	H	4.57424800	-3.44168700	-1.52582100
Cl	4.22757600	-1.78688200	-2.71405600	Cl	-0.31007300	0.99224300	4.96610500
<b>[LCI]-, 18Cl, E<sub>0</sub>=-2191.171246 au</b>				<b>[LCI]-, 19Cl, E<sub>0</sub>=-2191.169724 au</b>			
N	-0.22581000	-0.00774400	-1.69963900	O	-1.11693300	1.14185100	-0.85895300
C	-1.37007600	-0.74655300	-2.26310700	O	2.95367500	-1.13150300	-2.15351500
H	-1.24916400	-1.79142100	-1.98241900	O	-3.29061800	-0.50192700	-0.94411500
H	-1.35474700	-0.67234400	-3.36699400	N	-1.03046800	2.54430600	-0.62823600
C	1.05732600	-0.55746400	-2.15715900	N	2.96014100	-0.33196400	-0.96637200
H	1.82243900	0.09686200	-1.76712800	N	-2.90706400	-1.38310800	0.13784400
H	1.11828800	-0.51002900	-3.26136000	N	-0.02950900	-0.37966400	1.98710600
C	-0.35185700	1.41474300	-2.06334900	C	-1.07915100	0.67177500	1.91710200
H	-1.28128000	1.76080200	-1.63221800	C	-0.45657200	2.04556600	1.80471900
H	-0.45990500	1.50052500	-3.16097600	C	0.21625400	2.50944700	2.94261700
C	-2.71159300	-0.27151400	-1.76081500	C	0.93726500	3.69492500	2.95457900
C	-3.56508600	0.45800300	-2.58697000	C	1.02770600	4.43910600	1.78087900
C	-3.12199900	-0.59228000	-0.44903100	C	0.38014200	3.99441800	0.63755100
C	-4.81893100	0.87277200	-2.14538100	C	-0.39950700	2.82672300	0.62839300
H	-3.23914600	0.69880600	-3.59377300	C	-2.37376800	3.17186000	-0.86718400
C	-4.37918800	-0.16356900	-0.01115700	C	-3.42278400	2.71989100	0.16439400
C	-5.22311300	0.55638200	-0.85246800	C	-2.23259300	4.69951800	-0.80491300
H	-5.46974800	1.43883200	-2.80249200	C	-2.80507100	2.78638400	-2.28918200
H	-4.69289800	-0.37705200	0.99913400	C	1.04556800	-0.17101700	1.01404900
H	-6.19135800	0.88260300	-0.48782000	C	2.28013800	-1.00051800	1.24916700
C	0.80432600	2.29649100	-1.65397800	C	2.54061100	-1.65811200	2.45174200
C	1.70424600	2.67922400	-2.65738000	C	3.60139500	-2.55427300	2.55835400
C	1.05614700	2.71184200	-0.33085200	C	4.40546400	-2.81264000	1.44903100
C	2.85221600	3.41203000	-2.38740600	C	4.19584900	-2.11111300	0.26416400
H	1.50348600	2.35500500	-3.67332000	C	3.17444700	-1.16370500	0.17718000
C	2.23209500	3.43118800	-0.06269500	C	3.89619400	0.81994100	-1.14063700
C	3.12051200	3.77588000	-1.07062600	C	5.32261100	0.36457400	-1.50135700
H	3.53594600	3.67333700	-3.18733700	C	3.32718300	1.69085900	-2.26726900
H	2.44245200	3.68483700	0.96507300	C	3.92241700	1.63918900	0.15649400
H	4.02149600	4.32830300	-0.82572500	C	-0.62065100	-1.73788600	1.97460200
C	1.30596200	-1.98165300	-1.72420500	C	-0.73315000	-2.40924500	0.61123400
C	0.98794800	-3.00868000	-2.62093500	C	0.32957300	-3.21625400	0.18826700
C	1.79836200	-2.32488300	-0.45065300	C	0.40882300	-3.70105300	-1.11122200
C	1.09210100	-4.34979600	-2.27601500	C	-0.59465800	-3.38785200	-2.02070400
H	0.62450200	-2.73420700	-3.60616900	C	-1.69066500	-2.64432400	-1.60665100
C	1.87255000	-3.68049900	-0.09904700	C	-1.78313400	-2.17806700	-0.29305000
C	1.52225500	-4.68132000	-0.99380300	C	-4.14682900	-2.12082900	0.51727300
H	0.82258100	-5.12154500	-2.98855400	C	-3.80566800	-3.13602900	1.61393700
H	2.18180900	-3.92407300	0.90587500	C	-4.79126100	-2.85572300	-0.67319800
H	1.58849000	-5.72038500	-0.68880000	C	-5.12383300	-1.07836400	1.07924000
N	-2.17275800	-1.31247500	0.32571700	H	-1.78683200	0.48421600	1.12008000
N	2.17114300	-1.31110000	0.49627200	H	-1.63348500	0.62265900	2.86273300
N	0.17894000	2.34956800	0.74069900	H	0.18542200	1.88492300	3.82892000
O	-1.25728700	-0.35680800	0.88926800	H	1.44666800	4.01765000	3.85576700
H	-0.59372600	-0.21849400	0.17978500	H	1.62280100	5.34506100	1.74509400
O	0.99729800	2.23435000	1.91065200	H	0.48816000	4.53075900	-0.29503600
H	0.72122700	1.40340600	2.37853300	H	-3.11022500	2.98877700	1.17675600
O	1.90824900	-1.85335700	1.79662200	H	-3.58536900	1.64439800	0.11868600
H	1.39699200	-1.16717400	2.29855000	H	-4.37910300	3.21230600	-0.03714100
C	-2.55155500	-2.27685400	1.38629400	H	-1.95461000	5.04657100	0.19088100
C	-0.92223600	3.32991300	1.08727400	H	-3.19386200	5.15050000	-1.06445800
C	3.63386000	-0.91037700	0.49746800	H	-1.48458800	5.04853900	-1.51979200
C	-1.72699300	2.68810400	2.22493000	H	-2.00888600	3.02088400	-2.99823000
H	-2.61027900	3.29886800	2.43801900	H	-3.70456800	3.34612000	-2.56128100
H	-2.03412000	1.68386800	1.93213300	H	-3.02517900	1.72458400	-2.37843000
H	-1.13076100	2.60117000	3.13209700	H	1.32479400	0.87760200	1.05894200
C	-0.34197700	4.68247600	1.53362200	H	0.72815100	-0.33804000	-0.01759600
H	0.16039900	5.19428300	0.70799700	H	1.87571400	-1.47881200	3.28798700

H	-1.14741400	5.32836900	1.89500200	H	3.78194300	-3.07186300	3.49489800
H	0.37190200	4.53008400	2.34271800	H	5.20463600	-3.54397100	1.51141900
C	-1.85931400	3.54796000	-0.10432000	H	4.81329100	-2.29434100	-0.60479100
H	-1.32868500	3.90602500	-0.98947700	H	5.28324700	-0.32037300	-2.34974900
H	-2.40776400	2.63688800	-0.34603300	H	5.80686300	-0.13668300	-0.66002500
H	-2.59369500	4.30952700	0.17125900	H	5.93456800	1.22861000	-1.77754400
C	3.78313300	0.17768300	1.56722800	H	3.93787600	2.59224900	-2.38377300
H	4.79882300	0.58491400	1.53583700	H	2.29788500	1.97315400	-2.04471200
H	3.06945500	0.98279200	1.39187000	H	3.31411100	1.14714800	-3.21091300
H	3.59315300	-0.22107900	2.56270000	H	2.93479200	2.03974700	0.38856800
C	4.04176700	-0.32231700	-0.85751800	H	4.60488600	2.48392900	0.02779000
H	3.85381200	-1.01327600	-1.68232100	H	4.27011900	1.04837400	1.00610400
H	3.53625700	0.62447200	-1.05011900	H	-1.59196000	-1.65759500	2.45666000
H	5.11584300	-0.11918800	-0.83421800	H	-0.00265600	-2.38834900	2.60011800
C	4.54304800	-2.10677600	0.82677400	H	1.14047500	-3.41344400	0.87812300
H	5.57419100	-1.76228400	0.94741000	H	1.27837800	-4.26742300	-1.42241000
H	4.22069700	-2.57193700	1.75810200	H	-0.51348400	-3.69171600	-3.05723500
H	4.52540600	-2.85563700	0.03056400	H	-2.45371300	-2.35467800	-2.31350500
C	-2.91832300	-1.60964800	2.72531700	H	-3.42850500	-2.63993900	2.50962700
H	-3.80660000	-0.97806200	2.65284000	H	-3.05909900	-3.85589800	1.27583300
H	-3.12133200	-2.38338900	3.47204800	H	-4.71253300	-3.68279000	1.88551900
H	-2.08255500	-1.00368700	3.07823400	H	-4.14643000	-3.65968400	-1.03271800
C	-1.30840700	-3.15402400	1.60306800	H	-4.97175100	-2.16112700	-1.49344000
H	-1.50420000	-3.89757700	2.38182500	H	-5.74568600	-3.29403500	-0.36636500
H	-1.04406200	-3.66908700	0.67669800	H	-6.02316500	-1.56992100	1.46214200
H	-0.46120900	-2.54638600	1.91157900	H	-5.41143200	-0.36766700	0.30544100
C	-3.68747800	-3.16349000	0.85659000	H	-4.64883600	-0.52564000	1.89317200
H	-4.64059100	-2.63851600	0.78018400	H	-0.56948900	0.93684200	-1.67594900
H	-3.43311700	-3.55580400	-0.13204300	H	2.07677000	-0.90179500	-2.54184800
H	-3.82088800	-4.00907600	1.53568400	H	-2.54969300	0.14265400	-0.95741800
Cl	0.52673800	-0.06247400	3.81210000	Cl	0.25346200	0.06118500	-3.27025000
<b>[LCI]-, 20Cl, E<sub>0</sub>=-2191.166022 au</b>				<b>[LCI]-, 22Cl, E<sub>0</sub>=-2191.159262 au</b>			
N	-0.75372900	-0.04619800	-0.68852200	N	0.16265000	0.07474800	1.25357600
C	-1.60650800	0.24683800	-1.82341700	C	0.01720200	1.54353200	1.43814000
H	-1.57030300	-0.62318100	-2.48630300	H	0.86672500	1.99252400	0.93102300
H	-1.21839700	1.09296600	-2.41975300	H	0.06835800	1.78160400	2.50679600
C	-0.76469300	0.94780200	0.39232400	C	1.37796900	-0.35552500	1.99530600
H	-0.19334600	0.53750500	1.21480700	H	1.46614000	-1.43323800	1.86150200
H	-1.78595000	1.03206300	0.75787400	H	1.25111500	-0.12513600	3.06055700
C	0.55365800	-0.52614300	-1.09724000	C	-1.02515400	-0.66547300	1.75105200
H	1.22944600	0.28049700	-1.42334300	H	-1.89182000	-0.18529100	1.31311700
H	0.38513800	-1.13735700	-1.98812300	H	-1.09843900	-0.57582800	2.84171800
C	-3.05734200	0.57588100	-1.50889100	C	-1.26353600	2.11730500	0.89256600
C	-3.63637200	1.57459200	-2.30578600	C	-2.29402500	2.41333700	1.79485500
C	-3.84194800	0.00634600	-0.48309500	C	-1.45553000	2.38744200	-0.46997700
C	-4.92415900	2.04649000	-2.09851900	C	-3.50018200	2.94657900	1.35362500
H	-3.02600500	2.02088500	-3.08433700	H	-2.12509700	2.19535800	2.84771900
C	-5.12223900	0.53457900	-0.24219700	C	-2.67073200	2.93228400	-0.90411700
C	-5.66340100	1.53399200	-1.03443000	C	-3.69306400	3.20375600	-0.00197700
H	-5.32805300	2.82899200	-2.73154700	H	-4.28862300	3.15659700	2.06775600
H	-5.66644000	0.14552000	0.60518700	H	-2.83127500	3.13696500	-1.95668200
H	-6.65802400	1.91163300	-0.82155000	H	-4.63164700	3.61558300	-0.35715800
C	1.23546900	-1.39787400	-0.05769700	C	-0.98224900	-2.11080600	1.32130800
C	0.45193100	-1.96339500	0.95076900	C	-0.46798400	-3.07868500	2.19113100
C	2.61633300	-1.67028300	-0.05728900	C	-1.40282300	-2.51535900	0.04433000
C	0.99950100	-2.77478300	1.93540900	C	-0.31052600	-4.40186400	1.79348900
H	-0.59419000	-1.69885800	0.99742500	H	-0.17623500	-2.77028300	3.18882800
C	3.16145300	-2.50981000	0.91804700	C	-1.20784700	-3.83671200	-0.36720500
C	2.36016400	-3.06379400	1.90898800	C	-0.66078100	-4.77623000	0.49807600
H	0.35953300	-3.12282500	2.73644000	H	0.10093700	-5.13070400	2.48315100
H	4.23144200	-2.65842900	0.93229600	H	-1.46025200	-4.10913300	-1.38220200
H	2.80740800	-3.68585600	2.67690500	H	-0.51012000	-5.79673700	0.16225400
C	-0.25042900	2.31595300	-0.02156800	C	2.64369500	0.28102300	1.47772800
C	-1.13957800	3.25968200	-0.54896800	C	3.30239100	1.24253700	2.24323200
C	1.11108300	2.65545300	0.04078600	C	3.18762700	-0.10773900	0.23346500
C	-0.69598000	4.47350400	-1.06229900	C	4.49569700	1.81540600	1.80912300

H	-2.19598700	3.02183600	-0.56651300	H	2.86543800	1.53379600	3.19231900
C	1.56363300	3.86238000	-0.50373200	C	4.38014900	0.48157900	-0.19821200
C	0.66666000	4.76590700	-1.06017500	C	5.03517200	1.42769800	0.58722200
H	-1.40883900	5.18062400	-1.47275800	H	4.99692200	2.55723700	2.42090500
H	2.62511300	4.06787800	-0.50077600	H	4.79920700	0.21341400	-1.15616100
H	1.02883700	5.69915800	-1.47871000	H	5.96023900	1.86988500	0.23195800
N	-3.35060000	-1.04436100	0.35826100	N	-0.40011500	2.05362000	-1.38987400
N	2.00981100	1.71615500	0.65042000	N	2.42983200	-1.07287600	-0.49100000
N	3.49361800	-0.98163300	-0.99133000	N	-2.01670400	-1.53790500	-0.81537900
O	-3.92614700	-0.87738700	1.65509900	O	-0.88887600	1.15045200	-2.39687200
H	-3.13609000	-0.78572400	2.26035500	H	-1.74109800	1.48948400	-2.70711000
O	4.73481900	-0.66654900	-0.30416800	O	-1.42187900	-1.63723900	-2.12413600
H	4.54631400	0.22135600	0.04215400	H	-0.92348700	-0.80309400	-2.17497400
O	3.21493100	1.66059500	-0.15912000	O	1.33251900	-0.39399500	-1.13846300
H	3.02510500	0.89622800	-0.74097300	H	0.70303800	-0.23180900	-0.37556000
C	-3.65238200	-2.44410200	-0.09850200	C	0.37927600	3.15026500	-2.03268700
C	3.90588900	-1.71772900	-2.23233700	C	-3.50079400	-1.63456100	-0.97129600
C	2.40791200	1.97502100	2.07258100	C	3.01857700	-2.02659700	-1.44938400
Cl	-1.55913700	-0.69702100	3.53695300	C	-3.94406800	-0.40302000	-1.77064300
C	3.35351900	3.18384600	2.19174800	H	-5.03362500	-0.38857900	-1.86570500
H	2.84705800	4.10947300	1.90984400	H	-3.62520400	0.50475200	-1.25939300
H	3.68681200	3.28516600	3.22799600	H	-3.50828200	-0.42381400	-2.77059600
H	4.23140900	3.05626400	1.55645500	C	-3.94955600	-2.91267900	-1.70400000
C	3.08970700	0.70470000	2.59291000	H	-3.76990500	-3.80319900	-1.09950900
H	2.42553600	-0.15132200	2.48054200	H	-5.02150900	-2.86045400	-1.91583500
H	4.01823300	0.49406200	2.06186700	H	-3.41343200	-3.01131600	-2.64917800
H	3.32712100	0.82253300	3.65343700	C	-4.14366100	-1.58247000	0.42009900
C	1.14608500	2.22793900	2.91036800	H	-3.82014800	-2.41567800	1.04558200
H	0.58763600	3.09331100	2.54980400	H	-3.90283700	-0.65022400	0.93236300
H	0.48044000	1.36389800	2.94492300	H	-5.23006200	-1.63973200	0.31207100
H	1.45777600	2.43511100	3.93718900	C	1.94980000	-3.11357100	-1.65782000
C	4.69292900	-0.72588200	-3.09805200	H	2.31436300	-3.87489800	-2.35502800
H	5.60526000	-0.41260200	-2.59219200	H	1.71192500	-3.58772700	-0.70483500
H	4.95893700	-1.18923600	-4.05212900	H	1.03145700	-2.67935400	-2.04926100
H	4.08587000	0.16035100	-3.29939700	C	4.24925900	-2.67729700	-0.80385600
C	4.77059900	-2.94822400	-1.91067200	H	5.08570500	-1.98692500	-0.69410000
H	5.10450800	-3.41500300	-2.84151600	H	3.99194800	-3.06024400	0.18651600
H	5.64788800	-2.66048600	-1.33138000	H	4.57784400	-3.51587700	-1.42340300
H	4.20215500	-3.68712900	-1.34322800	C	3.36146800	-1.40406500	-2.81954000
C	2.65260700	-2.16284600	-2.98916600	H	3.62619100	-2.19259000	-3.53032900
H	2.02877400	-2.81845800	-2.37989600	H	2.49279300	-0.86710800	-3.20012600
H	2.06041900	-1.30477900	-3.30744800	H	4.19981400	-0.70758100	-2.76987200
H	2.95811600	-2.71530300	-3.88107600	C	-0.44906700	4.02915600	-2.98982800
C	-3.04915700	-3.40457700	0.93347600	H	-1.19436800	4.62018400	-2.45444800
H	-3.24696600	-4.43735500	0.62964300	H	0.21292300	4.72153400	-3.51673700
H	-1.97214500	-3.26318000	1.00934100	H	-0.95131300	3.42117600	-3.74757300
H	-3.47953300	-3.23162100	1.91776500	C	1.52903900	2.47988800	-2.79784800
C	-5.16726500	-2.69473900	-0.20676900	H	2.22996300	3.23998500	-3.15558100
H	-5.35680200	-3.74394400	-0.45215900	H	2.04133300	1.77695100	-2.14172100
H	-5.64740200	-2.46860300	0.74633300	H	1.15041900	1.91956900	-3.65324000
H	-5.62034300	-2.07519200	-0.98440000	C	0.96026200	4.02254900	-0.91297800
C	-2.98073000	-2.68503100	-1.45254500	H	0.17743000	4.44166100	-0.27797400
H	-3.39531100	-2.04062700	-2.23065600	H	1.64624500	3.44851300	-0.29000700
H	-1.90775900	-2.50875800	-1.37293600	H	1.51798900	4.84991900	-1.35907200
H	-3.14327800	-3.72330200	-1.75434600	Cl	-0.65514500	1.14899400	4.87185100
<b>[LBr]<sup>-</sup>, 10Br, E<sub>0</sub> = -4305.105809 au</b>				<b>[LBr]<sup>-</sup>, 11Br, E<sub>0</sub> = -4305.102217 au</b>			
O	-3.48441200	-1.25500700	0.00851600	N	-0.00092500	-0.00055400	-1.79819000
H	-3.15225100	-0.82368200	-0.81712100	C	0.34286200	-1.34756900	-2.25255400
O	-2.32012400	3.01273100	-1.89505300	H	1.33072900	-1.56469200	-1.87181300
H	-2.28700400	2.12623100	-2.32471900	H	0.41184100	-1.37314800	-3.36098500
O	3.27032800	-0.35463800	1.51588500	C	0.99350200	0.97110800	-2.25248900
H	2.31362600	-0.15099400	1.27996500	H	0.68785300	1.93478200	-1.87051300
N	-2.41183900	-2.14769900	0.32509300	H	0.98002000	1.04473700	-3.36081000
N	-2.00298200	2.67387000	-0.54303100	C	-1.33945500	0.37506500	-2.25271000
N	3.94324400	-0.02397700	0.27624800	H	-2.02137900	-0.37170400	-1.87148700
N	0.86632500	-0.15365300	0.39735000	H	-1.39601500	0.32731800	-3.36110200

C	0.34924200	-1.54651500	0.56139600	C	-0.63930600	-2.41566500	-1.83191400
H	-0.23348600	-1.82518100	-0.31780900	C	-1.58157700	-2.85050100	-2.77184300
H	1.21605700	-2.20622500	0.63789100	C	-0.69434100	-2.94872900	-0.53063900
C	-0.52711200	-1.67270100	1.77766200	C	-2.59354400	-3.74528700	-2.44828300
C	0.00518700	-1.46947500	3.05501900	H	-1.52995800	-2.43797700	-3.77419200
H	1.07754500	-1.34117600	3.15931500	C	-1.73558800	-3.83003500	-0.20168700
C	-0.82396500	-1.37588000	4.16610200	C	-2.67705200	-4.22242500	-1.14286600
H	-0.39869100	-1.20457400	5.14896700	H	-3.31901100	-4.04522700	-3.19639300
C	-2.20740500	-1.46592300	4.00500700	H	-1.80383800	-4.17462300	0.81922400
H	-2.86402800	-1.35269700	4.86108300	H	-3.47287900	-4.90166600	-0.85592000
C	-2.74604600	-1.70886700	2.74715500	C	-1.77350400	1.75993900	-1.83322900
H	-3.81678200	-1.76495100	2.60703200	C	-1.67881700	2.79265900	-2.77396400
C	-1.91221200	-1.85531400	1.63281100	C	-2.20813100	2.07519100	-0.53237700
C	-2.82406200	-3.55401700	0.05353700	C	-1.94847600	4.11660900	-2.45169100
C	-3.10163600	-3.65204400	-1.45191500	H	-1.34671900	2.54106700	-3.77593900
H	-2.24633400	-3.28567900	-2.02095900	C	-2.45144900	3.41777500	-0.20472500
H	-3.95846000	-3.03801200	-1.72737600	C	-2.32076300	4.42852700	-1.14675500
H	-3.30834600	-4.69134300	-1.72588200	H	-1.84551100	4.89421900	-3.20046500
C	-1.64810600	-4.47153600	0.41368100	H	-2.71612700	3.64983600	0.81593300
H	-0.75348000	-4.19271900	-0.14663800	H	-2.51173500	5.45752900	-0.86086300
H	-1.90573300	-5.50278900	0.15814600	C	2.41008800	0.65429400	-1.83378000
H	-1.41476600	-4.43288000	1.47949600	C	3.25637000	0.05561500	-2.77500000
C	-4.07934300	-3.96930300	0.84217000	C	2.90138500	0.87303600	-0.53327300
H	-4.42955500	-4.94892800	0.50346200	C	4.53775600	-0.37341300	-2.45347100
H	-4.87378600	-3.24005300	0.67523600	H	2.87181800	-0.10596200	-3.77677500
H	-3.87626100	-4.03633900	1.91341400	C	4.18581400	0.41203600	-0.20640100
C	-0.22478300	0.82855800	0.61138700	C	4.99490700	-0.20706600	-1.14882600
H	-0.57360100	0.70402600	1.63640600	H	5.15901000	-0.85176500	-3.20257700
H	-1.06953000	0.62100300	-0.05081100	H	4.51985200	0.52530400	0.81400500
C	0.19277100	2.26074400	0.40281200	H	5.98154700	-0.55660100	-0.86349600
C	1.45110600	2.72689400	0.79809700	N	0.25821000	-2.55285100	0.46374900
H	2.13092200	2.04559700	1.29282700	N	2.08380200	1.49945700	0.46276400
C	1.85274300	4.02695400	0.51717300	N	-2.34088600	1.05336700	0.46316800
H	2.83554600	4.36686100	0.82552700	O	-0.43107800	-2.57495300	1.72142600
C	1.00212000	4.87883600	-0.18928600	H	-0.26498100	-1.69405700	2.12719000
H	1.32363300	5.88308900	-0.44518300	O	-2.01506600	1.66293600	1.71998200
C	-0.26190600	4.43985400	-0.56005000	H	-1.33489900	1.07933000	2.12615800
H	-0.92727600	5.07614500	-1.12731700	O	2.44929400	0.91261100	1.71956800
C	-0.69270900	3.14938600	-0.22874700	H	1.60377300	0.61653900	2.12670000
C	-3.12516400	3.08804000	0.34447000	C	1.47806300	-3.42722800	0.62902400
C	-3.44753600	4.58807700	0.21051200	C	-3.70768500	0.43368000	0.62964900
H	-3.62329400	4.83552800	-0.83746600	C	2.23105900	2.99298700	0.62878800
H	-2.62766600	5.20450400	0.58682500	Br	0.00157800	0.00232400	3.57507800
H	-4.34646500	4.83354800	0.78393300	C	-4.74976500	1.47616700	1.07123600
C	-4.34294500	2.24725400	-0.05948700	H	-4.93371800	2.21316000	0.28498700
H	-4.13059600	1.18719100	0.08226900	H	-5.69687700	0.97903300	1.30000800
H	-4.58695700	2.41261100	-1.10824600	H	-4.40313300	1.99303000	1.96605000
H	-5.20708600	2.52137300	0.55414500	C	-3.55860100	-0.65740400	1.69749700
C	-2.75254300	2.76029000	1.79551800	H	-4.49624300	-1.21460200	1.78900600
H	-1.86656900	3.30897600	2.12183500	H	-2.76052200	-1.34847900	1.42276300
H	-2.57151900	1.69166700	1.91701700	H	-3.30930500	-0.22718200	2.66653300
H	-3.58452400	3.03917300	2.44788400	C	-4.16796900	-0.22291800	-0.67617800
C	1.40714000	-0.01834900	-0.98610400	H	-3.54705500	-1.08273100	-0.92883900
H	1.85583400	0.97179000	-1.06150300	H	-5.18992000	-0.58601500	-0.53756900
H	0.58182600	-0.08563700	-1.70483900	H	-4.17536500	0.48036300	-1.51171300
C	2.45089200	-1.05618400	-1.31204000	C	1.09603800	-4.85047900	1.07184100
C	2.16414600	-2.02567900	-2.27288200	H	0.54813700	-5.37820200	0.28667400
H	1.18967400	-2.00505000	-2.74866300	H	2.00009600	-5.42264400	1.29942100
C	3.10329600	-2.98923400	-2.63135100	H	0.47649800	-4.80794200	1.96759000
H	2.86369600	-3.72706100	-3.38876600	C	2.27524300	-3.49862400	-0.67776000
C	4.34518900	-2.99510500	-2.00707000	H	2.70924700	-2.53123400	-0.93166400
H	5.08532200	-3.74544700	-2.26467500	H	3.10071900	-4.20213300	-0.53955800
C	4.64215200	-2.04430600	-1.03333300	H	1.66891400	-3.85720300	-1.51236500
H	5.60264700	-2.08178100	-0.54347100	C	2.35013400	-2.75239600	1.69533300
C	3.71601400	-1.05687300	-0.68201400	H	3.30130600	-3.28631700	1.78600800
C	5.28480200	0.50047200	0.60033800	H	2.54984400	-1.71598500	1.41969600

C	6.02231000	0.81596800	-0.70834700	H	1.85417700	-2.75070100	2.66503000
H	5.39061000	1.43077300	-1.35352300	C	3.65493800	3.37368600	1.07080200
H	6.30264000	-0.07884600	-1.26271800	H	4.38540800	3.16419000	0.28484000
H	6.93342300	1.37540800	-0.48058100	H	3.69834500	4.44245800	1.29956700
C	6.11529500	-0.42593700	1.51438500	H	3.92870300	2.81496100	1.96571500
H	6.47707200	-1.31546100	0.99761500	C	1.21133900	3.41005500	1.69612400
H	5.50149400	-0.74490500	2.35692400	H	1.19862100	4.50065500	1.78805400
H	6.98784500	0.11080000	1.89823900	H	0.21365300	3.06555900	1.42050200
C	5.04992700	1.82899800	1.34325200	H	1.45809400	2.97842400	2.66518800
H	4.49612400	1.65424600	2.26496100	C	1.89328800	3.71984600	-0.67726200
H	4.47204500	2.50694600	0.71350500	H	0.83822800	3.61239400	-0.93023800
H	6.00685800	2.29892900	1.58785400	H	2.09021200	4.78635000	-0.53864600
Br	-2.14631800	-0.13631400	-2.76791600	H	2.50614000	3.37431600	-1.51259800
<b>[LBr], 12Br, E<sub>0</sub>=-4305.103262 au</b>				<b>[LBr], 13Br, E<sub>0</sub>=-4305.104089 au</b>			
N	-1.14674600	0.12851500	1.74871600	N	0.09145500	-0.09951800	0.95751100
C	-0.25641000	-0.66045000	2.59858900	C	-0.26257500	1.09652800	1.78080700
H	-0.34598400	-1.69406000	2.28268800	H	0.52578200	1.83156900	1.61762600
H	-0.57368600	-0.60822000	3.66065900	H	-0.28888900	0.81865100	2.83986400
C	-2.48383800	-0.45292300	1.67390000	C	1.45252700	-0.59476200	1.30979300
H	-3.08162400	0.19570100	1.04419300	H	1.59020100	-1.51187500	0.75047600
H	-2.96516800	-0.45697000	2.67448400	H	1.48098300	-0.82306700	2.38172500
C	-1.19936800	1.52933800	2.17024800	C	-0.90949200	-1.17848400	1.22582800
H	-0.17417500	1.87397300	2.26440500	H	-1.88579400	-0.72903400	1.08409300
H	-1.68455400	1.62631800	3.16364000	H	-0.81284300	-1.49586300	2.27076700
C	1.18306400	-0.22207900	2.49739500	C	-1.57139800	1.70042000	1.34873500
C	1.74034000	0.55404800	3.51818200	C	-2.68492700	1.61301300	2.18338900
C	1.96955500	-0.53318900	1.37595700	C	-1.68154400	2.37452500	0.11254900
C	3.03729400	1.04799300	3.42872500	C	-3.89947900	2.19387800	1.82572700
H	1.13114900	0.78474800	4.38656600	H	-2.57749100	1.09075600	3.12809800
C	3.25838700	0.00015100	1.26904100	C	-2.91329400	2.92714900	-0.24999900
C	3.79001400	0.78139800	2.28889100	C	-4.00904700	2.85363600	0.60669900
H	3.44676100	1.65287300	4.23075300	H	-4.75170500	2.12638800	2.49243300
H	3.83355700	-0.16695400	0.36528800	H	-3.03086400	3.40899000	-1.20847500
H	4.78931000	1.18805400	2.18070300	H	-4.95330200	3.29349100	0.30431900
C	-1.93675600	2.38955400	1.17348900	C	-0.75486300	-2.34864700	0.28969600
C	-3.27114700	2.74165900	1.39656400	C	-0.00491100	-3.46243700	0.68555600
C	-1.32740200	2.77281700	-0.03078700	C	-1.32576900	-2.34209500	-0.99279200
C	-4.01686400	3.40933900	0.43068700	C	0.23094600	-4.51922200	-0.18689700
H	-3.73492400	2.45484700	2.33497800	H	0.40059300	-3.47955600	1.69131500
C	-2.09512600	3.39522300	-1.02067300	C	-1.04626500	-3.38285500	-1.88405500
C	-3.42971800	3.71225600	-0.79544100	C	-0.27186400	-4.46606400	-1.48584900
H	-5.05422500	3.66191500	0.62074700	H	0.82136500	-5.36873500	0.13781200
H	-1.63833500	3.60781900	-1.97622600	H	-1.42077500	-3.31844000	-2.89591200
H	-4.00916100	4.19360000	-1.57574200	H	-0.06024700	-5.26568200	-2.18757300
C	-2.51391800	-1.86639600	1.14019000	C	2.54217600	0.38244200	0.95493200
C	-2.75113600	-2.91161800	2.04037100	C	3.06712500	1.21007700	1.95386500
C	-2.27012200	-2.18411200	-0.20784400	C	3.03222100	0.50668100	-0.35482500
C	-2.71695000	-4.24461400	1.65001500	C	4.02106700	2.17755300	1.65828800
H	-2.93461500	-2.66061400	3.08009200	H	2.69643100	1.08963000	2.96647300
C	-2.21139000	-3.53071700	-0.59025000	C	3.96928700	1.50035100	-0.65369700
C	-2.43008900	-4.55289600	0.32294600	C	4.45960600	2.33381600	0.34436900
H	-2.88640400	-5.03145000	2.37658100	H	4.40663100	2.81661100	2.44492300
H	-1.95795300	-3.75901000	-1.61495200	H	4.27982800	1.63287800	-1.68050000
H	-2.37144400	-5.58635000	-0.00099600	H	5.18352600	3.10309400	0.09670800
N	1.41296700	-1.39311900	0.36385700	N	-0.48601400	2.45735800	-0.66059800
N	-2.01622600	-1.13800700	-1.16180300	N	2.49355500	-0.36719900	-1.36561900
N	0.06729900	2.48671600	-0.20491500	N	-2.17680800	-1.23836100	-1.34152100
O	1.40792000	-0.71423200	-0.90067800	O	-0.21910400	1.17571500	-1.29162900
H	2.33022200	-0.63501800	-1.30201000	H	-0.01966700	0.55313400	-0.47018000
O	0.22424600	1.80455400	-1.45607900	O	-1.73694100	-0.68412900	-2.59529800
H	0.58976000	0.94072000	-1.18253000	H	-1.28650700	0.12613800	-2.27996800
O	-0.97187500	-1.59518000	-2.03683600	O	2.15439100	0.42616800	-2.52563000
H	-0.15871600	-1.19613200	-1.66502100	H	1.24803000	0.70416900	-2.29332600
C	1.98043700	-2.78738500	0.28914800	C	-0.20300000	3.55591200	-1.60650500
C	0.99638000	3.66089600	-0.17909800	C	-3.64007500	-1.51038600	-1.42670200
C	-3.15706300	-0.73723200	-2.04761800	C	3.35660200	-1.48701600	-1.84170600

C	2.41822600	3.09288400	-0.20997000	C	-4.32803000	-0.14973100	-1.58535800
H	3.14734900	3.90646000	-0.14916900	H	-5.41500400	-0.27418100	-1.59174400
H	2.56906500	2.42570100	0.63601000	H	-4.05233400	0.50636200	-0.76094500
H	2.60721700	2.52797900	-1.12266300	H	-4.02395500	0.32446600	-2.51887300
C	0.80118900	4.62221500	-1.36591800	C	-4.02039900	-2.42472100	-2.60653300
H	-0.13974100	5.17220500	-1.29659100	H	-3.66653600	-3.44573300	-2.45322700
H	1.61495700	5.35250400	-1.38289300	H	-5.10865200	-2.45950500	-2.71226500
H	0.82457800	4.06191700	-2.30158800	H	-3.59439700	-2.03579600	-3.53274200
C	0.77673200	4.40755400	1.14259500	C	-4.08815400	-2.15049100	-0.10693700
H	-0.23700400	4.80643700	1.22233600	H	-3.59301800	-3.10723900	0.06706200
H	0.96372000	3.74969700	1.99373300	H	-3.87974400	-1.49346800	0.73874700
H	1.47728300	5.24466800	1.20113000	H	-5.16646600	-2.32646300	-0.14346200
C	-2.62851000	0.36673800	-2.97248600	C	2.49278800	-2.33290700	-2.78492400
H	-3.46462200	0.84406200	-3.49303100	H	3.03618300	-3.23446400	-3.08353400
H	-2.08967500	1.11275100	-2.39135700	H	1.57254800	-2.62693300	-2.28179900
H	-1.94007100	-0.04399900	-3.70960900	H	2.22989500	-1.76607900	-3.67760400
C	-4.28533600	-0.16985700	-1.18096400	C	3.76673400	-2.33670700	-0.63315500
H	-4.62250800	-0.88975300	-0.43152200	H	4.29828200	-1.74672700	0.11567000
H	-3.97217500	0.74862900	-0.68549900	H	2.89828300	-2.80061500	-0.16506700
H	-5.13799500	0.06927900	-1.82216200	H	4.43297500	-3.13420900	-0.97235600
C	-3.69255400	-1.90826100	-2.89241000	C	4.61720800	-0.99838500	-2.58008200
H	-4.42931000	-1.53547600	-3.60994200	H	5.13772400	-1.85188200	-3.02385900
H	-2.87776300	-2.37345000	-3.44887800	H	4.34349100	-0.30752800	-3.37874600
H	-4.17698500	-2.66617500	-2.27233100	H	5.30964300	-0.49817900	-1.90009500
C	3.51643000	-2.88336100	0.35430500	C	-0.89101600	3.38695000	-2.97526200
C	3.90364000	-2.53627400	1.31429700	H	-1.97909000	3.40012200	-2.90102800
H	3.80481000	-3.93280800	0.23734300	H	-0.58786100	4.19539800	-3.64662900
H	3.98776100	-2.31212200	-0.44777400	H	-0.59812300	2.44015600	-3.43010900
C	1.50483200	-3.43768700	-1.01414900	C	1.32308700	3.58812300	-1.80787100
H	1.76214200	-4.50036300	-0.98704800	H	1.59493100	4.44117000	-2.43696400
H	0.42881600	-3.33769900	-1.13151900	H	1.82221700	3.68452200	-0.84248500
H	1.99509900	-2.98794600	-1.87784800	H	1.69539700	2.68357800	-2.27998000
C	1.37203800	-3.54441400	1.48013000	C	-0.59440600	4.88684700	-0.94205200
H	1.63468800	-3.06753400	2.42794700	H	-1.67005400	5.03724000	-0.87349900
H	0.28556600	-3.59102600	1.39331600	H	-0.17962600	4.93583200	0.06715700
H	1.76300600	-4.56553900	1.50179500	H	-0.17246800	5.70739800	-1.52702900
Br	4.17821800	-0.27882900	-2.31970300	Br	0.20980500	-0.94504100	4.81933000
<b>[LBr]<sup>-</sup>, 14Br, E<sub>0</sub>=-4305.100401 au</b>				<b>[LBr]<sup>-</sup>, 15Br, E<sub>0</sub>=-4305.099953 au</b>			
N	-1.01504500	-0.03497400	1.79261500	N	-0.82671000	0.39790200	1.74175600
C	-1.00791100	1.35066000	2.25818100	C	-0.64469800	-0.85587800	2.47689400
H	0.02939000	1.67352400	2.28511900	H	-1.39110900	-1.55560700	2.10815800
H	-1.41622300	1.43320400	3.28616700	H	-0.82125200	-0.70743100	3.56262300
C	-0.06302600	-0.87244100	2.52376600	C	-2.19641300	0.88722700	1.84338400
H	-0.14789200	-1.87375700	2.11788100	H	-2.23993800	1.82994800	1.31098200
H	-0.34586500	-0.92904500	3.59550100	H	-2.46513400	1.09453500	2.90124800
C	-2.36106200	-0.61245300	1.83285700	C	0.15723200	1.40409600	2.15002400
H	-3.03213000	0.10323300	1.36878300	H	1.12397300	0.92030500	2.10958400
H	-2.69618500	-0.76598400	2.87914600	H	-0.01730300	1.72358900	3.19915500
C	-1.78981800	2.25704600	1.34003900	C	0.73141900	-1.43858300	2.28026500
C	-3.05621100	2.71646700	1.70917700	C	1.68964500	-1.33202000	3.29139600
C	-1.27585800	2.61785100	0.08432300	C	1.09112100	-2.03254700	1.06020400
C	-3.82327700	3.49721700	0.84962000	C	2.99609800	-1.76880000	3.09672900
H	-3.44493300	2.44517300	2.68558200	H	1.40458600	-0.87720700	4.23481800
C	-2.07452600	3.34779300	-0.79963700	C	2.41866400	-2.41701800	0.84729300
C	-3.33471200	3.79745500	-0.41840300	C	3.36401800	-2.29100700	1.86051000
H	-4.80266200	3.84648900	1.15774300	H	3.72702900	-1.67215100	3.89239000
H	-1.70486400	3.55088900	-1.79361300	H	2.72675900	-2.76339700	-0.12916300
H	-3.93689200	4.36992200	-1.11552100	H	4.38986400	-2.58708900	1.67207000
C	-2.42729700	-1.92501000	1.08975900	C	0.18374700	2.62763200	1.26325700
C	-2.32953000	-3.13431200	1.78345000	C	-0.68104900	3.69410900	1.53637100
C	-2.49501400	-1.95593400	-0.31129900	C	1.03445400	2.72580000	0.14771900
C	-2.22827500	-4.34937200	1.11388200	C	-0.78185700	4.79517400	0.69405800
H	-2.29767800	-3.11093500	2.86788100	H	-1.30002700	3.64215500	2.42605700
C	-2.32169900	-3.16951400	-0.98258500	C	0.89623900	3.81403200	-0.72408700
C	-2.18905400	-4.36016700	-0.27788900	C	-0.00638900	4.83571000	-0.46165900
H	-2.13821500	-5.27384600	1.67320400	H	-1.47322700	5.59807700	0.92491900

H	-2.27245100	-3.16331100	-2.06181500	H	1.49976800	3.82799500	-1.61958600
H	-2.05251600	-5.29230900	-0.81467200	H	-0.09622600	5.66572600	-1.15414100
C	1.37591900	-0.42086600	2.44272800	C	-3.22315400	-0.05898300	1.26711900
C	1.93141000	0.25449600	3.53478200	C	-4.01832600	-0.82238900	2.12716900
C	2.17947500	-0.65183600	1.31215300	C	-3.37361600	-0.22739500	-0.11905200
C	3.23971200	0.72450900	3.51402800	C	-4.92237800	-1.76231700	1.64467300
H	1.31002300	0.42477200	4.40851900	H	-3.89780500	-0.68868200	3.19753800
C	3.49093700	-0.16248300	1.28775900	C	-4.25958700	-1.19818500	-0.60004300
C	4.01664700	0.52177100	2.37728800	C	-5.03032300	-1.95910000	0.26985900
H	3.64180200	1.25528000	4.37044500	H	-5.51758700	-2.35128400	2.33388200
H	4.09005000	-0.27205200	0.39010400	H	-4.29988100	-1.37209900	-1.66551500
H	5.03102200	0.90140500	2.32611400	H	-5.70794800	-2.70878600	-0.12465200
N	0.07466900	2.24043200	-0.21776400	N	0.05125100	-2.22907700	0.08696300
N	1.60966400	-1.34224300	0.18563800	N	-2.55533500	0.55051800	-1.00508700
N	-2.75426100	-0.72586000	-1.00725300	N	2.04051800	1.72840100	-0.07995600
O	0.06229600	1.44740600	-1.42210800	O	0.24903200	-1.39548600	-1.04874800
H	0.69570600	0.71382400	-1.21017400	H	1.11567600	-1.58314500	-1.49957300
O	-1.81842200	-0.60313000	-2.08803800	O	2.15260400	1.56922800	-1.50229400
H	-1.24489200	0.13281600	-1.79537000	H	2.21083900	0.60395600	-1.65216800
O	1.75639100	-0.54861100	-0.99274200	O	-2.03559400	-0.33279900	-2.00877600
H	2.70921500	-0.45212100	-1.28616400	H	-1.15724200	-0.59317500	-1.65159100
C	1.05403400	3.36949400	-0.36423200	C	-0.28518300	-3.63125500	-0.29453800
C	-4.13620700	-0.59302200	-1.57073700	C	3.41562000	2.08849900	0.44152100
C	2.04310300	-2.75416900	-0.06364000	C	-3.20453100	1.68926500	-1.71928300
C	-4.24517600	0.82527500	-2.13678000	C	4.31489700	0.87925900	0.16687900
H	-5.25492400	1.00050900	-2.52012800	H	5.30810400	1.05304700	0.59310600
H	-4.03047000	1.55348500	-1.35794500	H	3.88774800	-0.01370800	0.62126500
H	-3.53103200	0.96815200	-2.94744900	H	4.41764300	0.68980700	-0.90049800
C	-4.44537600	-1.61147400	-2.68397200	C	3.99287200	3.33622900	-0.24869900
H	-4.52743400	-2.62728500	-2.29390000	H	3.43792000	4.23884800	0.01728800
H	-5.39685100	-1.35711900	-3.15995600	H	5.03354000	3.47518600	0.05806700
H	-3.66168700	-1.58287000	-3.44234500	H	3.96495700	3.20693900	-1.33073500
C	-5.14212600	-0.75400400	-0.42403300	C	3.35088700	2.32390100	1.95549300
H	-5.08442700	-1.74467600	0.03029700	H	2.66120600	3.12845200	2.21834600
H	-4.97130000	-0.00336100	0.35000300	H	3.05822900	1.41578000	2.48396900
H	-6.15426900	-0.61682000	-0.81398800	H	4.34701700	2.60735600	2.30602800
C	1.37081700	-3.19523500	-1.37065200	C	-2.08654200	2.41211400	-2.47999600
H	1.45396600	-4.28146500	-1.47395400	H	-2.47294900	3.32910800	-2.93588100
H	0.31818400	-2.91468900	-1.36136900	H	-1.27869500	2.66901400	-1.79633500
H	1.84427000	-2.72331500	-2.23049400	H	-1.67888100	1.77081400	-3.26014200
C	1.50297200	-3.60190200	1.09566400	C	-3.81501300	2.64378400	-0.68684500
H	1.87762700	-3.24501800	2.05847200	H	-4.53812800	2.13648100	-0.04402000
H	0.41371900	-3.59457700	1.10830400	H	-3.04022600	3.09701400	-0.06840000
H	1.83676600	-4.63556600	0.97062700	H	-4.33680300	3.44801300	-1.21258700
C	3.56561800	-2.95340900	-0.16945900	C	-4.29671500	1.23102900	-2.70502500
H	3.76941400	-3.99276600	-0.44653200	H	-4.63444400	2.08220800	-3.30353500
H	4.01136400	-2.30716700	-0.92848300	H	-3.89662000	0.47186600	-3.37798600
H	4.06031400	-2.75935300	0.78530400	H	-5.16423400	0.82178300	-2.18190500
C	0.83070300	4.23836500	-1.61552300	C	0.81294800	-4.37882800	-1.07500600
H	-0.03845400	4.89160300	-1.51681800	H	1.65998100	-4.63436800	-0.43646500
H	1.70621600	4.87241500	-1.77821100	H	0.40446800	-5.31274800	-1.47340300
H	0.70784900	3.59768100	-2.48989300	H	1.18472900	-3.78490900	-1.91216200
C	2.45054000	2.74454300	-0.42897500	C	-1.55817100	-3.56166700	-1.14752600
H	3.20934000	3.53195000	-0.43672700	H	-1.90078700	-4.57427300	-1.38108000
H	2.61909500	2.10941300	0.43846500	H	-2.34413000	-3.03445100	-0.60801800
H	2.59895300	2.14035100	-1.32286500	H	-1.37522100	-3.03026800	-2.08006000
C	0.95246800	4.22849700	0.90380100	C	-0.60228000	-4.38030600	1.00802100
H	-0.02613600	4.70316300	1.00224000	H	0.27278800	-4.44828000	1.65718300
H	1.14063400	3.62408700	1.79385900	H	-1.40386300	-3.87777600	1.55419500
H	1.71056700	5.01455600	0.86179700	H	-0.93022800	-5.39587600	0.77055100
Br	4.64195400	0.02433400	-2.23072400	Br	2.99613800	-1.49921600	-2.63095700
<b>[LBr]<sup>-</sup>, 16Br, E<sub>0</sub>=-4305.100503 au</b>				<b>[LBr]<sup>-</sup>, 17Br, E<sub>0</sub>=-4305.099351 au</b>			
N	-1.20433200	0.19989900	1.64519200	N	-0.03945900	0.61681600	0.79441300
C	-0.54196000	-0.87286200	2.40903400	C	-1.20577400	0.08801900	1.55125400
H	-0.89813900	-1.81163000	1.99875000	H	-2.03961500	0.07094700	0.85859100
H	-0.88238300	-0.83515500	3.46057000	H	-1.44998800	0.76842000	2.37552900



C	-2.66443100	0.06375900	1.78895400	C	-0.38174200	1.90341500	0.12473100
H	-3.11997700	0.88730700	1.24206500	H	0.49183800	2.18229700	-0.45203500
H	-2.94402900	0.15157000	2.85565300	H	-0.54536500	2.66633400	0.89412000
C	-0.75581200	1.53234600	2.08839600	C	1.10593200	0.86976400	1.71966200
H	0.32675500	1.50059900	2.11966400	H	1.32246000	-0.07228800	2.22255200
H	-1.12355300	1.73921200	3.11051800	H	0.81854400	1.62707500	2.45758700
C	0.96765900	-0.83599800	2.41552100	C	-0.93278000	-1.30233900	2.06320500
C	1.60442200	-0.46587500	3.60663000	C	-0.53420900	-1.48356900	3.39163600
C	1.76008200	-1.14531600	1.29447100	C	-1.00923700	-2.42494300	1.22370800
C	2.98753600	-0.37438300	3.70103500	C	-0.16298400	-2.73576300	3.86922300
H	0.98917700	-0.22604600	4.46814000	H	-0.49938400	-0.61498000	4.04008600
C	3.15331700	-1.03703500	1.39087700	C	-0.59518100	-3.67445400	1.69374400
C	3.76202900	-0.65499000	2.57927300	C	-0.17216600	-3.83130100	3.00838400
H	3.45188500	-0.07405300	4.63416000	H	0.15298700	-2.85126600	4.90008700
H	3.76899900	-1.21642900	0.51514100	H	-0.57924900	-4.51256500	1.01217900
H	4.84242300	-0.57148100	2.61739200	H	0.14888300	-4.80648600	3.35868700
C	-1.20280400	2.63159900	1.15570300	C	2.33336000	1.30210100	0.96312500
C	-2.39495100	3.32153900	1.39801700	C	2.75662800	2.62967100	1.02672100
C	-0.45927700	2.94835200	0.00725500	C	3.04863500	0.38096500	0.16792900
C	-2.88326200	4.26507800	0.50090800	C	3.87344400	3.06209700	0.31697600
H	-2.95276000	3.09875700	2.30187800	H	2.18846800	3.32039400	1.64060400
C	-0.97823200	3.86165100	-0.91600500	C	4.15300100	0.83232800	-0.56170100
C	-2.17913400	4.51671100	-0.67440900	C	4.56915200	2.15882800	-0.47992200
H	-3.81384500	4.78258000	0.70643700	H	4.19056400	4.09693400	0.38003200
H	-0.43657900	4.02938200	-1.83546600	H	4.69209000	0.15460400	-1.20505800
H	-2.56486100	5.22219800	-1.40249400	H	5.43052400	2.48432800	-1.05344500
C	-3.22711400	-1.22520400	1.24219700	C	-1.59909700	1.84892200	-0.76145000
C	-3.66702900	-2.23193400	2.10011200	C	-2.77398500	2.44450800	-0.28350000
C	-3.34596900	-1.40357300	-0.15174600	C	-1.61546800	1.23703400	-2.02604000
C	-4.22925400	-3.40644700	1.60755100	C	-3.95106700	2.41532800	-1.02243300
H	-3.56913300	-2.08636800	3.17089200	H	-2.74538100	2.90804700	0.69852200
C	-3.90600000	-2.58803500	-0.63816500	C	-2.80694200	1.20196900	-2.76014500
C	-4.35073000	-3.57893500	0.23292100	C	-3.96763800	1.78233700	-2.26374700
H	-4.56507500	-4.17884600	2.29021600	H	-4.85119000	2.87022600	-0.62412700
H	-3.97866300	-2.74879900	-1.70265600	H	-2.81696900	0.67758200	-3.70514300
H	-4.77647800	-4.49256500	-0.16757700	H	-4.88286300	1.73666700	-2.84489600
N	1.12379600	-1.50708400	0.05615200	N	-1.48616500	-2.22295100	-0.12386200
N	-2.83004100	-0.33890800	-0.94539200	N	-0.42340600	0.58616800	-2.50743400
N	0.80796600	2.30788600	-0.18796500	N	2.55263700	-0.96029000	0.17590900
O	1.65585600	-0.71771900	-1.00706700	O	-0.54962600	-2.84847300	-1.05116800
H	2.60610800	-0.94137400	-1.22351600	H	0.26064900	-2.30262000	-0.91073000
O	0.85247700	1.83107100	-1.53980200	O	1.39240500	-1.01825900	-0.69879300
H	1.05850200	0.87822100	-1.41346400	H	0.71183500	-0.41069400	-0.21770100
O	-1.41617700	-0.55386400	-1.09751200	O	-0.81779800	-0.64924000	-3.14460400
H	-1.03122500	-0.20857500	-0.26137100	H	-0.66450200	-1.31885900	-2.45969500
C	1.10225000	-2.96676600	-0.31048600	C	-2.84507200	-2.76924800	-0.42317300
C	2.02110600	3.15910300	0.06486600	C	3.41053800	-2.13453200	-0.08393500
C	-3.38454500	0.03442600	-2.26449900	C	0.41680500	1.31947500	-3.50683200
C	3.24035500	2.23844200	-0.03754900	C	-2.93939100	-4.30159100	-0.29214100
H	4.15124700	2.80186500	0.18508400	H	-2.85550900	-4.62567800	0.74611900
H	3.15527900	1.42049000	0.67503500	H	-3.90799300	-4.63877300	-0.67145200
H	3.34367700	1.80398000	-1.03050500	H	-2.15472300	-4.78140200	-0.87942200
C	2.15933100	4.31464500	-0.94222200	C	-3.82994000	-2.10232300	0.54610300
H	1.38634100	5.07372800	-0.80192100	H	-3.58687600	-2.32175500	1.58696900
H	3.13183300	4.79761800	-0.81322500	H	-3.83924600	-1.02014500	0.40931800
H	2.10150500	3.92513400	-1.95926400	H	-4.83552600	-2.47994000	0.34437400
C	1.93264300	3.72058600	1.48990200	C	-3.20980600	-2.36175500	-1.85484200
H	1.05340800	4.35389200	1.62792400	H	-4.24353400	-2.65320300	-2.06178000
H	1.90800000	2.91550000	2.22674500	H	-3.11629400	-1.28520000	-1.98002500
H	2.82089600	4.32632300	1.68676000	H	-2.56125700	-2.85057700	-2.58160900
C	-2.83037200	1.43937500	-2.55092300	C	-0.33493900	1.57228900	-4.82684000
H	-3.18558200	1.79756600	-3.52215800	H	-1.16036300	2.27342000	-4.68569400
H	-3.15689700	2.13282900	-1.77541600	H	0.34995900	1.99889500	-5.56537200
H	-1.74103000	1.42647200	-2.55088900	H	-0.73067100	0.63623400	-5.22300900
C	-4.91099600	0.12014200	-2.14192300	C	0.86704300	2.65877700	-2.91259500
H	-5.37826200	-0.85600700	-2.00430500	H	0.02108000	3.26315400	-2.58039400

H	-5.18541300	0.75367900	-1.29461800	H	1.55157100	2.51145200	-2.07701400
H	-5.31917600	0.56742400	-3.05168900	H	1.39984400	3.22096400	-3.68404100
C	-2.96452800	-0.90419900	-3.41407400	C	1.65719900	0.45232500	-3.76159800
H	-3.26387600	-0.46770400	-4.37120100	H	2.37473500	1.00212900	-4.37805800
H	-1.88177700	-1.02500100	-3.41245900	H	2.11867400	0.19225700	-2.80955600
H	-3.42288700	-1.89205700	-3.34656500	H	1.38474100	-0.46940500	-4.27549000
C	2.47682400	-3.65271600	-0.22563400	C	2.62860300	-3.36325100	0.41599500
H	2.84567500	-3.68312900	0.80268300	H	3.27219200	-4.24758100	0.39116500
H	2.38250200	-4.68429300	-0.57935500	H	2.28638800	-3.19747200	1.43772300
H	3.22070000	-3.14945200	-0.84722000	H	1.75496800	-3.56582600	-0.20048100
C	0.55705400	-3.07210000	-1.74087100	C	3.76118800	-2.35091500	-1.57096800
H	0.35396400	-4.12383500	-1.96570500	H	4.45972300	-1.60759200	-1.95577600
H	-0.36097200	-2.49246400	-1.82807400	H	4.21936500	-3.33544800	-1.70241700
H	1.28021500	-2.69516300	-2.46273500	H	2.85477400	-2.30756100	-2.17479200
C	0.12356900	-3.66613900	0.64231400	C	4.67296100	-2.00655700	0.78193500
H	0.43612100	-3.56488700	1.68469600	H	5.32920500	-1.19951900	0.45949800
H	-0.88477200	-3.26638700	0.52377900	H	4.39445300	-1.82267400	1.82210500
H	0.09832600	-4.73377600	0.40843600	H	5.23417300	-2.94297000	0.73412900
Br	4.68212000	-1.08516600	-1.96440700	Br	-1.14559100	3.36182900	3.43250700
<b>[LBr]<sup>-</sup>, 18Br, E<sub>0</sub>=-4305.097018 au</b>				<b>[LBr]<sup>-</sup>, 19Br, E<sub>0</sub>=-4305.096298 au</b>			
N	0.33060500	-0.01341700	-1.92300400	O	1.13199800	1.15078700	0.68447600
C	1.47102000	0.76490900	-2.43972700	O	-3.04322300	-1.14051700	1.92940800
H	1.29381300	1.80768500	-2.18221400	O	3.28167300	-0.54256600	0.79185200
H	1.51682000	0.67407600	-3.54147200	N	1.07542800	2.55462400	0.44496600
C	-0.94870200	0.47762500	-2.45176300	N	-2.98183600	-0.32624300	0.75285200
H	-1.70600000	-0.20433500	-2.09481400	N	2.90571700	-1.40902600	-0.30462900
H	-0.95015900	0.41708200	-3.55701200	N	0.05554800	-0.37194500	-2.16673800
C	0.53088900	-1.43319000	-2.26249300	C	1.11108000	0.67140100	-2.08855500
H	1.45605400	-1.73439800	-1.79066000	C	0.49774200	2.04997900	-1.98442900
H	0.68522200	-1.52745000	-3.35395100	C	-0.17115700	2.51319400	-3.12488400
C	2.79918500	0.34875000	-1.85750800	C	-0.87798600	3.70704400	-3.14406900
C	3.71959900	-0.36947100	-2.61955300	C	-0.95725700	4.46151000	-1.97606000
C	3.12359800	0.70553800	-0.53152400	C	-0.31449300	4.01701100	-0.82997900
C	4.95622200	-0.74037800	-2.09819800	C	0.44926800	2.83911300	-0.81366700
H	3.45922700	-0.63802800	-3.63834200	C	2.43075100	3.15582800	0.68203100
C	4.36373500	0.31917400	-0.01293900	C	3.47353200	2.67302900	-0.34149300
C	5.27462400	-0.39144800	-0.78967200	C	2.31884900	4.68515200	0.60450000
H	5.65980000	-1.29880300	-2.70558100	C	2.84952400	2.77473200	2.10892400
H	4.61166900	0.55943700	1.00942100	C	-1.02366900	-0.16397200	-1.19846500
H	6.22796400	-0.68450600	-0.36298400	C	-2.26596800	-0.97464700	-1.46024700
C	-0.60085300	-2.35849200	-1.88373300	C	-2.51416200	-1.61472400	-2.67504300
C	-1.44967100	-2.79203300	-2.91038300	C	-3.58170700	-2.49859600	-2.81073500
C	-0.87637600	-2.76952700	-0.56457600	C	-4.40614200	-2.76279100	-1.71792000
C	-2.57219600	-3.57215400	-2.66663800	C	-4.20940800	-2.07753500	-0.52168500
H	-1.23067500	-2.47116700	-3.92362500	C	-3.18012800	-1.14151800	-0.40587900
C	-2.02659800	-3.53766200	-0.32325200	C	-3.90376600	0.84243200	0.90749800
C	-2.86621000	-3.93279800	-1.35445300	C	-5.35370200	0.40872400	1.19259100
H	-3.21791500	-3.87302600	-3.48403200	C	-3.37257600	1.68017300	2.07637100
H	-2.25864900	-3.78929600	0.70040100	C	-3.85451700	1.68778300	-0.37202300
H	-3.74938100	-4.52183900	-1.13119700	C	0.63606200	-1.73452800	-2.16548300
C	-1.27871600	1.89433900	-2.04999400	C	0.73291600	-2.42210700	-0.80940500
C	-0.97168100	2.92258400	-2.94913600	C	-0.33734700	-3.22899900	-0.40591100
C	-1.83907400	2.23198500	-0.80341800	C	-0.42825800	-3.73223000	0.88592000
C	-1.15431300	4.26189800	-2.63091200	C	0.56982100	-3.43674200	1.80720600
H	-0.55379700	2.65184900	-3.91357300	C	1.67180400	-2.69123000	1.41249500
C	-1.99428000	3.58718800	-0.47812700	C	1.77627100	-2.20689700	0.10646400
C	-1.65499400	4.59080800	-1.37401400	C	4.14745000	-2.14513500	-0.68175800
H	-0.89142100	5.03539900	-3.34399700	C	3.81366400	-3.14697700	-1.79289300
H	-2.35731600	3.83098400	0.50856700	C	4.77980000	-2.89493100	0.50580200
H	-1.78426500	5.62966500	-1.08938600	C	5.13154700	-1.09862000	-1.22335700
N	2.11347900	1.41757100	0.17228300	H	1.81109800	0.48018000	-1.28555200
N	-2.19901600	1.21510500	0.14597200	H	1.67357600	0.61701800	-3.02906100
N	-0.04826500	-2.35412900	0.52658900	H	-0.14827000	1.88233900	-4.00689000
O	1.19809800	0.45177500	0.72164500	H	-1.38469400	4.02937900	-4.04689700
H	0.59040800	0.25635700	-0.02360700	H	-1.54032200	5.37544900	-1.94675600
O	-0.91066600	-2.25120100	1.66702300	H	-0.41390000	4.56157100	0.09885700

H	-0.67624200	-1.41194700	2.13480300	H	3.16936300	2.93681600	-1.35773400
O	-2.01062400	1.79186000	1.44563700	H	3.61547300	1.59530900	-0.28323300
H	-1.49235700	1.14069000	1.97831500	H	4.43842700	3.14923700	-0.14216500
C	2.41413500	2.42686800	1.21602800	H	2.04924800	5.02742000	-0.39529400
C	1.07836700	-3.28334700	0.92747800	H	3.28802000	5.12025600	0.86152200
C	-3.64049900	0.74533800	0.10302200	H	1.57635600	5.05543400	1.31438900
C	1.82703800	-2.58282000	2.06877700	H	2.05598800	3.03085100	2.81347600
H	2.72646900	-3.15344000	2.32146300	H	3.75907900	3.31868600	2.37933000
H	2.10489100	-1.57542600	1.75780300	H	3.04804000	1.70953000	2.20866200
H	1.20437200	-2.49427300	2.95812700	H	-1.28749200	0.88895400	-1.22836000
C	0.53748100	-4.64567200	1.39290800	H	-0.71766600	-0.35271500	-0.16661900
H	0.07801400	-5.19670800	0.56756100	H	-1.83399000	-1.43137900	-3.49788700
H	1.35680200	-5.25068900	1.79171800	H	-3.75165300	-3.00253100	-3.75662800
H	-0.20335200	-4.50149100	2.17884800	H	-5.21122500	-3.48537300	-1.80204500
C	2.05462400	-3.49506400	-0.23374500	H	-4.84271200	-2.26461400	0.33484400
H	1.56048100	-3.88852700	-1.12499600	H	-5.36862800	-0.28992900	2.03052800
H	2.58115500	-2.57264000	-0.48104000	H	-5.80741100	-0.06928200	0.32132400
H	2.80505600	-4.22627300	0.07821700	H	-5.96080500	1.28055900	1.45434300
C	-3.77732600	-0.33098500	1.18629900	H	-3.96674700	2.59436400	2.17669500
H	-4.77139700	-0.78548500	1.12669200	H	-2.32671300	1.94062200	1.91239400
H	-3.02214200	-1.10515300	1.04984800	H	-3.42150300	1.12220000	3.01046500
H	-3.64141300	0.09071900	2.18125400	H	-2.85232400	2.08165200	-0.54516000
C	-3.96853600	0.11616200	-1.25506500	H	-4.53333300	2.53778700	-0.26013200
H	-3.78465600	0.80249600	-2.08468000	H	-4.16519500	1.11921500	-1.25058300
H	-3.40992900	-0.80705100	-1.41227500	H	1.61154900	-1.65646300	-2.63929500
H	-5.03131400	-0.14014000	-1.26697900	H	0.01808900	-2.37340000	-2.80288500
C	-4.61711400	1.90155700	0.37757300	H	-1.14413400	-3.41180200	-1.10466700
H	-5.63432700	1.50926500	0.46551500	H	-1.30241200	-4.29942500	1.18256800
H	-4.35385500	2.39601900	1.31237100	H	0.47920200	-3.75378300	2.83888500
H	-4.60522500	2.63801900	-0.43018600	H	2.42882400	-2.41296500	2.13021400
C	2.75260800	1.82015500	2.59049900	H	3.44613700	-2.63987300	-2.68642200
H	3.67895600	1.24160600	2.58087500	H	3.06228600	-3.86874200	-1.46981200
H	2.87409200	2.62554800	3.32123700	H	4.72158200	-3.69303100	-2.06230300
H	1.93768800	1.17708800	2.92642100	H	4.13054300	-3.70199400	0.85002000
C	1.13396900	3.26595400	1.35430900	H	4.95411500	-2.21042700	1.33578500
H	1.27722100	4.04823900	2.10599600	H	5.73620900	-3.33122700	0.20236300
H	0.88353300	3.73123200	0.39822400	H	6.03280100	-1.58801800	-1.60441200
H	0.29828000	2.64168400	1.66089000	H	5.41464200	-0.39779600	-0.43896700
C	3.53925200	3.33526800	0.69992200	H	4.66492100	-0.53522400	-2.03480200
H	4.50973300	2.83788500	0.67030600	H	0.59137000	0.97043100	1.50566500
H	3.30722500	3.69282100	-0.30722800	H	-2.17933800	-0.94068100	2.35721600
H	3.62361600	4.20212800	1.35974600	H	2.54951900	0.11050600	0.80041400
Br	-0.64600200	0.10092500	3.79188400	Br	-0.23830200	0.03233900	3.28338200
<b>[LBr]<sup>-</sup>, 20Br, E<sub>0</sub>=-4305.093150 au</b>				<b>[LBr]<sup>-</sup>, 21Br, E<sub>0</sub>=-4305.092857 au</b>			
N	-0.62127900	0.11247200	-0.90798700	N	0.13279100	0.59631500	-1.86214400
C	-1.39934400	0.58791800	-2.03560800	C	0.68955600	1.95056700	-2.01480600
H	-1.33802300	-0.17865600	-2.81424900	H	-0.05067700	2.64557300	-1.61923100
H	-0.95899100	1.49938800	-2.47935300	H	0.84906600	2.18479100	-3.08253700
C	-0.67734700	0.94664200	0.30040600	C	-1.22074300	0.46109900	-2.42792800
H	-0.14791300	0.41848800	1.08325800	H	-1.50427100	-0.57152000	-2.27312000
H	-1.71493300	0.99195100	0.62506200	H	-1.19229700	0.64634800	-3.51774900
C	0.70181600	-0.32660600	-1.31545400	C	1.04309700	-0.41918100	-2.43867900
H	1.39882800	0.50751700	-1.49325900	H	2.04906400	-0.11526600	-2.17641000
H	0.57244000	-0.80503400	-2.29015500	H	0.95610500	-0.41954700	-3.53933600
C	-2.86142700	0.90773700	-1.76762900	C	1.97867800	2.17529600	-1.26238400
C	-3.37011600	2.01816200	-2.45782600	C	3.16532500	2.37917300	-1.96348800
C	-3.72314900	0.22420000	-0.88340100	C	1.98194800	2.26716300	0.14968000
C	-4.66215600	2.48790700	-2.27482100	C	4.35351500	2.69608400	-1.30908600
H	-2.70104300	2.55100200	-3.12575500	H	3.14806200	2.31003200	-3.04663000
C	-5.01052700	0.74342400	-0.66081000	C	3.18741300	2.55619000	0.79698500
C	-5.48129800	1.85304100	-1.34361200	C	4.35642200	2.78676200	0.07744100
H	-5.00972600	3.35821100	-2.82058700	H	5.26325600	2.86036200	-1.87542300
H	-5.61938300	0.25576900	0.08549000	H	3.21936000	2.58774800	1.87433100
H	-6.48328900	2.22081800	-1.14902400	H	5.27545300	3.00766500	0.60932000
C	1.32511300	-1.34516600	-0.37852800	C	0.76584000	-1.79548700	-1.88601200
C	0.49022600	-2.03890900	0.50015500	C	-0.13583400	-2.65075900	-2.52575900

C	2.70267300	-1.63326600	-0.35244900	C	1.32442800	-2.19673900	-0.66006700
C	0.98428900	-2.99028100	1.38264100	C	-0.55280400	-3.83504100	-1.92667800
H	-0.55535500	-1.76990600	0.53411500	H	-0.53358400	-2.36536900	-3.49465000
C	3.19487200	-2.60929200	0.51814200	C	0.83015700	-3.33333500	-0.01445700
C	2.34297500	-3.28902400	1.38017000	C	-0.09944900	-4.14893800	-0.64721700
H	0.30461800	-3.44068800	2.09504700	H	-1.26683700	-4.47747400	-2.42995200
H	4.26201900	-2.77211000	0.56151100	H	1.14819800	-3.53168500	0.99824200
H	2.74836800	-4.01986000	2.07162600	H	-0.47975500	-5.02272300	-0.13083800
C	-0.13542700	2.35291100	0.10799200	C	-2.24387900	1.37579800	-1.79856500
C	-0.99421300	3.37373500	-0.31584900	C	-2.46860400	2.63372300	-2.37019900
C	1.22433700	2.66250800	0.27527400	C	-2.94613900	1.02883800	-0.63044000
C	-0.52016800	4.64194000	-0.63297700	C	-3.31179800	3.56717800	-1.78096300
H	-2.05057600	3.15517300	-0.41106800	H	-1.94466200	2.88583500	-3.28674800
C	1.70886400	3.92781600	-0.07403200	C	-3.76456600	1.98831800	-0.01973300
C	0.84332400	4.91273000	-0.53377400	C	-3.94449800	3.24383300	-0.58253700
H	-1.20975400	5.40936700	-0.96784300	H	-3.45608100	4.53969300	-2.23842800
H	2.77070600	4.11659400	0.00245500	H	-4.23075300	1.73130500	0.91969900
H	1.22994100	5.89075100	-0.80075500	H	-4.58292200	3.96808000	-0.08773200
N	-3.30557900	-0.94009200	-0.15953700	N	0.72846900	2.10276500	0.79753600
N	2.08778600	1.63623500	0.78720800	N	-2.79668600	-0.27845900	-0.06197600
N	3.62756400	-0.83227500	-1.13907000	N	2.36679500	-1.38653300	-0.09055100
O	-3.97630200	-0.93644800	1.10311600	O	0.37074000	0.70981000	0.86067100
H	-3.23699300	-0.95414600	1.76869600	H	0.06394800	0.50669800	-0.05596400
O	4.83588200	-0.63085500	-0.35742600	O	2.20337400	-1.34738600	1.33343100
H	4.63822700	0.20555500	0.09566800	H	1.49382500	-0.68362200	1.44907700
O	3.32658000	1.67427200	0.02939900	O	-2.87353600	-0.12732000	1.35906700
H	3.15842500	0.99655000	-0.65707800	H	-2.12070700	-0.65954100	1.73945900
C	-3.58790800	-2.26116800	-0.81939500	C	0.40191400	2.70327800	2.11535200
C	4.09437200	-1.39355600	-2.45034600	C	3.76064200	-1.88211700	-0.32695500
C	2.42529000	1.69354800	2.24743900	C	-3.86294800	-1.28008400	-0.45112600
Br	-1.66154700	-1.13000600	3.30584900	C	4.70646000	-0.82071400	0.24531300
C	3.39375300	2.84675900	2.56671800	H	5.74711700	-1.11029700	0.06814100
H	2.92436400	3.81638500	2.38693200	H	4.51972200	0.14038900	-0.23176100
H	3.67810600	2.80164500	3.62133100	H	4.54375900	-0.70765500	1.31583700
H	4.29821000	2.77681400	1.96059000	C	4.02020100	-3.23971100	0.35279100
C	3.04998800	0.34493500	2.62204000	H	3.42453200	-4.03241200	-0.10447400
H	2.36631500	-0.46690400	2.37641100	H	5.07666200	-3.50701600	0.25403100
H	3.99165100	0.17371000	2.10012500	H	3.76840000	-3.18257600	1.41154200
H	3.24952000	0.31673900	3.69645800	C	4.00949600	-2.01073700	-1.83470000
C	1.13311900	1.87393600	3.05670000	H	3.32105900	-2.71629200	-2.30250200
H	0.61722000	2.79915200	2.79483800	H	3.91713100	-1.04447400	-2.33414100
H	0.44283300	1.03620000	2.94436500	H	5.02827700	-2.37441800	-1.99309800
H	1.40119700	1.92759200	4.11480600	C	-3.45442300	-2.61030300	0.19026800
C	4.92560500	-0.29974700	-3.13245100	H	-4.14350300	-3.40064500	-0.12574800
H	5.81431800	-0.06940600	-2.54632600	H	-2.44239700	-2.87512300	-0.11323200
H	5.23460800	-0.62926700	-4.12825700	H	-3.46017500	-2.54430500	1.27725000
H	4.33243500	0.61225000	-3.23671600	C	-3.90594800	-1.45054400	-1.97439400
C	2.87626900	-1.71575100	-3.31873900	H	-4.08751600	-0.50533300	-2.49071800
H	2.22052700	-2.44154100	-2.83553700	H	-2.98315900	-1.89436200	-2.34862200
H	2.30450000	-0.81522400	-3.54321700	H	-4.72457300	-2.13076700	-2.22439400
H	3.22125600	-2.14394500	-4.26302200	C	-5.25423600	-0.85679600	0.05095300
C	4.93768900	-2.66597700	-2.26353500	H	-5.96976300	-1.66461300	-0.12781900
H	5.31354800	-3.00238700	-3.23379000	H	-5.21417100	-0.65683000	1.12133600
H	5.78772300	-2.47088600	-1.60982200	H	-5.61490900	0.03600100	-0.46643200
H	4.33997700	-3.47048100	-1.83157800	C	0.96508000	1.90125500	3.30417100
C	-3.06664100	-3.36132600	0.11286900	H	2.05342000	1.81802600	3.28024400
H	-3.24957400	-4.34031600	-0.34106000	H	0.68658600	2.39476900	4.24022900
H	-1.99682400	-3.24939200	0.28201600	H	0.54431600	0.89373400	3.31256800
H	-3.56362900	-3.31684300	1.07982400	C	-1.13261600	2.69861800	2.20417000
C	-5.09377200	-2.46565600	-1.06326600	H	-1.44843700	3.11909900	3.16390600
H	-5.27545500	-3.46822400	-1.46160300	H	-1.55673700	3.29971300	1.39679400
H	-5.63788400	-2.36161100	-0.12353200	H	-1.52324100	1.68734600	2.12045500
H	-5.48508000	-1.73825600	-1.77852300	C	0.86916100	4.16701000	2.12768200
C	-2.82556600	-2.33173200	-2.14451700	H	1.94899800	4.28092100	2.21843500
H	-3.17964300	-1.58238900	-2.85558700	H	0.54790800	4.67302900	1.21321200
H	-1.75942200	-2.18683600	-1.96917000	H	0.40515500	4.67255100	2.97783400

H	-2.97605900	-3.31758100	-2.59264000	Br	-0.85021500	-1.88895700	3.03538700
<b>[LBr]<sup>-</sup>, 22Br, E<sub>0</sub>=-4305.087269 au</b>				<b>[Li]<sup>-</sup>, 10I, E<sub>0</sub>=-8650.493764 au</b>			
N	0.04564200	0.49584300	0.85499000	O	-3.42522000	-1.35082900	0.51323200
C	-0.24855600	1.84008800	0.29102800	H	-3.22121200	-0.92173900	-0.34802700
H	0.62251300	2.11312800	-0.29805000	O	-2.34703500	3.17640800	-1.58120300
H	-0.36649300	2.56084500	1.10856400	H	-2.37962100	2.32399300	-2.06661900
C	1.17958100	0.64054900	1.80767500	O	3.47372900	-0.31979300	1.43083000
H	1.37921000	-0.35013500	2.21463000	H	2.50842900	-0.11648100	1.23821800
H	0.88752400	1.32036400	2.61775200	N	-2.26834600	-2.17171500	0.71422800
C	-1.13281800	-0.08122500	1.55036500	N	-1.91333400	2.74688100	-0.28655000
H	-1.96728900	0.00455800	0.86480000	N	4.08684600	-0.01496600	0.15376500
H	-1.36608000	0.50099100	2.45039100	N	1.01548800	-0.12812400	0.42652900
C	-1.48402300	1.89867300	-0.56752000	C	0.49676400	-1.51044700	0.64878700
C	-2.65207500	2.43922700	-0.01376200	H	-0.17292400	-1.78746800	-0.16760400
C	-1.50589200	1.45666100	-1.89820100	H	1.35635900	-2.18357700	0.64522800
C	-3.82609500	2.51897700	-0.75471200	C	-0.25475900	-1.61139100	1.94910000
H	-2.61574700	2.77917600	1.01921000	C	0.39856000	-1.35809400	3.15996700
C	-2.69098300	1.54671500	-2.63915600	H	1.47362000	-1.21301700	3.15320200
C	-3.84915200	2.06594000	-2.07194000	C	-0.31706900	-1.23800600	4.34477900
H	-4.72138600	2.92996700	-0.30171100	H	0.20151700	-1.02713000	5.27358000
H	-2.71954100	1.19897500	-3.66573000	C	-1.70799600	-1.35251300	4.32660200
H	-4.76083100	2.11842200	-2.65733400	H	-2.27788700	-1.21870000	5.23984400
C	-0.90532900	-1.53386600	1.88650800	C	-2.36482300	-1.64816700	3.13852600
C	-0.43920400	-1.88649600	3.15775100	H	-3.44285700	-1.72639900	3.10730900
C	-1.10050900	-2.55116000	0.93897300	C	-1.64334000	-1.82031700	1.95160200
C	-0.11030300	-3.20082600	3.47078700	C	-2.63456900	-3.60797800	0.53061000
H	-0.32198700	-1.10288200	3.89800400	C	-3.08879500	-3.77057800	-0.92486100
C	-0.73180700	-3.86476400	1.24202600	H	-2.32814300	-3.38882800	-1.60699400
C	-0.23470700	-4.19046700	2.49804600	H	-4.00289900	-3.20756800	-1.11091400
H	0.25978200	-3.44692800	4.46000200	H	-3.27617000	-4.82702600	-1.14015400
H	-0.80996100	-4.61891900	0.47177900	C	-1.37700800	-4.45493300	0.76597500
H	0.05262100	-5.21350400	2.71652700	H	-0.57364000	-4.15336900	0.09123700
C	2.44333800	1.13624900	1.15139600	H	-1.61163300	-5.50467400	0.57124800
C	2.89819600	2.42930400	1.40777900	H	-1.01689800	-4.37165700	1.79308400
C	3.18972500	0.29286100	0.29906500	C	-3.75822900	-4.05729600	1.48159200
C	4.08456600	2.89859400	0.84840100	H	-4.08552100	-5.06871400	1.22344700
H	2.30718400	3.06368600	2.05983800	H	-4.61082700	-3.38275500	1.38822800
C	4.37339400	0.77768700	-0.26611300	H	-3.42364800	-4.06626800	2.52137100
C	4.82328700	2.06629900	0.01398100	C	-0.06055300	0.86017500	0.67317700
H	4.42637500	3.90487700	1.06372000	H	-0.38094300	0.73139500	1.70615700
H	4.94610600	0.15568100	-0.93721200	H	-0.92764400	0.65708800	0.03749400
H	5.74580100	2.41994100	-0.43480900	C	0.35177600	2.29364800	0.46456500
N	-0.30568000	0.88527500	-2.44960900	C	1.64125800	2.74332600	0.76721200
N	2.63083900	-0.99885500	0.07462300	H	2.35529400	2.04629500	1.18489300
N	-1.66977300	-2.19905600	-0.33511400	C	2.02583700	4.05049100	0.49485200
O	-0.56425500	-0.44570600	-2.92708200	H	3.03316000	4.37644500	0.73034100
H	-1.38105000	-0.41919600	-3.44647800	C	1.12410400	4.92797400	-0.10848500
O	-0.88854000	-2.81771500	-1.37586200	H	1.42835200	5.93921900	-0.35752900
H	-0.46330800	-2.04447500	-1.78576200	C	-0.16927800	4.50533800	-0.38504900
O	1.57836700	-0.87332900	-0.90577100	H	-0.87661700	5.16224600	-0.87220300
H	0.83630000	-0.46429100	-0.37124400	C	-0.57757800	3.20554700	-0.06280300
C	0.45810500	1.65023400	-3.47689100	C	-2.95240600	3.11815700	0.71792000
C	-3.10206800	-2.57462400	-0.54452500	C	-3.25340500	4.62813600	0.70711600
C	3.43136100	-2.19352100	-0.25160900	H	-3.51028300	4.94769900	-0.30389700
C	-3.53475000	-1.94961500	-1.87656400	H	-2.39317300	5.20611200	1.05301400
H	-4.59622200	-2.14363100	-2.05552800	H	-4.09710000	4.84790200	1.36799600
H	-3.37560100	-0.87209100	-1.84945100	C	-4.21539300	2.32390500	0.36310800
H	-2.95977400	-2.37648000	-2.69956100	H	-4.00549400	1.25459200	0.39614400
C	-3.32648500	-4.09748800	-0.59354000	H	-4.55726600	2.57610400	-0.63989300
H	-3.15616800	-4.55761100	0.38114900	H	-5.01247900	2.55068800	1.07799800
H	-4.35769600	-4.31004600	-0.89036600	C	-2.47264100	2.69078200	2.11022900
H	-2.65463100	-4.55254600	-1.32295100	H	-1.54019000	3.18563500	2.38960900
C	-3.93877900	-1.96408900	0.58652000	H	-2.32991600	1.61083400	2.15786200
H	-3.63503400	-2.34303300	1.56336300	H	-3.23425100	2.96270800	2.84594400
H	-3.85735300	-0.87651700	0.59563200	C	1.49067800	-0.02298900	-0.98220300
H	-4.98922900	-2.22463900	0.43202900	H	1.93549800	0.96496500	-1.09941600

C	2.50464900	-3.39405600	0.00818900	H	0.63325500	-0.10228700	-1.66085500
H	3.03092800	-4.33113600	-0.20040500	C	2.51421100	-1.07103400	-1.33882200
H	2.17833800	-3.39249600	1.04897000	C	2.17647500	-2.05830300	-2.26441600
H	1.61541600	-3.33558600	-0.61711500	H	1.17959500	-2.04426100	-2.69159800
C	4.61304500	-2.27605400	0.72392300	C	3.09317900	-3.03298200	-2.64956900
H	5.36086000	-1.50198500	0.55094900	H	2.81340900	-3.78459900	-3.37902800
H	4.25531100	-2.17984900	1.75175700	C	4.36454100	-3.03182000	-2.08779700
H	5.09853100	-3.24966400	0.61722200	H	5.08831900	-3.79036700	-2.36672600
C	3.90563200	-2.24603000	-1.71948400	C	4.71286900	-2.06329200	-1.14928800
H	4.33938300	-3.22704000	-1.93520500	H	5.69640800	-2.09530900	-0.70726600
H	3.05393600	-2.08694200	-2.38059600	C	3.80887000	-1.06500400	-0.77212800
H	4.66091400	-1.49227100	-1.94690700	C	5.44554400	0.50730000	0.40312200
C	-0.29903100	1.84012500	-4.80575800	C	6.12137200	0.79236200	-0.94531600
H	-1.16457100	2.49486400	-4.68906500	H	5.46209100	1.39643700	-1.57279500
H	0.36697700	2.29296900	-5.54503000	H	6.37280900	-0.11461200	-1.49370000
H	-0.62891500	0.88006300	-5.21275600	H	7.04384900	1.35268900	-0.77232800
C	1.76107900	0.87604300	-3.72050000	C	6.31349900	-0.40624000	1.29476100
H	2.43509600	1.47055600	-4.34437300	H	6.64054200	-1.31086300	0.78123400
H	2.23469600	0.65190600	-2.76532900	H	5.74146100	-0.70006900	2.17494700
H	1.56109700	-0.07146600	-4.22171400	H	7.20908600	0.13071700	1.62075000
C	0.79157600	3.02303900	-2.87995500	C	5.25422100	1.85179600	1.12955500
H	-0.10879400	3.57216900	-2.59808400	H	4.74203600	1.70010000	2.07899900
H	1.42854400	2.92035000	-2.00141200	H	4.65357900	2.52242000	0.51337500
H	1.33254400	3.61285300	-3.62427900	H	6.22472200	2.31849900	1.32073900
Br	-1.29771200	3.12207600	3.56441600	I	-2.36747200	-0.18175800	-2.67545600
<b>[Li]<sup>-</sup>, 11l, E<sub>0</sub>=-8650.485753 au</b>				<b>[Li]<sup>-</sup>, 12l, E<sub>0</sub>=-8650.491012 au</b>			
N	-0.00237900	0.00059000	-2.03729300	N	-1.65400700	0.12322400	1.66852900
C	-1.38259100	-0.16354100	-2.49333300	C	-0.89337600	-0.65127600	2.64759900
H	-1.72848500	-1.11418700	-2.11283300	H	-0.92633700	-1.68814900	2.33127600
H	-1.41539700	-0.22889100	-3.60159900	H	-1.36507600	-0.59475200	3.65029300
C	0.83044500	-1.11213100	-2.49353000	C	-2.95849800	-0.47487100	1.39758400
H	1.82622400	-0.93614700	-2.11199900	H	-3.46316300	0.16508500	0.68329100
H	0.90441700	-1.10719700	-3.60173000	H	-3.58317000	-0.48156700	2.31534100
C	0.54490200	1.27871800	-2.49230400	C	-1.78774000	1.52426300	2.07301500
H	-0.10453600	2.05278400	-2.10862800	H	-0.79281500	1.88343100	2.31757500
H	0.50201500	1.34189100	-3.60033800	H	-2.41651400	1.61484500	2.98278800
C	-2.31238700	0.95092300	-2.07456800	C	0.54133600	-0.19951400	2.75802100
C	-2.62008600	1.94060200	-3.01601300	C	0.93381300	0.58933300	3.84351700
C	-2.83449200	1.07717200	-0.77415000	C	1.49002100	-0.51244900	1.77066600
C	-3.37558500	3.06084300	-2.69421800	C	2.22565300	1.09438500	3.94506200
H	-2.21767500	1.83428900	-4.01811200	H	0.19976300	0.82133300	4.60877100
C	-3.57367600	2.22396200	-0.44696600	C	2.77633800	0.02967300	1.85514700
C	-3.83916600	3.20744600	-1.38957700	C	3.14367000	0.82480600	2.93466800
H	-3.57818200	3.81808200	-3.44348000	H	2.50496500	1.70998200	4.79334100
H	-3.90865600	2.33810900	0.57302300	H	3.48642600	-0.14174400	1.05481300
H	-4.40945400	4.08506000	-1.10423400	H	4.14497700	1.23848900	2.97309000
C	1.97592600	1.52594000	-2.07653200	C	-2.38002500	2.37361900	0.97531200
C	2.98492500	1.29673300	-3.01984100	C	-3.73679000	2.70970500	0.99672700
C	2.34892600	1.91502200	-0.77692100	C	-1.60305300	2.76303700	-0.12590300
C	4.33347200	1.39003400	-2.70053600	C	-4.33806700	3.36790100	-0.07100000
H	2.68953000	1.00144500	-4.02133200	H	-4.33174400	2.41816200	1.85636100
C	3.71231400	1.98093300	-0.45220700	C	-2.22182200	3.37553800	-1.22061700
C	4.69483400	1.71819500	-1.39659900	C	-3.57863600	3.67700900	-1.19691400
H	5.08905000	1.18612500	-3.45111400	H	-5.39497800	3.60835100	-0.03801300
H	3.98076800	2.21407000	0.56720300	H	-1.63054500	3.59236800	-2.09824500
H	5.74057700	1.77256200	-1.11319200	H	-4.04115000	4.15105100	-2.05575100
C	0.33050600	-2.47504800	-2.07594800	C	-2.89471900	-1.89010800	0.87161400
C	-0.37366800	-3.23508000	-3.01772300	C	-3.25067100	-2.93467500	1.73264200
C	0.48358300	-2.99205800	-0.77634300	C	-2.45561300	-2.21017400	-0.42557000
C	-0.96595600	-4.44980800	-2.69698500	C	-3.14973100	-4.26858200	1.35731800
H	-0.48365100	-2.83208000	-4.01919300	H	-3.58516800	-2.68198700	2.73360100
C	-0.13992700	-4.20595000	-0.45018500	C	-2.33315400	-3.55749400	-0.79006800
C	-0.85995300	-4.92623900	-1.39304600	C	-2.67312400	-4.57864900	0.08646700
H	-1.52127700	-5.00280800	-3.44642100	H	-3.41603800	-5.05446000	2.05526300
H	-0.07043200	-4.55459800	0.56924000	H	-1.93396500	-3.78726700	-1.76694100
H	-1.33477500	-5.85917700	-1.10839300	H	-2.56135600	-5.61252900	-0.22164700

N	-2.56693000	0.08126200	0.22163700	N	1.09813100	-1.38295300	0.69238100
N	1.21346500	-2.26387100	0.21972600	N	-2.07146000	-1.16549400	-1.33678900
N	1.35440300	2.18235400	0.22031000	N	-0.19500400	2.49213400	-0.08955900
O	-2.50009100	0.77399200	1.47788700	O	1.27889300	-0.71061700	-0.56341400
H	-1.66257500	0.48402600	1.89423500	H	2.24157200	-0.62730800	-0.81831000
O	1.92233200	1.77797100	1.47586900	O	0.15297900	1.80971900	-1.30207200
H	1.25299400	1.19744600	1.89279800	H	0.47731700	0.94959100	-0.97516600
O	0.58213800	-2.55499400	1.47638300	O	-0.90788400	-1.62034200	-2.04831500
H	0.41407300	-1.68552600	1.89429300	H	-0.16218000	-1.20989000	-1.56786200
C	-3.59747700	-1.01052600	0.39039300	C	1.67722400	-2.77367500	0.71060100
C	0.92578400	3.62127600	0.38927600	C	0.70787800	3.67645800	0.07012600
C	2.67465300	-2.61008500	0.38621600	C	-3.07197900	-0.77333500	-2.38213200
C	2.10031800	4.51308700	0.82736200	C	2.12416400	3.12371800	0.25304500
H	2.85361700	4.59569900	0.03947800	H	2.82691200	3.94406900	0.42623700
H	1.73538300	5.51849200	1.05585900	H	2.15299400	2.45347600	1.10971600
H	2.56771500	4.10189000	1.72199600	H	2.45601400	2.56768700	-0.62358000
C	-0.17252700	3.62103400	1.45992600	C	0.68164800	4.63329900	-1.13557600
H	-0.59804100	4.62508500	1.55190100	H	-0.26444800	5.17390300	-1.20852400
H	-0.96678800	2.92458000	1.18704000	H	1.48169700	5.37171400	-1.03385800
H	0.22072500	3.31789000	2.42945300	H	0.84980900	4.07202000	-2.05566500
C	0.33385500	4.16415100	-0.91571600	C	0.28564800	4.42273100	1.34198900
H	-0.60139300	3.66301700	-1.16659600	H	-0.73302700	4.81011800	1.26880900
H	0.11023900	5.22523300	-0.77668800	H	0.35129200	3.76893900	2.21408100
H	1.03028700	4.07796000	-1.75255000	H	0.96026400	5.26798200	1.50090800
C	-4.95779900	-0.44119000	0.82882700	C	-2.41916300	0.33178000	-3.22249800
H	-5.40667300	0.17012800	0.04152200	H	-3.17198600	0.80179000	-3.86285800
H	-5.64512100	-1.26097000	1.05642200	H	-1.97756300	1.08352700	-2.57080800
H	-4.83626600	0.16836900	1.72415300	H	-1.62663600	-0.07580000	-3.84842000
C	-3.77063500	-1.79437100	-0.91483200	C	-4.31812200	-0.21004900	-1.69255900
H	-2.86829100	-2.35257800	-1.16572800	H	-4.75896600	-0.92989200	-0.99892900
H	-4.57689100	-2.51959200	-0.77616900	H	-4.08560800	0.71126100	-1.15946100
H	-4.04485700	-1.14815100	-1.75145000	H	-5.06798100	0.02331300	-2.45313500
C	-3.04712400	-1.96136000	1.46074000	C	-3.47105300	-1.94967600	-3.29208300
H	-3.70268300	-2.83288800	1.55192900	H	-4.09773100	-1.58341900	-4.11038300
H	-2.04630000	-2.29941800	1.18800700	H	-2.58131400	-2.41096300	-3.72280500
H	-2.98228000	-1.46972700	2.43058800	H	-4.03597500	-2.70918100	-2.74658800
C	2.86269600	-4.07355300	0.82180600	C	3.18828000	-2.85758700	0.99548100
H	2.55705900	-4.76657700	0.03355400	H	3.43332200	-2.50053900	1.99749100
H	3.91661300	-4.25898500	1.04789900	H	3.49803800	-3.90495500	0.92808600
H	2.27505100	-4.27497500	1.71737500	H	3.76944100	-2.29129800	0.26522600
C	3.22348700	-1.65982600	1.45783300	C	1.39491300	-3.43737500	-0.64117900
H	4.30605600	-1.79210000	1.54827900	H	1.65038400	-4.49814000	-0.56830300
H	3.01582800	-0.62352800	1.18706700	H	0.34612900	-3.34430800	-0.91093800
H	2.76572200	-1.85116200	2.42754300	H	2.00042900	-2.99414700	-1.43217000
C	3.43886800	-2.36547800	-0.91925900	C	0.90888300	-3.52507500	1.80897200
H	3.47063700	-1.30448100	-1.16834800	H	1.02919600	-3.03879500	2.78035900
H	4.47027300	-2.70104600	-0.78208200	H	-0.15335500	-3.58080600	1.56668700
H	3.01584300	-2.92474300	-1.75650200	H	1.29930000	-4.54280000	1.89542500
I	0.00219600	-0.00093900	3.72501500	I	4.43958900	-0.16023400	-1.73714800
<b>[Li]<sup>-</sup>, 13I, E<sub>0</sub>=-8650.496006 au</b>				<b>[Li]<sup>-</sup>, 14I, E<sub>0</sub>=-8650.488657 au</b>			
N	-0.66130100	-0.07605200	-0.10644300	N	-1.51467100	-0.01907400	1.76916100
C	-1.08684100	-0.54159500	-1.45987500	C	-1.53712400	1.36457000	2.24097300
H	-0.96044800	0.30440900	-2.13547300	H	-0.50497000	1.66721900	2.39485000
H	-2.14225100	-0.83174400	-1.43882600	H	-2.06478300	1.45072000	3.21265700
C	-1.42451100	1.13785800	0.29571100	C	-0.66770900	-0.87587000	2.59976300
H	-1.13773300	1.34674400	1.31889900	H	-0.72765000	-1.87531600	2.18507600
H	-2.49705000	0.91357700	0.27008400	H	-1.06916300	-0.92768000	3.63304000
C	-0.91473500	-1.16933600	0.88078100	C	-2.86765400	-0.57081000	1.65522300
H	-0.45590900	-2.06190100	0.47104000	H	-3.46574900	0.15438600	1.11243900
H	-1.99524700	-1.33498100	0.96056800	H	-3.32457800	-0.70922900	2.65641800
C	-0.23334200	-1.67801000	-1.95485300	C	-2.18572200	2.28851000	1.24015100
C	-0.77624600	-2.95761000	-2.06499900	C	-3.48078300	2.76657900	1.45261000
C	1.10973500	-1.45863900	-2.33147100	C	-1.51564400	2.64517200	0.05927400
C	-0.01998300	-4.01952000	-2.55556600	C	-4.12425200	3.56077500	0.50809200
H	-1.81068000	-3.10457200	-1.77307500	H	-3.99116400	2.49874700	2.37229000
C	1.86855300	-2.53777000	-2.79330200	C	-2.18745300	3.38980400	-0.91325400

C	1.30406400	-3.80456100	-2.92149700	C	-3.47864700	3.85669700	-0.68875300
H	-0.46209100	-5.00515000	-2.64611400	H	-5.12900800	3.92383900	0.69436800
H	2.90865700	-2.40090200	-3.04648800	H	-1.69453300	3.58936400	-1.85297500
H	1.91206700	-4.62536900	-3.28614200	H	-3.98177500	4.43972000	-1.45239700
C	-0.32042700	-0.87251100	2.23310500	C	-2.87563700	-1.88792000	0.91765000
C	-1.11516400	-0.29917000	3.23259100	C	-2.89871800	-3.09300300	1.62525500
C	1.02986800	-1.13499000	2.51320600	C	-2.77009900	-1.92962500	-0.48075200
C	-0.57541700	0.06713700	4.46059700	C	-2.75182400	-4.31652500	0.98008600
H	-2.16734600	-0.13587400	3.02641100	H	-2.99969900	-3.06057500	2.70520300
C	1.58060900	-0.72070900	3.72996200	C	-2.55156500	-3.15399500	-1.11866300
C	0.78461200	-0.12215000	4.69931900	C	-2.54251400	-4.34144800	-0.39628800
H	-1.20770000	0.51661000	5.21801200	H	-2.75874100	-5.23801200	1.55138100
H	2.64095800	-0.85055400	3.89412700	H	-2.37007100	-3.16026600	-2.18363700
H	1.22473700	0.19644900	5.63805800	H	-2.36953200	-5.28217800	-0.90692100
C	-1.12735300	2.33519100	-0.56875200	C	0.78098400	-0.45589000	2.68332500
C	-2.01199000	2.66758100	-1.60075800	C	1.22320700	0.20258200	3.83578800
C	0.02415800	3.11707300	-0.38490600	C	1.70534400	-0.70329000	1.65290700
C	-1.74221900	3.72017100	-2.46822200	C	2.53643800	0.63877900	3.97097700
H	-2.91080600	2.07162600	-1.72013800	H	0.50880900	0.38656500	4.63211800
C	0.30645800	4.15586600	-1.27697600	C	3.02318200	-0.25173300	1.78749000
C	-0.56798900	4.45521500	-2.31464700	C	3.43678500	0.41624500	2.93359900
H	-2.43563400	3.95403500	-3.26826700	H	2.84828300	1.15793600	4.87085800
H	1.23396400	4.69981900	-1.16727400	H	3.72483200	-0.37959600	0.97099400
H	-0.33345400	5.26187300	-3.00118000	H	4.46025800	0.76684900	3.00300100
N	1.57274300	-0.11311800	-2.23151000	N	-0.14450100	2.24633800	-0.07693100
N	0.91416600	2.77176200	0.69411300	N	1.25615900	-1.36901900	0.45870200
N	1.80138900	-1.81954400	1.51318600	N	-2.90163900	-0.69777500	-1.20845700
O	1.83476100	0.21293600	-0.83911800	O	-0.02188800	1.47290400	-1.28895900
H	0.88142500	0.18618400	-0.41815600	H	0.57585200	0.73285400	-1.01777100
O	3.01021600	-1.07774200	1.26545500	O	-1.82159900	-0.60205900	-2.14851000
H	2.79036300	-0.66587100	0.40527400	H	-1.28616100	0.13186400	-1.78873200
O	2.26798900	2.76275400	0.18645500	O	1.57843100	-0.57517100	-0.68524200
H	2.33088000	1.84590100	-0.14098900	H	2.55618900	-0.51690600	-0.85158800
C	2.63679800	0.44665100	-3.09008400	C	0.86322600	3.36047300	-0.08313600
C	2.16177400	-3.23996800	1.79060900	C	-4.18897300	-0.53139500	-1.95593800
C	0.90913800	3.65036800	1.90064300	C	1.66794100	-2.79386100	0.24849200
C	2.77546400	-3.79424100	0.49995200	C	-4.18507800	0.89024700	-2.52425600
H	3.00530400	-4.85738200	0.61730600	H	-5.12619100	1.08960400	-3.04550800
H	2.07803500	-3.67317600	-0.32769500	H	-4.06609700	1.61225300	-1.71948000
H	3.69508700	-3.26190800	0.25560600	H	-3.36075000	1.01821800	-3.22555500
C	3.16326000	-3.39667400	2.95019300	C	-4.36669400	-1.53989800	-3.10640600
H	2.70835700	-3.14621700	3.91012900	H	-4.52855700	-2.55372300	-2.73665600
H	3.50836200	-4.43331000	3.00336100	H	-5.23608900	-1.26022200	-3.70837500
H	4.02798300	-2.75158400	2.78690200	H	-3.48504100	-1.53069800	-3.74886400
C	0.87414500	-4.01038000	2.10790300	C	-5.34543500	-0.67030400	-0.95804600
H	0.38052200	-3.62319700	3.00077600	H	-5.37540100	-1.66401300	-0.50760800
H	0.17154800	-3.96215900	1.27465900	H	-5.26226000	0.07250300	-0.16233800
H	1.12079700	-5.06067800	2.28370000	H	-6.29125200	-0.50490600	-1.48081200
C	1.82351000	2.97955000	2.93263000	C	1.14085900	-3.20382200	-1.13322300
H	1.77384600	3.51849500	3.88351300	H	1.19214800	-4.29207700	-1.23371600
H	1.50752500	1.94990200	3.09501700	H	0.10719300	-2.87994600	-1.24842100
H	2.85586700	2.97121600	2.58421100	H	1.73240700	-2.75080800	-1.92766900
C	-0.51884400	3.71292600	2.45529400	C	0.96685300	-3.62926000	1.32716500
H	-1.22645600	4.08740900	1.71341100	H	1.23679600	-3.29217000	2.33119400
H	-0.85167700	2.73294300	2.79785600	H	-0.11518700	-3.58551900	1.21078000
H	-0.53498000	4.39187700	3.31175600	H	1.27868000	-4.67263900	1.23096300
C	1.40928400	5.07663300	1.60353800	C	3.18459800	-3.04205500	0.32292800
H	1.51421400	5.63172900	2.54003800	H	3.38715500	-4.08628100	0.06545000
H	2.38260600	5.04193700	1.11208600	H	3.73988700	-2.41406900	-0.37659100
H	0.70923300	5.62075000	0.96644200	H	3.57049900	-2.86460900	1.32943500
C	4.06134000	0.08644400	-2.62547100	C	0.80664300	4.25337100	-1.33586800
H	4.25461500	-0.98633600	-2.66118500	H	-0.06107100	4.91585500	-1.33303600
H	4.79733700	0.58397600	-3.26331100	H	1.70238400	4.87853500	-1.37643300
H	4.21991400	0.42119800	-1.59983900	H	0.78663300	3.63039700	-2.23112500
C	2.46830300	1.97665800	-3.06637300	C	2.24685500	2.71144400	0.01011600
H	3.18345900	2.43806500	-3.75399300	H	3.01446100	3.48344200	0.10992500



H	1.45610800	2.24283000	-3.37446800	H	2.29808400	2.05675100	0.87804200
H	2.62950000	2.39304700	-2.07622300	H	2.49157000	2.12400900	-0.87368200
C	2.38653400	-0.00916800	-4.53765500	C	0.62269800	4.20094600	1.17847500
H	2.61176300	-1.06051300	-4.70600100	H	-0.35471400	4.68789600	1.16820300
H	1.34213800	0.16188600	-4.80762600	H	0.69707400	3.58115000	2.07469100
H	3.01524400	0.58479800	-5.20500200	H	1.38985200	4.97684800	1.23921400
I	-4.82058400	-0.97492000	-0.19119400	I	4.84621900	-0.00656000	-1.72590300
<b>[Li]<sup>-</sup>, 16l, E<sub>0</sub>=-8650.489020 au</b>				<b>[Li]<sup>-</sup>, 17l, E<sub>0</sub>=-8650.491259 au</b>			
N	-1.67236600	0.21038100	1.60171500	N	0.64820500	0.20111800	-0.24342000
C	-1.01342700	-0.76852800	2.48450300	C	1.36223100	0.20970200	1.06288400
H	-1.25534000	-1.75114200	2.09444400	H	1.00389200	1.08139600	1.59710000
H	-1.46008400	-0.70780800	3.49432500	H	2.43429300	0.34405600	0.88054600
C	-3.12429300	-0.04383800	1.59711300	C	1.01121400	1.44771900	-0.98019300
H	-3.58183400	0.71705400	0.96736000	H	0.50984100	1.40391900	-1.94638800
H	-3.52443100	0.05945100	2.62300600	H	2.09562400	1.48624300	-1.13115700
C	-1.38274200	1.59298500	2.02312000	C	1.02176300	-0.99793700	-1.03873200
H	-0.31120000	1.65398900	2.17106600	H	0.87313100	-1.85493700	-0.39158000
H	-1.87601100	1.80934800	2.98868500	H	2.08248400	-0.94881900	-1.31130300
C	0.48108900	-0.61295200	2.63457800	C	1.17272600	-1.03176400	1.89647100
C	0.96823100	-0.13574500	3.85743900	C	2.25012300	-1.92320700	1.98327800
C	1.40171500	-0.91853300	1.61532200	C	-0.01538100	-1.33765100	2.58170200
C	2.32541000	0.06366800	4.07912100	C	2.15445000	-3.10726900	2.70497300
H	0.25475400	0.10073600	4.64045700	H	3.16173400	-1.67632200	1.44740300
C	2.76679400	-0.70343900	1.84013200	C	-0.10877700	-2.53715200	3.29740700
C	3.22664900	-0.21629300	3.05656400	C	0.96363800	-3.41826800	3.35776200
H	2.67165500	0.44590300	5.03320300	H	2.99852100	-3.78662300	2.74354800
H	3.48094200	-0.88226900	1.04366700	H	-1.04840700	-2.78413800	3.77064400
H	4.28940500	-0.05111800	3.19252800	H	0.86686800	-4.34622900	3.91162300
C	-1.80958300	2.61166500	0.99485600	C	0.16393800	-1.12576200	-2.27070300
C	-3.07031000	3.21129400	1.07666800	C	0.65685200	-0.68736400	-3.50400500
C	-0.97297600	2.93944000	-0.08428900	C	-1.14710200	-1.62345700	-2.20670000
C	-3.52952400	4.07398000	0.08756800	C	-0.14359600	-0.68525800	-4.64113300
H	-3.70386900	2.98117400	1.92719200	H	1.67841300	-0.32626100	-3.55123900
C	-1.45703300	3.76904300	-1.10062600	C	-1.96238600	-1.58141100	-3.34117800
C	-2.72356700	4.33364000	-1.01850700	C	-1.46636800	-1.11357100	-4.55228600
H	-4.51382500	4.52179300	0.16854100	H	0.25608400	-0.33120400	-5.58481100
H	-0.83348500	3.94255900	-1.96546700	H	-2.99440900	-1.88962700	-3.25724900
H	-3.08090100	4.97500800	-1.81691100	H	-2.11156200	-1.08441500	-5.42378700
C	-3.51683700	-1.39554600	1.05338700	C	0.53709400	2.67501700	-0.24900000
C	-3.95761100	-2.40635500	1.90607600	C	1.45713800	3.49367600	0.40586400
C	-3.47270400	-1.63288400	-0.33633100	C	-0.83679300	2.99414100	-0.20092700
C	-4.36270300	-3.64319700	1.41180800	C	1.04135600	4.62035400	1.10985000
H	-3.98595700	-2.21463100	2.97368700	H	2.50811400	3.22922800	0.35676400
C	-3.87597600	-2.87916600	-0.82370000	C	-1.24562200	4.11320100	0.53113100
C	-4.32367900	-3.87430700	0.04101600	C	-0.31422600	4.92581400	1.17259100
H	-4.70166100	-4.41775000	2.09040700	H	1.77001800	5.24768400	1.61055100
H	-3.82334700	-3.08374300	-1.88176900	H	-2.29378900	4.35495100	0.61258600
H	-4.62562400	-4.83583600	-0.35973500	H	-0.65568900	5.79009100	1.73215300
N	0.91911500	-1.38673600	0.34370400	N	-1.14413300	-0.44900500	2.46904700
N	-2.97045300	-0.55455700	-1.12029500	N	-1.70318800	2.10932100	-0.91637700
N	0.35324600	2.39568000	-0.11491600	N	-1.61194200	-2.12899200	-0.93682900
O	1.49742500	-0.60985500	-0.70555300	O	-2.33420600	-1.25855100	2.34221500
H	2.47041500	-0.77236300	-0.80933700	H	-2.50355300	-1.26927400	1.38714600
O	0.58298400	1.88126800	-1.43449400	O	-2.90507600	-1.52291800	-0.63777700
H	0.83371400	0.95098500	-1.25155600	H	-2.65864800	-0.57303900	-0.53582100
O	-1.53421300	-0.63911900	-1.11165700	O	-1.89960000	0.91737700	-0.10626400
H	-1.27858700	-0.23970600	-0.25010100	H	-0.95979800	0.50542500	-0.07352000
C	1.03642200	-2.85833700	0.05325300	C	-1.40324400	0.49436800	3.60398900
C	1.46282900	3.35114300	0.22872400	C	-1.78220200	-3.61204300	-0.84846800
C	-3.40692700	-0.28526700	-2.50754400	C	-3.00620600	2.53483400	-1.46811800
C	2.75507600	2.53202600	0.28255900	C	-1.72551500	-0.24606400	4.91500600
H	3.58959300	3.17238400	0.58210400	H	-0.85692700	-0.79457400	5.28571500
H	2.66017000	1.72497400	1.00643100	H	-2.02377700	0.47490800	5.68154200
H	2.99778100	2.08919300	-0.68193000	H	-2.54708900	-0.94713400	4.76240200
C	1.61282300	4.48564300	-0.80009500	C	-0.17836800	1.39162300	3.81246800
H	0.77030400	5.18023700	-0.76818900	H	0.73039900	0.81048000	3.97889500

H	2.52380300	5.05207800	-0.58859200	H	-0.02735600	2.05865400	2.96348700
H	1.69572700	4.06545800	-1.80308800	H	-0.34678100	2.01197700	4.69660200
C	1.18339400	3.94267400	1.61642900	C	-2.59084000	1.37258200	3.18730300
H	0.24370300	4.49885800	1.64443100	H	-2.73546500	2.17220900	3.91990600
H	1.15472100	3.16021200	2.37709800	H	-2.39440700	1.80740100	2.20805500
H	1.99192100	4.63074000	1.87597200	H	-3.50483100	0.78222500	3.12519900
C	-2.94798600	1.15194000	-2.80211200	C	-4.12935700	2.66942900	-0.41876800
H	-3.22755500	1.43877800	-3.82051400	H	-3.99531600	3.52761100	0.24002400
H	-3.41309400	1.84249000	-2.09800500	H	-5.09270200	2.78664200	-0.92332600
H	-1.86774400	1.23696800	-2.69043900	H	-4.16923800	1.77212400	0.19877400
C	-4.93925800	-0.33379300	-2.55157900	C	-2.79326700	3.84588900	-2.23984400
H	-5.33329600	-1.34200400	-2.41648500	H	-2.56395000	4.68901000	-1.58979300
H	-5.35864400	0.30527100	-1.77036800	H	-1.97134100	3.73141800	-2.95022200
H	-5.28187300	0.03809000	-3.52038400	H	-3.70243600	4.08248800	-2.79791100
C	-2.78329600	-1.22606200	-3.55872200	C	-3.41832900	1.45776500	-2.48827600
H	-3.00736200	-0.85376400	-4.56234100	H	-4.30150300	1.78996900	-3.04173800
H	-1.70141200	-1.25146500	-3.43296900	H	-2.60343600	1.27627300	-3.18932500
H	-3.16296500	-2.24701700	-3.49569500	H	-3.66027600	0.51325500	-2.00478000
C	2.44591000	-3.42849500	0.28572600	C	-2.18062400	-3.95398300	0.59129600
H	2.72922300	-3.38095000	1.33992700	H	-2.20386600	-5.04081800	0.71159600
H	2.46099700	-4.47913600	-0.01981500	H	-1.46232000	-3.53822200	1.29448900
H	3.20212000	-2.90195100	-0.30032900	H	-3.16730100	-3.55883500	0.83224200
C	0.62229800	-3.07134300	-1.40871400	C	-2.84322300	-4.17202900	-1.81510900
H	0.51638100	-4.14454500	-1.59434700	H	-2.52097100	-4.10344400	-2.85505700
H	-0.32463300	-2.56797100	-1.59901900	H	-3.01948100	-5.22694600	-1.58770000
H	1.37273000	-2.67365700	-2.09059000	H	-3.78518200	-3.63371300	-1.69791200
C	0.03581300	-3.58793800	0.95915900	C	-0.41825300	-4.24772900	-1.14773900
H	0.24579200	-3.40950800	2.01669100	H	-0.06131100	-3.99253700	-2.14679200
H	-0.98662500	-3.28107200	0.73350500	H	0.32797000	-3.93197300	-0.41742900
H	0.11563300	-4.66399100	0.78429700	H	-0.51371100	-5.33477100	-1.08813200
I	4.89149800	-0.72405300	-1.47728900	I	4.87643100	0.28235300	-0.80492700
<b>[Li]<sup>-</sup>, 18l, E<sub>0</sub>=-8650.484122 au</b>				<b>[Li]<sup>-</sup>, 19l, E<sub>0</sub>=-8650.483859 au</b>			
N	-0.72097400	0.20297400	-2.09111300	O	1.16811600	1.15920000	0.53496500
C	-1.86771200	-0.63343100	-2.49018800	O	-3.18697400	-1.17057900	1.65714000
H	-1.56063900	-1.67288000	-2.39027600	O	3.26746200	-0.62738200	0.61444300
H	-2.12518000	-0.43836800	-3.54826100	N	1.16773100	2.56787400	0.30173000
C	0.48251600	-0.11158100	-2.87227700	N	-3.02526200	-0.31142800	0.52038700
H	1.23109400	0.61021400	-2.58017900	N	2.88659200	-1.44660400	-0.51616800
H	0.28448300	0.04275200	-3.95021000	N	0.07123200	-0.30587900	-2.36036400
C	-1.08847000	1.62065200	-2.24919600	C	1.14130500	0.71717100	-2.24981500
H	-1.95603300	1.78674000	-1.62529600	C	0.54947100	2.10326000	-2.12434800
H	-1.40792700	1.79962300	-3.29325400	C	-0.12435400	2.59153100	-3.25132500
C	-3.08810600	-0.40873200	-1.63321000	C	-0.80669300	3.79964100	-3.24766100
C	-4.18496300	0.30095000	-2.12079400	C	-0.85429200	4.54432100	-2.07154700
C	-3.12204900	-0.92484200	-0.32136400	C	-0.20620000	4.07465800	-0.93854700
C	-5.31475600	0.51218300	-1.33533500	C	0.53041900	2.87995200	-0.94553700
H	-4.14768700	0.69270500	-3.13220400	C	2.54998300	3.11246000	0.51752800
C	-4.25519600	-0.69471800	0.46518200	C	3.55876400	2.58985800	-0.51990500
C	-5.34430100	0.01149600	-0.03760200	C	2.49295200	4.64475200	0.43920900
H	-6.15855100	1.06690500	-1.73030300	C	2.97544600	2.71574500	1.93786000
H	-4.27984100	-1.05553700	1.48166700	C	-1.01025900	-0.11204000	-1.39211600
H	-6.20989600	0.18127800	0.59366000	C	-2.26713900	-0.88304200	-1.70410500
C	0.00390700	2.61201000	-1.92969900	C	-2.50370700	-1.46800900	-2.94899700
C	0.65374100	3.23319800	-3.00353700	C	-3.58518200	-2.32301000	-3.14356900
C	0.42914100	2.91130900	-0.62140700	C	-4.43749000	-2.61466100	-2.07965900
C	1.72634500	4.09625900	-2.82106400	C	-4.25268200	-1.98261700	-0.85312200
H	0.32024500	2.99765800	-4.00895800	C	-3.20709700	-1.07403600	-0.67722700
C	1.52911100	3.76476700	-0.44548300	C	-3.91882100	0.88291400	0.67900900
C	2.17330300	4.34868600	-1.52690100	C	-5.39447500	0.48536200	0.86615200
H	2.21901000	4.54529100	-3.67615500	C	-3.42718200	1.65073400	1.91055500
H	1.88410000	3.93294900	0.56002300	C	-3.77540600	1.78222700	-0.55565500
H	3.02424500	4.99944200	-1.35679000	C	0.62863400	-1.67723900	-2.40350400
C	0.99780100	-1.51634400	-2.67756600	C	0.70446500	-2.41198700	-1.07170300
C	0.63949800	-2.48676600	-3.62088500	C	-0.38074800	-3.21624700	-0.70476100
C	1.78761700	-1.90261000	-1.57860400	C	-0.48739700	-3.76528000	0.56725100
C	0.99789800	-3.82102700	-3.48076000	C	0.50853200	-3.51805000	1.50510600

H	0.04186900	-2.17760600	-4.47250300	C	1.62345500	-2.77354500	1.14535600
C	2.12427400	-3.25531800	-1.43008900	C	1.74375100	-2.24356900	-0.14138100
C	1.73441200	-4.20502700	-2.36341300	C	4.12098600	-2.18684100	-0.91131400
H	0.69121800	-4.55131600	-4.22130900	C	3.78109600	-3.14386400	-2.05950300
H	2.66985800	-3.54747500	-0.54584700	C	4.73400000	-2.98697000	0.25314500
H	2.00724700	-5.24455600	-2.21639100	C	5.12374500	-1.13639500	-1.40914300
N	-1.95439800	-1.62917400	0.08937300	H	1.83016800	0.49864500	-1.44415300
N	2.20031000	-0.94145900	-0.59197200	H	1.71360900	0.67228900	-3.18485800
N	-0.19854900	2.29844500	0.51029000	H	-0.12532000	1.97013800	-4.14022400
O	-1.01071400	-0.66712200	0.60243100	H	-1.31848300	4.14202000	-4.14015900
H	-0.60091600	-0.29854500	-0.20961900	H	-1.41630300	5.47062300	-2.02622800
O	0.83298500	2.14174000	1.49648800	H	-0.27828500	4.61247100	-0.00314200
H	0.71693900	1.25113900	1.89304800	H	3.25177300	2.86426300	-1.53239900
O	2.26902900	-1.65085000	0.65527100	H	3.66147100	1.50788200	-0.46135700
H	1.76747700	-1.11995400	1.30947600	H	4.54325900	3.02974400	-0.33395000
C	-2.00379700	-2.79010800	1.01052800	H	2.22059600	4.99503700	-0.55713300
C	-1.31609200	3.06949400	1.17983100	H	3.48104500	5.04456500	0.68064300
C	3.57020900	-0.32373900	-0.79317500	H	1.77532000	5.04288800	1.15943700
C	-1.83080700	2.17760600	2.31733400	H	2.20834900	3.01013700	2.65657300
H	-2.72954900	2.62306800	2.75504300	H	3.91369700	3.21764200	2.19054700
H	-2.06626800	1.18674100	1.92780100	H	3.12747900	1.64280700	2.03736600
H	-1.08310000	2.05726200	3.10076900	H	-1.24719900	0.94739500	-1.37930600
C	-0.81661200	4.41368600	1.73451500	H	-0.71864600	-0.35282000	-0.36621400
H	-0.52832500	5.09634400	0.93043800	H	-1.80281000	-1.26477500	-3.74926200
H	-1.61138100	4.88947800	2.31597100	H	-3.74455500	-2.78389800	-4.11288200
O	0.04070500	4.25108200	2.38718300	H	-5.25473200	-3.31644700	-2.20928700
C	-2.46547100	3.31852000	0.19831000	H	-4.90746400	-2.19064800	-0.01800500
H	-2.13716200	3.85142800	-0.69703000	H	-5.48026700	-0.24201700	1.67473100
H	-2.95259300	2.38536400	-0.08655300	H	-5.81266300	0.05500600	-0.04659500
H	-3.21448200	3.93931000	0.69679900	H	-5.98728800	1.36708600	1.12685700
C	3.78083700	0.65251700	0.37016300	H	-4.00034100	2.57660500	2.02268000
H	4.70467800	1.21729500	0.21074200	H	-2.36819200	1.89037500	1.81218800
H	2.94513800	1.34908500	0.43765800	H	-3.54041900	1.05494800	2.81524000
H	3.85093900	0.12607100	1.32118900	H	-2.75614500	2.15698000	-0.65471800
C	3.61857100	0.46156000	-2.10781600	H	-4.43807500	2.64443100	-0.44157000
H	3.36807500	-0.16013700	-2.97036600	H	-4.05046200	1.26327500	-1.47566800
H	2.95937700	1.32968300	-2.07774600	H	1.60829900	-1.59945000	-2.86844200
H	4.63766700	0.83052100	-2.25062100	H	0.00432400	-2.28320500	-3.06627800
C	4.67715400	-1.39139100	-0.79508400	H	-1.18520200	-3.36120000	-1.41522800
H	5.65565200	-0.90338800	-0.81733000	H	-1.37082400	-4.33149900	0.83734200
H	4.61316900	-1.99616400	0.10929200	H	0.40691400	-3.87070700	2.52396400
H	4.60371500	-2.04571600	-1.66756200	H	2.37808900	-2.53202900	1.87869000
C	-2.16273700	-2.41380000	2.49500400	H	3.43032800	-2.60028100	-2.93821800
H	-3.14214200	-1.98767300	2.72206400	H	3.01557600	-3.86433700	-1.76838100
H	-2.04561300	-3.31043000	3.11050100	H	4.68263100	-3.69488500	-2.33980100
H	-1.39035200	-1.70349100	2.79119200	H	4.07169700	-3.79701600	0.56377600
C	-0.66173600	-3.51656500	0.82936900	H	4.91159600	-2.33524600	1.10837600
H	-0.63100400	-4.40943700	1.46085500	H	5.68659700	-3.42511200	-0.05930100
H	-0.53233500	-3.81232400	-0.21393100	H	6.01982200	-1.62557000	-1.80231400
H	0.16689900	-2.86929700	1.10596000	H	5.41289900	-0.46876000	-0.59846100
C	-3.13032000	-3.72128000	0.54025200	H	4.67113100	-0.53715000	-2.20265000
H	-4.12390400	-3.30540400	0.71409700	H	0.64086500	1.00893000	1.36111300
H	-3.02910800	-3.93238000	-0.52796000	H	-2.34313700	-1.03651200	2.13756800
H	-3.05872500	-4.66570200	1.08505100	H	2.55452800	0.04404900	0.63630500
I	1.25782100	-0.42005600	3.74502600	I	-0.21761200	-0.07504600	3.38756500
<b>[Li]<sup>-</sup>, 20I, E<sub>0</sub>=<b>-8650.482783</b> au</b>				<b>[Li]<sup>-</sup>, 21I, E<sub>0</sub>=<b>-8650.482959</b> au</b>			
N	-0.44582600	0.73908800	-0.87938400	N	-0.38776600	1.22520000	1.76379200
C	-1.11648900	1.79058200	-1.62092500	C	-1.07043000	2.50676800	1.51841900
H	-1.01878600	1.54539800	-2.68287600	H	-0.36772500	3.14389700	0.98229500
H	-0.60924100	2.76355600	-1.49202000	H	-1.32436900	2.99840000	2.47421400
C	-0.55901800	0.82528300	0.58415200	C	0.93202200	1.38801800	2.39984400
H	-0.08534500	-0.05723000	0.99689400	H	1.31559800	0.38677400	2.54496000
H	-1.61433700	0.74707600	0.83917500	H	0.81303100	1.85447200	3.39507400
C	0.89149700	0.50021900	-1.39669400	C	-1.23993100	0.31456100	2.56446600
H	1.61891300	1.26372000	-1.08054200	H	-2.25217300	0.43703600	2.19841300
H	0.81639000	0.60737600	-2.48226100	H	-1.21445200	0.61512200	3.62613800

C	-2.58385600	2.03078100	-1.30397600	C	-2.31726000	2.39061500	0.67593500
C	-2.99114000	3.37295600	-1.34680500	C	-3.56329800	2.65940700	1.23831200
C	-3.54485100	1.05778800	-0.95735800	C	-2.22797900	2.09709600	-0.70504400
C	-4.27818700	3.77769800	-1.02709700	C	-4.72337800	2.66975700	0.46738100
H	-2.24670400	4.12125700	-1.59840000	H	-3.61781800	2.88783400	2.29802500
C	-4.83099200	1.48355500	-0.58148000	C	-3.40339100	2.07883800	-1.46197200
C	-5.20065200	2.81804500	-0.61612600	C	-4.63551500	2.37985000	-0.88863400
H	-4.54502900	4.82820500	-1.06144500	H	-5.68146600	2.89150400	0.92364300
H	-5.52385700	0.72988400	-0.23924600	H	-3.36080200	1.81556900	-2.50674700
H	-6.20434300	3.10703700	-0.32293600	H	-5.52936000	2.35721700	-1.50233100
C	1.42353600	-0.89025200	-1.10486100	C	-0.81469100	-1.12483400	2.40952400
C	0.51274200	-1.89566300	-0.77295200	C	0.12659500	-1.68848000	3.27527700
C	2.78952500	-1.22435700	-1.16169200	C	-1.27524900	-1.88798800	1.32246600
C	0.92151600	-3.19420400	-0.50022700	C	0.67608800	-2.94158500	3.02241500
H	-0.52777000	-1.62484400	-0.66728000	H	0.44911800	-1.12172000	4.14306600
C	3.19768000	-2.53626600	-0.90693200	C	-0.65386000	-3.10134400	1.01626300
C	2.27175700	-3.51931500	-0.58069500	C	0.31522100	-3.62471800	1.86323600
H	0.18412800	-3.91750000	-0.17552100	H	1.41913500	-3.35522900	3.69513700
H	4.25548700	-2.75570200	-0.89815700	H	-0.90336100	-3.59371000	0.08789500
H	2.61053700	-4.52468000	-0.35560800	H	0.79739000	-4.56015000	1.60476000
C	0.02104100	2.09849300	1.17765500	C	1.91185200	2.20057800	1.58788600
C	-0.79328300	3.22810600	1.31831800	C	1.97584700	3.58441100	1.78996000
C	1.37535700	2.21424200	1.53204000	C	2.73460400	1.62357400	0.60467400
C	-0.27760600	4.45376900	1.72483800	C	2.77511800	4.40413100	1.00351400
H	-1.84709400	3.13926400	1.08579800	H	1.36163600	4.02200500	2.57044300
C	1.90346400	3.45394500	1.90848400	C	3.50984400	2.45868300	-0.21037000
C	1.08395400	4.57239700	1.99739600	C	3.52860600	3.83298600	-0.01963400
H	-0.93301000	5.31328500	1.81496800	H	2.79406100	5.47491900	1.17320000
H	2.96310900	3.52691300	2.11061100	H	4.07301900	2.00493200	-1.01218000
H	1.50383800	5.52851800	2.29186700	H	4.13611600	4.45699900	-0.66634200
N	-3.23437000	-0.34196600	-0.91633000	N	-0.92108400	1.88917000	-1.22456800
N	2.18648100	1.03174800	1.47516500	N	2.75267400	0.20054200	0.42798200
N	3.78407400	-0.18398900	-1.36936400	N	-2.35385800	-1.35852300	0.53265000
O	-4.03490300	-0.93492400	0.11222200	O	-0.45061600	0.56923200	-0.88874200
H	-3.37711500	-1.35745900	0.71573200	H	-0.19804800	0.65266900	0.06422700
O	4.93845000	-0.48347800	-0.53994700	O	-2.10724300	-1.65050700	-0.84998300
H	4.73677500	0.02123500	0.26542000	H	-1.48170700	-0.94082300	-1.10085800
O	3.46695700	1.39209200	0.89273100	O	2.92491700	-0.04082600	-0.97446600
H	3.32884400	1.16105600	-0.04905400	H	2.26111400	-0.73104200	-1.21860000
C	-3.49137200	-1.11150600	-2.18361600	C	-0.54999200	2.14937800	-2.63844500
C	4.32824600	-0.00897400	-2.75768500	C	-3.70743500	-1.91995600	0.83957900
C	2.43981300	0.31665800	2.76991300	C	3.87753500	-0.52582900	1.13502100
C	3.44341100	1.07502900	3.65699200	C	-4.71137700	-1.12975000	-0.00651500
H	3.03629500	2.03600800	3.97899800	H	-5.73023800	-1.46999100	0.20358200
H	3.65576400	0.48391600	4.55164800	H	-4.63725400	-0.06768800	0.22346400
H	4.38031300	1.25100100	3.12683300	H	-4.50097100	-1.26489600	-1.06616900
C	2.97227500	-1.07747200	2.41975400	C	-3.80709000	-3.42078400	0.50920700
H	2.25787200	-1.60518400	1.78843500	H	-3.17213100	-4.01553600	1.16890400
H	3.92576200	-1.02847700	1.89367400	H	-4.83996500	-3.75943500	0.63457000
H	3.11990900	-1.65786700	3.33418600	H	-3.50062400	-3.59884700	-0.52137800
C	1.11403000	0.15794700	3.52654500	C	-4.02270200	-1.70060900	2.32425100
H	0.67000600	1.12339300	3.77419400	H	-3.30365500	-2.20488800	2.97173600
H	0.38552600	-0.44062300	2.97841100	H	-4.03443500	-0.63750200	2.57247000
H	1.31736900	-0.36924600	4.46165000	H	-5.01513800	-2.10651600	2.53748300
C	5.23089000	1.23077500	-2.72898200	C	3.65192300	-2.01944900	0.87873000
H	6.08278900	1.07219100	-2.06905000	H	4.37972900	-2.60675500	1.44800100
H	5.59944400	1.44968800	-3.73488000	H	2.64607100	-2.30372300	1.18597600
H	4.66914600	2.09638500	-2.36890200	H	3.75154600	-2.26117300	-0.17852700
C	3.16677000	0.23594500	-3.72342400	C	3.81313400	-0.26039900	2.64379000
H	2.46252500	-0.59729700	-3.72316600	H	3.86354700	0.80515800	2.87804100
H	2.63279100	1.15229000	-3.47145500	H	2.90835400	-0.68299500	3.08130000
H	3.56715000	0.34278600	-4.73447600	H	4.66871500	-0.74807700	3.11829400
C	5.12603600	-1.23909200	-3.22138200	C	5.25718200	-0.10191900	0.60299700
H	5.56177800	-1.04371200	-4.20509900	H	6.02942200	-0.74128500	1.04007900
H	5.93201600	-1.46033200	-2.52179700	H	5.28613200	-0.21367300	-0.48055300
H	4.48072300	-2.11550900	-3.30226600	H	5.48864400	0.93430000	0.86227700

C	-3.10934100	-2.57255500	-1.91849200	C	-0.96440600	1.01692600	-3.59679800
H	-3.24896000	-3.15717800	-2.83293900	H	-2.04247100	0.84605300	-3.61023200
H	-2.06794600	-2.65084900	-1.60991200	H	-0.65249800	1.26927200	-4.61448900
H	-3.72350000	-2.99790300	-1.12729500	H	-0.47353600	0.08329500	-3.31631000
C	-4.96864200	-1.03536600	-2.60729900	C	0.98248200	2.26670100	-2.65010800
H	-5.13955400	-1.67311700	-3.47945500	H	1.33187800	2.44803000	-3.67096600
H	-5.60694300	-1.38301200	-1.79388900	H	1.29986200	3.09552000	-2.01369900
H	-5.25715800	-0.01464700	-2.86918500	H	1.44551100	1.35480200	-2.28115000
C	-2.59641100	-0.55716300	-3.29424800	C	-1.12955800	3.50778700	-3.06213700
H	-2.85197700	0.47527300	-3.54140000	H	-2.20642800	3.49033800	-3.22725400
H	-1.55051300	-0.60755700	-2.99144400	H	-0.91213700	4.26410900	-2.30313400
H	-2.73019000	-1.16059900	-4.19594000	H	-0.65098400	3.81368100	-3.99533100
I	-1.87306700	-2.62607600	2.22565900	I	1.22669500	-2.65340900	-2.41388300
<b>[L(HCI)], 23Cl, E<sub>0</sub>=-2191.695342 au</b>				<b>[L(HCI)], 24Cl, E<sub>0</sub>=-2191.689689 au</b>			
N	-0.00039400	0.00045800	1.17382800	N	-0.11608300	0.04157800	-1.22459300
C	1.44105700	-0.07448400	1.64223800	C	0.99154900	-0.89881200	-1.69668700
H	1.80967600	-1.01031800	1.24851800	H	1.90853800	-0.33418600	-1.58232000
H	1.40032000	-0.12501700	2.73267600	H	0.79640500	-1.08047900	-2.75532600
C	-0.78557100	-1.21058800	1.64242800	C	0.17052200	1.44180900	-1.70286300
H	-1.78061800	-1.06160100	1.24963100	H	-0.66073000	2.04953100	-1.37298900
H	-0.80804300	-1.15054000	2.73291400	H	0.15126900	1.40065800	-2.79346600
C	-0.65625200	1.28564800	1.64362200	C	-1.48311800	-0.46328900	-1.68718100
H	-0.03028800	2.07315100	1.25044100	H	-1.65321900	-1.35421400	-1.09418700
H	-0.59177500	1.27472500	2.73402500	H	-1.36191200	-0.72059100	-2.74083100
C	2.31246000	1.06051800	1.18177800	C	1.08849000	-2.16381000	-0.89781100
C	2.36394900	2.25774000	1.90593200	C	0.19470700	-3.21909200	-1.09974700
C	3.08573900	0.93347600	0.01526900	C	2.05188400	-2.26402500	0.11863800
C	3.09387600	3.34515700	1.44573000	C	0.19073000	-4.31950100	-0.25431000
H	1.81286900	2.33955800	2.83651000	H	-0.51706900	-3.16981200	-1.91596700
C	3.77923400	2.04808200	-0.46913600	C	2.01311800	-3.35056500	0.99235200
C	3.77956300	3.24367100	0.23545200	C	1.08388500	-4.36525200	0.81390200
H	3.11303400	4.26758000	2.01320700	H	-0.51940900	-5.12246100	-0.41075200
H	4.29525300	1.95854500	-1.41385100	H	2.69245100	-3.36439500	1.83172800
H	4.32631300	4.09564500	-0.15178800	H	1.05799700	-5.19745900	1.50740300
C	-2.07515100	1.47288900	1.18406200	C	-2.61795000	0.50815800	-1.49388200
C	-3.13732100	0.92100300	1.91038900	C	-2.81792800	1.56662800	-2.39135300
C	-2.35232500	2.20374700	0.01626200	C	-3.49353900	0.37264800	-0.40269100
C	-4.44445000	1.00963200	1.45143100	C	-3.77729600	2.54055200	-2.15297600
H	-2.93193800	0.40419600	2.84158200	H	-2.19901500	1.63693100	-3.27889800
C	-3.66488400	2.24742000	-0.46667100	C	-4.42070200	1.38803700	-0.13573500
C	-4.70020800	1.65225500	0.24028800	C	-4.55514300	2.46765500	-0.99624300
H	-5.25262200	0.56668000	2.02056400	H	-3.90890400	3.35698600	-2.85268800
H	-3.84595500	2.73732700	-1.41218000	H	-5.02352500	1.30937100	0.75778800
H	-5.71181400	1.69996700	-0.14587900	H	-5.28435800	3.24062300	-0.78246400
C	-0.23878700	-2.53246800	1.18081300	C	1.47838100	2.01926100	-1.23975600
C	0.77177200	-3.17686500	1.90458700	C	2.45530300	2.35065700	-2.18233500
C	-0.73525000	-3.13691600	0.01338000	C	1.72154200	2.26678600	0.11863700
C	1.34820700	-4.35241700	1.44318800	C	3.66854500	2.90350800	-1.78930900
H	1.11814300	-2.74157800	2.83567500	H	2.26216000	2.16551100	-3.23375800
C	-0.11698000	-4.29441400	-0.47223400	C	2.96429400	2.76726600	0.51311400
C	0.91771600	-4.89381200	0.23207100	C	3.92636000	3.09501200	-0.43417800
H	2.13712600	-4.83120100	2.01031500	H	4.41628700	3.15669600	-2.53106800
H	-0.45217000	-4.69509900	-1.41767500	H	3.16927200	2.88260100	1.56736500
H	1.38197100	-5.79299100	-0.15612300	H	4.88300200	3.49012700	-0.11346100
N	3.09936100	-0.32526000	-0.66387300	N	3.02500100	-1.21157400	0.24004000
N	-1.83140300	-2.51761400	-0.66556000	N	0.68531700	1.94078200	1.05236100
N	-1.26898500	2.84151600	-0.66593100	N	-3.39086500	-0.79310800	0.40295100
O	3.05463200	-0.07768800	-2.07341800	O	3.19888900	-0.89422400	1.63022100
H	2.09171400	-0.12232900	-2.24923700	H	2.65312800	-0.09547600	1.74358200
O	-1.46337500	2.67535200	-2.07472500	O	-3.45363900	-0.41095600	1.77656300
H	-0.94254000	1.86399600	-2.24963200	H	-2.52238400	-0.58360500	2.05231100
O	-1.59380900	-2.60136300	-2.07510000	O	1.30311200	1.23741300	2.14679800
H	-1.14924700	-1.74575200	-2.24964400	H	0.69973200	0.44641600	2.23146800
C	4.27096000	-1.23067500	-0.41542500	C	4.38694100	-1.52598100	-0.31464600
C	-1.06779500	4.30925800	-0.42197900	C	-4.36804300	-1.89973000	0.15933200
C	-3.20184100	-3.07907200	-0.41871800	C	-0.10531900	3.09725400	1.61725400

H	-0.00051000	0.00098900	0.11374500	Cl	-0.51499300	-1.03598800	1.81649700
C	5.57320300	-0.65534400	-0.99785100	C	-3.87016100	-3.09684400	0.97869200
H	5.87847300	0.25146800	-0.47052000	H	-4.49356700	-3.97304800	0.78097100
H	6.37804600	-1.38798500	-0.89813400	H	-2.83313500	-3.32380600	0.72320900
H	5.44494500	-0.42278300	-2.05463000	H	-3.90942100	-2.87274400	2.04396000
C	4.44545700	-1.45113600	1.09224100	C	-5.79418600	-1.51451500	0.58598000
H	4.60373000	-0.51372100	1.62893300	H	-6.20201800	-0.72576400	-0.05081400
H	3.58996500	-1.97257700	1.52492400	H	-6.45478400	-2.38198200	0.50925300
H	5.32469800	-2.07871600	1.25246600	H	-5.79350300	-1.17002500	1.62032600
C	3.92721300	-2.56548100	-1.08723700	C	-4.35641600	-2.26130300	-1.33099500
H	4.71915800	-3.29575800	-0.90013300	H	-4.66081100	-1.42214600	-1.95948500
H	2.98729100	-2.95470600	-0.69152200	H	-3.36938000	-2.60228400	-1.65071400
H	3.81796100	-2.43209000	-2.16246200	H	-5.05961200	-3.07925700	-1.50119700
C	-3.35509900	-4.49379800	-1.00279900	C	-1.19827200	2.49952500	2.51029700
H	-2.72392400	-5.21266800	-0.47515900	H	-1.85379000	3.29953600	2.86388700
H	-4.39246600	-4.82364100	-0.90505200	H	-1.79715400	1.77265700	1.96208000
H	-3.08796500	-4.49822900	-2.05918200	H	-0.76844900	1.99888800	3.37712600
C	-3.48124500	-3.12137000	1.08867900	C	-0.77283000	3.85216600	0.46149600
H	-2.74920100	-3.72790900	1.62539100	H	-0.04816600	4.20251200	-0.27711100
H	-3.50523700	-2.12018000	1.52231400	H	-1.52908400	3.23683000	-0.02927900
H	-4.46460400	-3.56895800	1.24761600	H	-1.28276900	4.72960200	0.86459600
C	-4.18503200	-2.11278000	-1.09018600	C	0.77307100	4.05762700	2.43289400
H	-5.21367600	-2.43356200	-0.90450600	H	0.13986800	4.78894000	2.94091700
H	-4.05245600	-1.10476800	-0.69286700	H	1.33173300	3.50491700	3.18888000
H	-4.01384800	-2.08334800	-2.16520400	H	1.47303200	4.60613300	1.79912300
C	0.26023300	4.67422000	-1.09604200	C	5.09276600	-2.65102300	0.46063500
H	0.49942200	5.72509300	-0.91180800	H	4.58746400	-3.60908700	0.32745000
H	1.06616700	4.05383300	-0.69962600	H	6.11798900	-2.75922300	0.09754300
H	0.19790500	4.51036100	-2.17079900	H	5.12673400	-2.41393100	1.52421200
C	-2.21611900	5.14963400	-1.00603800	C	5.20843800	-0.23691600	-0.22627600
H	-3.15398700	4.96351400	-0.47751100	H	6.20213200	-0.39639700	-0.65304900
H	-1.98227000	6.21286400	-0.90944300	H	4.71341900	0.56245600	-0.77647400
H	-2.35448500	4.91955900	-2.06207900	H	5.31872300	0.07603600	0.81118300
C	-0.96246000	4.57521200	1.08475300	C	4.24063900	-1.92885000	-1.78724500
H	-1.85346400	4.24663300	1.62325300	H	3.63544300	-2.82859500	-1.90679100
H	-0.08342600	4.09529000	1.51825800	H	3.79745700	-1.12311400	-2.37708300
H	-0.85693200	5.65080800	1.24142100	H	5.23213100	-2.13281400	-2.19742900
Cl	0.00343700	-0.00091200	-1.93368800	H	-0.13736900	0.02286000	-0.17522500
<b>[L(HCl)], 25Cl, E<sub>0</sub>=-2191.687647</b>				<b>[L(HCl)], 26Cl, E<sub>0</sub>=-2191.687392 au</b>			
N	-0.24084600	0.18862500	1.54630500	O	-3.06991100	-0.80184000	-0.92883800
C	1.14712600	0.71432700	1.88054400	H	-2.61632900	0.06681700	-0.86256600
H	1.81896700	-0.06061500	1.53999200	O	-2.48320200	2.04218500	-2.46879800
H	1.18299500	0.77438900	2.97028400	H	-2.61268200	1.12205100	-2.72769700
C	-0.43974600	-1.15668600	2.22822600	O	4.11429400	-0.66269700	1.48383900
H	-1.44862400	-1.46957000	1.97306400	H	3.51915500	-0.35403000	2.21036300
H	-0.35862700	-0.96546600	3.29972400	N	-2.08601500	-1.76481500	-0.47505600
C	-1.32393200	1.16257300	1.93743100	N	-2.31236800	1.95197000	-1.03383200
H	-1.03752800	2.10846200	1.50041700	N	3.50136100	-0.07660800	0.32812600
H	-1.27431400	1.24990700	3.02478200	N	0.57909300	-0.17050200	0.56949700
C	1.49637400	2.02892500	1.24748000	H	1.43694800	0.14015200	1.07978400
C	1.11284600	3.23179200	1.85435500	C	0.31897200	-1.58720500	1.10661800
C	2.22303500	2.06780400	0.04515400	H	0.47599600	-2.25883000	0.27276900
C	1.35390300	4.45440900	1.24289000	H	1.09643700	-1.75004000	1.84841900
H	0.61051100	3.20488600	2.81549500	C	-1.03208200	-1.77605100	1.73423000
C	2.41691600	3.30083100	-0.59043800	C	-1.12194300	-1.79810300	3.12860500
C	1.98080500	4.47956000	-0.00249500	H	-0.21372200	-1.68285300	3.70863100
H	1.04388400	5.37464600	1.72285500	C	-2.35676300	-1.89271900	3.75985700
H	2.90467500	3.30693600	-1.55384500	H	-2.41138400	-1.89657000	4.84167500
H	2.14758900	5.42391900	-0.50755200	C	-3.51945300	-1.94101300	2.99490900
C	-2.70414900	0.76077000	1.50224600	H	-4.48883900	-1.98394400	3.47796700
C	-3.60288900	0.24099700	2.43828400	C	-3.44346700	-1.92081700	1.60646400
C	-3.10780800	0.91043000	0.16585400	H	-4.34456800	-1.91040400	1.01137500
C	-4.88036200	-0.15414800	2.06068500	C	-2.20384500	-1.86586600	0.96553400
H	-3.29000200	0.13824800	3.47214300	C	-2.33105300	-3.02387600	-1.25458800
C	-4.38423800	0.48671300	-0.21194100	C	-2.16259600	-2.67650400	-2.73926600
C	-5.26424300	-0.03716100	0.72632300	H	-1.22850600	-2.13900000	-2.90662100

H	-5.56430900	-0.56056300	2.79578000	H	-2.98399400	-2.05178800	-3.08787200
H	-4.65932900	0.54022800	-1.25491900	H	-2.14478600	-3.59194900	-3.33486300
H	-6.25082400	-0.35975100	0.41466700	C	-1.27090000	-4.04757500	-0.83319100
C	0.55204200	-2.18374200	1.77401300	H	-0.26460900	-3.71038600	-1.08397600
C	1.65714900	-2.52066200	2.55660000	H	-1.45104500	-4.98581900	-1.36218800
C	0.35873600	-2.80607900	0.52758900	H	-1.31809700	-4.25478200	0.23745500
C	2.57649500	-3.46319000	2.10879500	C	-3.73432900	-3.61439200	-1.03501500
H	1.79541200	-2.04484400	3.52176000	H	-3.89035400	-4.44238100	-1.73079900
C	1.30240600	-3.72846800	0.07236200	H	-4.50329800	-2.86384300	-1.22320300
C	2.39852700	-4.05850500	0.86257200	H	-3.85501800	-4.00299400	-0.02305400
H	3.43224200	-3.72086400	2.72095500	C	-0.49307600	0.82691100	0.96414500
H	1.20279100	-4.15357200	-0.91380500	H	-0.43465400	0.88203600	2.04951900
H	3.12846500	-4.76718100	0.49027600	H	-1.44444200	0.41442600	0.67468600
N	2.73475200	0.85180200	-0.49955500	C	-0.26168400	2.16301900	0.32587200
N	-0.80359500	-2.39456200	-0.18950600	C	0.84515600	2.91652600	0.73274500
N	-2.14621400	1.40265300	-0.78263600	H	1.43352800	2.55022300	1.56763200
O	2.65307500	0.96771200	-1.92213200	C	1.19144100	4.08481300	0.06864100
H	2.28527400	0.09794100	-2.21578600	H	2.05755500	4.65151000	0.38794200
O	-2.24652400	0.58476700	-1.96168000	C	0.43647000	4.50240200	-1.02624500
H	-1.58361300	-0.10860700	-1.77426900	H	0.71720400	5.39334500	-1.57565200
O	-0.48785700	-1.19403000	-0.91852600	C	-0.69589300	3.79261800	-1.40504900
H	0.27164800	-1.40340300	-1.57053700	H	-1.29006300	4.11766300	-2.24611800
C	4.17831800	0.53761600	-0.14150600	C	-1.07742700	2.64053900	-0.71062000
C	-2.28633300	2.82736800	-1.24442400	C	-3.55039400	2.56080800	-0.37764100
C	-1.67569600	-3.34308900	-0.93715400	C	-3.70008900	4.05498300	-0.69086100
H	-0.29589700	0.01104100	0.51893900	H	-2.90099100	4.64865200	-0.24614500
C	4.35708700	0.50792800	1.38181200	H	-4.64903200	4.41057700	-0.28332000
H	3.79239300	-0.30673700	1.83926800	C	-4.78080600	1.80956500	-0.90283200
H	5.41217500	0.32980400	1.60014100	H	-4.70952200	0.73870300	-0.71240400
H	4.07874600	1.45266800	1.85320700	H	-4.91136400	1.97363200	-1.97217500
C	4.46703000	-0.85820200	-0.70226300	H	-5.66858100	2.18784200	-0.39168800
H	3.74422700	-1.58040800	-0.31967100	C	-3.42944100	2.34276900	1.13469600
H	4.39790500	-0.87014900	-1.78837400	H	-2.55732700	2.84704400	1.55282800
H	5.47363000	-1.17065100	-0.41056900	H	-3.38137800	1.28109600	1.38350700
C	5.14391600	1.56785600	-0.74654900	H	-4.31509500	2.75784300	1.62007300
H	6.17461400	1.24168200	-0.58710900	C	0.89011400	-0.16266300	-0.90706200
H	4.97067500	1.65797400	-1.81826800	H	1.15603500	0.85845100	-1.15941800
H	5.02789200	2.55031900	-0.28243600	H	-0.03403500	-0.42770700	-1.41723400
C	-1.17939000	-3.72324800	-2.33929000	C	1.98128700	-1.14170900	-1.25625400
H	-0.23990000	-4.27357900	-2.31983400	C	1.72665400	-2.12902000	-2.21252400
H	-1.93011300	-4.35348400	-2.82401100	H	0.78210100	-2.11871500	-2.74049300
H	-1.02068600	-2.84091500	-2.95762700	C	2.65013700	-3.13353000	-2.47547200
C	-1.83410500	-4.59217000	-0.05718100	H	2.43108900	-3.89104600	-3.21840500
H	-0.91856300	-5.18095100	-0.00077100	C	3.83544300	-3.17956500	-1.74525200
H	-2.13011500	-4.31659200	0.95836000	H	4.54516500	-3.98245200	-1.90724400
H	-2.61694800	-5.22437800	-0.48056700	C	4.11507800	-2.18978400	-0.81149200
C	-3.04634900	-2.65763200	-1.05401200	H	5.02084500	-2.22299900	-0.22442100
H	-3.75944700	-3.33280000	-1.53358400	C	3.21967000	-1.13853700	-0.59573200
H	-3.42441300	-2.39110600	-0.06518900	C	4.41753800	1.00735000	-0.19163300
H	-2.98859500	-1.74849900	-1.64900300	C	3.76920300	1.65308100	-1.42046600
C	-1.06750400	3.11195800	-2.12930500	H	2.82594400	2.13546900	-1.16343600
H	-1.04865700	4.16888700	-2.40758300	H	3.59860100	0.92820400	-2.21919000
H	-0.14631300	2.87462000	-1.59628200	H	4.43789700	2.42371800	-1.81041200
H	-1.09968400	2.51035000	-3.03617800	C	5.80777100	0.46634700	-0.55937700
C	-3.58496600	3.05245700	-2.03654600	H	5.77292200	-0.18378500	-1.43577500
H	-4.46646100	2.96562400	-1.39721500	H	6.23010200	-0.08637500	0.28039700
H	-3.58068200	4.05834000	-2.46323700	H	6.47356600	1.30176000	-0.78972200
H	-3.66365500	2.33434900	-2.85248100	C	4.55400700	2.04489500	0.92768700
C	-2.26487300	3.75957700	-0.02853900	H	5.08652200	1.62642800	1.78015600
H	-3.03700400	3.50217600	0.70034400	H	3.57502700	2.36912700	1.27637800
H	-1.28796600	3.76242500	0.45574600	H	5.10802400	2.91182500	0.55850300
H	-2.45879000	4.77933300	-0.36752200	Cl	1.92518600	0.45541100	3.27043300
Cl	1.65113900	-1.76159700	-2.80546800				
<b>[L(HCl)], 27Cl, E<sub>0</sub>=-2191.682213 au</b>				<b>[L(HCl)], 28Cl, E<sub>0</sub>=-2191.679696 au</b>			
N	0.48956100	-0.08313900	-1.74982900	N	-0.42847200	0.33346300	1.69805900
C	0.80023700	1.24320700	-2.33443600	C	-0.07744000	-0.96419500	2.39987100

H	-0.12128200	1.82423400	-2.31435100	H	-0.83211200	-1.67792700	2.09386600
H	1.12043700	1.12788800	-3.38146800	H	-0.17927700	-0.76541300	3.46828600
C	-0.69569500	-0.69384000	-2.38990700	C	-1.88057300	0.69399000	1.90901000
H	-0.76263800	-1.70515600	-2.00793400	H	-2.01409600	1.66465500	1.45050400
H	-0.53360000	-0.75652800	-3.47811500	H	-2.01183500	0.79801100	2.98730400
C	1.66821000	-0.97512100	-1.89007900	C	0.48894100	1.45600800	2.15115000
H	2.52563700	-0.40844200	-1.54534700	H	1.49474100	1.07506500	2.02804900
H	1.81940800	-1.21198000	-2.95527500	H	0.28037900	1.59977700	3.21266100
C	1.85445500	1.99298500	-1.55951600	C	1.30824600	-1.41831300	2.05810600
C	3.12598100	2.18680300	-2.09553600	C	2.33621200	-1.29625000	2.99748100
C	1.54804700	2.53598600	-0.29333200	C	1.58714200	-1.91115100	0.77462500
C	4.09253700	2.92161600	-1.41369300	C	3.64165100	-1.63569800	2.66291300
H	3.35334500	1.77023300	-3.07097300	H	2.10914100	-0.92431600	3.99129500
C	2.53344700	3.24512700	0.39679900	C	2.90856000	-2.20713800	0.43038300
C	3.78988000	3.45288800	-0.16573700	C	3.92395000	-2.07347200	1.37119900
H	5.07163800	3.07295100	-1.85209900	H	4.43303400	-1.54284100	3.39703300
H	2.32925000	3.63490600	1.38162800	H	3.14165800	-2.50860900	-0.58470900
H	4.53658700	4.01165400	0.38612400	H	4.94244600	-2.30837200	1.08564500
C	1.55349800	-2.25268600	-1.09732200	C	0.26803900	2.71846800	1.37332300
C	1.10155800	-3.42506300	-1.71134700	C	-0.50924600	3.75167000	1.90655700
C	1.87792300	-2.28647200	0.26812100	C	0.79779900	2.84285500	0.08094000
C	0.91706000	-4.59659300	-0.98564500	C	-0.80746200	4.87842500	1.15047300
H	0.88421200	-3.41111000	-2.77420000	H	-0.89467400	3.66117100	2.91673600
C	1.64156900	-3.45028700	1.00528000	C	0.44766700	3.95294000	-0.69271900
C	1.16635200	-4.59922500	0.38449300	C	-0.34754200	4.96168800	-0.16264600
H	0.56271200	-5.49303500	-1.48061300	H	-1.41147100	5.67269200	1.57174200
H	1.81502900	-3.43601200	2.07145200	H	0.79337000	4.00755500	-1.71418100
H	0.99181100	-5.49484200	0.96935300	H	-0.60483000	5.81833600	-0.77432800
C	-1.99250700	0.03447400	-2.12794900	C	-2.82392100	-0.33549000	1.35955300
C	-2.49036000	0.91850900	-3.09002400	C	-3.54282400	-1.13696000	2.25292900
C	-2.72538100	-0.15296400	-0.94356800	C	-2.96740800	-0.53904900	-0.02246200
C	-3.66101500	1.63790500	-2.87993000	C	-4.37773400	-2.14905600	1.79891000
H	-1.93870900	1.04778500	-4.01506300	H	-3.42838900	-0.97050300	3.31894100
C	-3.89365600	0.58308200	-0.72877600	C	-3.78625600	-1.58042900	-0.46959500
C	-4.35834000	1.47574000	-1.68626800	C	-4.48527600	-2.37564500	0.42862900
H	-4.02068500	2.32465600	-3.63701700	H	-4.92174000	-2.76512200	2.50419100
H	-4.42669500	0.47688000	0.20452000	H	-3.84469200	-1.76918600	-1.53072000
H	-5.26338800	2.04110800	-1.49807400	H	-5.11421800	-3.17595000	0.05696900
N	0.21265600	2.32872900	0.16341500	N	0.47414700	-2.06842900	-0.12790900
N	-2.19726100	-1.06247600	0.04260600	N	-2.21220600	0.28063900	-0.93875100
N	2.43289300	-1.10125100	0.85948400	N	1.65608900	1.79531700	-0.39303500
O	0.10029900	0.96876800	0.68392300	O	0.71354600	-1.32037100	-1.33128400
H	0.18606500	0.41557100	-0.16056500	H	1.44812600	-1.74247400	-1.93268300
O	1.69990700	-0.81255600	2.06491500	O	1.21255700	1.44682400	-1.71301200
H	1.19697500	-0.02365500	1.79109600	H	1.08137400	0.48274600	-1.63695300
O	-2.18611100	-0.39099400	1.32691100	O	-1.82117600	-0.55847200	-2.03517500
H	-1.35374600	0.12538500	1.28600500	H	-0.88351500	-0.78429700	-1.85088800
C	-0.49286000	3.27405900	1.06393000	C	0.06269300	-3.51198200	-0.38858900
C	3.89322500	-1.14021900	1.19351400	C	3.12746900	2.14189000	-0.45791700
C	-2.88959000	-2.37763100	0.22810200	C	-2.97968800	1.43073400	-1.56539200
C	4.27313200	0.27312200	1.64567500	C	3.85652900	0.88452900	-0.93440500
H	5.34903900	0.33192200	1.82985200	H	4.93460900	1.06341500	-0.93317400
H	4.00865500	0.99619600	0.87574300	H	3.64569700	0.05240300	-0.26738500
H	3.74882800	0.53679100	2.56412000	H	3.55887900	0.59288900	-1.94040200
C	4.23458100	-2.14989300	2.30263600	C	3.42164300	3.30409600	-1.41838900
H	4.11632000	-3.18032600	1.96341600	H	3.04519600	4.25744900	-1.04218100
H	5.27537300	-2.01879700	2.60963600	H	4.50235000	3.40141800	-1.54406800
H	3.59732100	-1.98464200	3.17232900	H	2.98517300	3.10210400	-2.39728700
C	4.66971400	-1.48728400	-0.08252700	C	3.59476000	2.49706000	0.95847600
H	4.38764700	-2.46500100	-0.47729400	H	3.05383400	3.35207700	1.37058700
H	4.51161500	-0.73421600	-0.85695600	H	3.48949300	1.64430000	1.63336800
H	5.73739600	-1.51252200	0.14675300	H	4.65414500	2.75954400	0.92590400
C	-2.09948800	-3.14695200	1.29207800	C	-2.03221700	2.10577500	-2.56240500
H	-2.45814300	-4.17816800	1.34214000	H	-2.46354700	3.05729600	-2.88461700
H	-1.04058800	-3.15550700	1.03870900	H	-1.06148800	2.28753400	-2.10695600
H	-2.21583200	-2.69050700	2.27415200	H	-1.87804100	1.47692600	-3.43723900



C	-2.81135400	-3.12922000	-1.10688300	C	-3.36919600	2.43297600	-0.47622900
H	-3.26611800	-2.55984900	-1.92021500	H	-3.97730900	1.97422500	0.30725900
H	-1.77856900	-3.36558900	-1.36370000	H	-2.48863900	2.90253200	-0.03691600
H	-3.35676300	-4.07055300	-1.01284300	H	-3.96798300	3.22609700	-0.92866200
C	-4.36214700	-2.25125800	0.65368600	C	-4.24159900	0.94908700	-2.29786400
H	-4.76348800	-3.24894300	0.84791100	H	-4.68260300	1.78851900	-2.84069500
H	-4.46949300	-1.67067800	1.57004100	H	-3.98968200	0.17386400	-3.02177900
H	-4.97245500	-1.79489200	-0.12742400	H	-4.99521400	0.56363500	-1.60787400
C	-0.13446800	3.09761100	2.54998400	C	1.23111400	-4.48802700	-0.60550000
H	0.92294300	3.27233000	2.75149900	H	1.85460100	-4.58758200	0.28473500
H	-0.71304200	3.80127300	3.15277800	H	0.81682600	-5.47455500	-0.82957900
H	-0.37900400	2.09059600	2.88898900	H	1.85254800	-4.18551700	-1.44942300
C	-1.99506000	3.02073500	0.86646500	C	-0.84220500	-3.55605400	-1.62197500
H	-2.57800200	3.70249100	1.48948900	H	-1.24440800	-4.56754700	-1.71573200
H	-2.26655300	3.17116700	-0.17943200	H	-1.67025200	-2.85838000	-1.53507500
H	-2.26999600	2.00828500	1.13920200	H	-0.28218000	-3.32823900	-2.52876900
C	-0.20782500	4.70610700	0.58213700	C	-0.74073600	-3.94210100	0.84729700
H	0.79639000	5.05278800	0.81826300	H	-0.13732500	-3.88544300	1.75740400
H	-0.34907500	4.77769300	-0.49869900	H	-1.63576900	-3.32772200	0.96414500
H	-0.91893300	5.38048100	1.06285500	H	-1.05608700	-4.98140400	0.73175900
H	-3.37660200	0.26103800	2.32611000	H	-0.29620800	0.18610300	0.68526400
Cl	-4.25405300	0.80637500	3.16089400	Cl	2.79041800	-2.27816500	-3.06579900
<b>[L(HCl)], 29Cl, E<sub>0</sub>=-2191.679670 au</b>				<b>[L(HCl)], 30Cl, E<sub>0</sub>=-2191.678523 au</b>			
O	-1.53582400	0.48377000	-1.45625300	O	-2.80381100	-0.49276400	-0.13182400
O	3.26622200	-0.58647000	-2.36870900	H	-2.47605300	-0.25655000	-1.03987100
O	-1.89782600	-2.28010300	-1.38671700	O	-1.19575200	3.21273200	-1.74240100
N	-2.44607200	1.60116000	-1.30310500	H	-1.32479100	2.37377900	-2.24100300
N	2.56736500	0.43490900	-1.62464400	O	3.58756300	-2.48901900	0.80530700
N	-1.35233600	-2.53761600	-0.07168100	H	2.69563800	-2.81458800	0.97139400
N	0.07622600	0.17557500	1.66767500	N	-2.76630100	-1.92478600	-0.07364700
C	-1.41172200	0.39658900	1.43235800	N	-1.38468900	2.77532800	-0.39226300
C	-1.72233100	1.84692900	1.13571200	N	3.37817700	-1.13274600	0.32731900
C	-1.53292600	2.75427400	2.18819000	N	0.73547400	-0.17372600	0.30292900
C	-1.69530500	4.12247000	2.01628300	H	1.58705100	-0.42175800	0.83318600
C	-2.03429800	4.62088800	0.76293500	C	0.04874000	-1.47838700	-0.05886200
C	-2.23053000	3.73925600	-0.29094200	H	-0.62034800	-1.26648800	-0.88696800
C	-2.11729900	2.35419700	-0.12139000	H	0.83611200	-2.13256300	-0.43092200
C	-3.86132700	1.11388000	-1.43958700	C	-0.65483800	-2.10413400	1.10961600
C	-4.27101200	0.14334100	-0.32428600	C	0.09185600	-2.51009400	2.21490500
C	-4.78142700	2.34196000	-1.41260300	H	1.16466200	-2.33169900	2.22922800
C	-3.98132000	0.43845200	-2.81186300	C	-0.50005100	-3.13337500	3.30802500
C	0.89793200	0.83610600	0.60727200	H	0.09871400	-3.44392200	4.15523100
C	2.38643700	0.76949400	0.79306700	C	-1.87264300	-3.35187900	3.28532300
C	2.98126700	0.89738900	2.05180700	H	-2.36209700	-3.82960700	4.12608800
C	4.35728600	0.76641500	2.19834000	C	-2.63514300	-2.94187300	2.19654800
C	5.15503500	0.51366900	1.08355700	H	-3.70051800	-3.09802100	2.22323700
C	4.57895100	0.42419200	-0.17719300	C	-2.05298200	-2.31883900	1.08352400
C	3.19874100	0.57084000	-0.33669000	C	-4.08268800	-2.49529500	-0.47328700
C	2.53326000	1.65070900	-2.50435500	C	-4.30934500	-2.05111400	-1.93001100
C	3.94224600	2.09909500	-2.92561700	H	-3.45254100	-2.31573400	-2.55076500
C	1.70941600	1.27676800	-3.74232000	H	-4.44856600	-0.97335800	-2.00347800
C	1.83286000	2.79056400	-1.75690000	H	-5.20339200	-2.54014200	-2.32414600
C	0.39720000	-1.28481200	1.94451700	C	-3.97535600	-4.02674000	-0.46204200
C	0.90708400	-2.10106700	0.78213000	H	-3.11463500	-4.34587600	-1.05402000
C	2.28599300	-2.33189200	0.70329400	H	-4.87557400	-4.44779500	-0.91439400
C	2.84556400	-3.04321200	-0.34947800	H	-3.87702000	-4.44764700	0.53792200
C	2.02173400	-3.51564700	-1.37040800	C	-5.25880800	-1.98408100	0.37966900
C	0.64698800	-3.32343200	-1.29499600	H	-6.20384600	-2.24328600	-0.10384500
C	0.07597200	-2.66377000	-0.20172900	H	-5.20279700	-0.89813400	0.46217700
C	-2.07088300	-3.75474400	0.45527600	H	-5.28096500	-2.40617800	1.38512400
C	-1.46643500	-4.15101200	1.80682300	C	-0.17298100	0.72856500	1.13860000
C	-1.98625100	-4.94893900	-0.51025000	H	-0.22284800	0.26543100	2.12196400
C	-3.53581200	-3.35426500	0.65930700	H	-1.14720200	0.67839300	0.66929500
H	0.25829100	0.61581200	2.64011400	C	0.33830200	2.13522600	1.19841900
H	-1.71755200	-0.29506100	0.66272500	C	1.42401600	2.46307000	2.01557900
H	-1.87615500	0.10908500	2.37651200	H	1.81579000	1.71924100	2.70158400

H	-1.22044500	2.36949600	3.15399100	C	2.01739600	3.71761200	1.94365000
H	-1.53604800	4.78993200	2.85429500	H	2.86080700	3.95954400	2.57923300
H	-2.13384200	5.68755200	0.59963700	C	1.53268100	4.65057100	1.02708600
H	-2.47687100	4.10605800	-1.27823200	H	2.00944100	5.61988100	0.93703600
H	-4.20576900	0.61948200	0.65619200	C	0.42433800	4.35283200	0.24300200
H	-3.65301200	-0.75105100	-0.32969700	H	0.04573600	5.06802700	-0.47295500
H	-5.30606600	-0.17375800	-0.47241500	C	-0.21353400	3.11275200	0.35278400
H	-4.75533400	2.85035300	-0.44882800	C	-2.68500800	3.31689100	0.13593000
H	-5.80667700	2.01265100	-1.59323500	C	-2.73180700	4.85274600	0.10310200
H	-4.50730900	3.05492700	-2.19232600	H	-2.50236800	5.21258500	-0.90104100
H	-3.62038000	1.10844900	-3.59582200	H	-2.02727500	5.29518100	0.81079500
H	-5.02876000	0.20504400	-3.01359800	H	-3.73342900	5.19800300	0.37114600
H	-3.42036700	-0.49452000	-2.85952200	C	-3.80016700	2.74403600	-0.74602000
H	0.56589100	1.87128700	0.59083600	H	-3.78507700	1.65505800	-0.72327200
H	0.63269000	0.38645000	-0.34399500	H	-3.68488900	3.07036500	-1.77866400
H	2.36486400	1.06855900	2.92889300	H	-4.76959200	3.08956500	-0.37713600
H	4.79963100	0.85062200	3.18365000	C	-2.86830700	2.80820000	1.57125200
H	6.22678300	0.39457300	1.19445800	H	-2.08244900	3.16942400	2.23816600
H	5.18233900	0.20453000	-1.04612200	H	-2.88944200	1.71719500	1.59513800
H	4.47971600	1.27947000	-3.40306500	H	-3.82382000	3.17135100	1.95652500
H	4.51809600	2.44511000	-2.06532900	C	1.27982000	0.48863600	-0.94045100
H	3.87037800	2.92523100	-3.63721300	H	1.78434700	1.39400800	-0.61460600
H	1.55800700	2.15366700	-4.37554400	H	0.42094500	0.75899700	-1.55418600
H	0.72924600	0.89313900	-3.44248400	C	2.20293700	-0.42073100	-1.71059400
H	2.20761900	0.50306400	-4.32433900	C	2.00778700	-0.50930100	-3.09189400
H	0.79594500	2.54431900	-1.52487100	H	1.18397900	0.03785800	-3.53476500
H	1.82872100	3.67756600	-2.39349300	C	2.81001900	-1.33218700	-3.87362900
H	2.34983400	3.04803300	-0.83123700	H	2.63674300	-1.39391700	-4.94106300
H	-0.50549700	-1.69720500	2.37919000	C	3.79995100	-2.10652400	-3.27475800
H	1.14689500	-1.26055900	2.73260000	H	4.40886900	-2.77436900	-3.87268100
H	2.92936400	-1.92224800	1.47132200	C	3.99782100	-2.04066200	-1.90061800
H	3.91656800	-3.19567600	-0.38927300	H	4.72729500	-2.67554700	-1.41968100
H	2.44495000	-4.05207000	-2.21249700	C	3.22323400	-1.18344100	-1.11731700
H	-0.00348400	-3.67988500	-2.07979800	C	4.54217600	-0.33018100	0.85348200
H	-1.61661000	-3.37625300	2.55995500	C	4.43776200	1.08973900	0.28950400
H	-0.40094500	-4.37283800	1.73222500	H	3.52454100	1.58935900	0.61110600
H	-1.97001600	-5.05252500	2.16119100	H	4.48272200	1.09449900	-0.80053100
H	-0.96767900	-5.33330600	-0.58545700	H	5.28014800	1.67612800	0.66181400
H	-2.33423200	-4.66753900	-1.50412900	C	5.89793300	-0.93955600	0.46599800
H	-2.62050800	-5.75792500	-0.14040900	H	6.06837100	-0.88111600	-0.60973800
H	-4.08469900	-4.18144600	1.11509300	H	5.96446900	-1.98079500	0.78126500
H	-4.00766000	-3.10871900	-0.29124200	H	6.69529100	-0.38028800	0.96062700
H	-3.60604100	-2.48843700	1.32079400	C	4.39723500	-0.29908400	2.37920600
H	-1.01500400	0.73199900	-2.22903200	H	4.50280100	-1.29825100	2.80021800
H	2.73348000	-1.37178100	-2.18911500	H	3.41983200	0.09738500	2.66436500
H	-1.87157300	-1.30835500	-1.43497100	H	5.16461100	0.34487400	2.81386800
Cl	0.34246200	0.90651800	4.50751500	Cl	-1.58659300	0.30970800	-2.82007900
<b>[L(HCl)], 31Cl, E<sub>0</sub>=-2191.675367 au</b>				<b>[L(HCl)], 32Cl, E<sub>0</sub>=-2191.674476 au</b>			
N	0.07561700	-0.17263900	1.24817800	N	-0.38918000	-0.04853100	1.71293000
C	0.60409000	1.18750100	1.66612800	C	-0.20835100	1.38232100	2.18365300
H	1.59642500	1.25516900	1.23768200	H	0.83809000	1.61276700	2.01944300
H	0.65564600	1.14759500	2.75821300	H	-0.41747000	1.37356300	3.25475800
C	0.99479300	-1.25944400	1.76333400	C	0.59703800	-0.97439000	2.39485400
H	0.54712600	-2.19644700	1.45882500	H	0.33544300	-1.97243800	2.06655600
H	0.95667100	-1.17199200	2.85180200	H	0.39889700	-0.89100000	3.46473400
C	-1.34878400	-0.40396000	1.72824800	C	-1.81910300	-0.51533400	1.92308600
H	-1.90600400	0.46980900	1.42110100	H	-2.44544700	0.26837700	1.51806900
H	-1.28469700	-0.44065300	2.81873700	H	-1.95773600	-0.57275800	3.00394000
C	-0.28189900	2.30262500	1.20122300	C	-1.11529200	2.33273700	1.45916900
C	-1.18754600	2.86971600	2.10363200	C	-2.26004600	2.83532800	2.08285300
C	-0.22885700	2.77995800	-0.11531700	C	-0.82909800	2.69208700	0.13443700
C	-2.05766600	3.87423200	1.69473000	C	-3.13504000	3.66693600	1.39305800
H	-1.20231800	2.49636900	3.12286200	H	-2.46744500	2.56844900	3.11382800
C	-1.12160600	3.77300500	-0.52511500	C	-1.73883200	3.48381200	-0.56833300
C	-2.03459900	4.31479600	0.37359800	C	-2.87920300	3.97453200	0.05907500
H	-2.75719800	4.30410500	2.40131200	H	-4.01618700	4.05860800	1.88647300

H	-1.12078000	4.12369900	-1.54859100	H	-1.55360100	3.69922800	-1.60973100
H	-2.72433500	5.08139900	0.04095800	H	-3.57226600	4.59467000	-0.49716500
C	-1.91383800	-1.65222400	1.11965900	C	-2.09077800	-1.83243000	1.26045900
C	-1.92321700	-2.84334900	1.85257100	C	-2.05000300	-3.01965500	1.99816800
C	-2.38518000	-1.65258500	-0.20186400	C	-2.34348500	-1.88179800	-0.11864800
C	-2.33718800	-4.03371700	1.26593800	C	-2.19407600	-4.25084100	1.37111000
H	-1.58422600	-2.82468800	2.88232000	H	-1.88639300	-2.97502000	3.06962600
C	-2.75439800	-2.85929000	-0.80081600	C	-2.41421900	-3.12475400	-0.75237200
C	-2.72588900	-4.04315100	-0.07241000	C	-2.34147800	-4.29942000	-0.01362700
H	-2.33527600	-4.95119400	1.84189400	H	-2.15824800	-5.16458400	1.95133200
H	-3.04673200	-2.86487600	-1.84083200	H	-2.51696500	-3.15899700	-1.82669700
H	-3.01533500	-4.97270800	-0.54851200	H	-2.40528600	-5.25525700	-0.51969400
C	2.39419400	-1.09870700	1.24501600	C	2.02442100	-0.63117600	2.08825700
C	3.40075000	-0.78306300	2.16399700	C	2.83037900	-0.11614800	3.10849800
C	2.71309100	-1.20117400	-0.11877000	C	2.55278300	-0.79277800	0.79634800
C	4.70574600	-0.55455900	1.74514100	C	4.14479300	0.25658100	2.85694300
H	3.13290900	-0.68898000	3.21062200	H	2.41550100	-0.00000600	4.10459200
C	4.02214100	-0.94382100	-0.53530800	C	3.86748500	-0.39091000	0.54410300
C	5.01079700	-0.62431200	0.38785400	C	4.65355000	0.12733000	1.56701700
H	5.47160200	-0.30414000	2.46913900	H	4.75970400	0.65555500	3.65474900
H	4.24797700	-0.97299500	-1.59088500	H	4.26513100	-0.44945300	-0.46428800
H	6.02018600	-0.42904100	0.04439900	H	5.66902800	0.43430000	1.34642700
N	0.77488900	2.20871300	-0.98216200	N	0.41036500	2.22227100	-0.41030900
N	1.66067800	-1.50129600	-1.06903800	N	1.68352200	-1.30927900	-0.23459000
N	-2.45172600	-0.38782900	-0.88910700	N	-2.51735800	-0.63710100	-0.81571400
O	0.15108500	1.60048300	-2.13458900	O	0.11625500	1.51332900	-1.63550100
H	-0.20107600	2.30051100	-2.70664800	H	0.78369400	0.77342100	-1.60043700
O	-1.88198000	-0.56278400	-2.20488600	O	-1.73963700	-0.69496900	-2.02181500
H	-1.16262100	0.08580400	-2.19515700	H	-1.15768100	0.08235300	-1.93263900
O	1.92801800	-0.72565000	-2.25966000	O	1.76386900	-0.47638300	-1.38948700
H	1.27018300	-0.01724500	-2.23032200	H	2.66832100	-0.49741200	-1.87471600
C	1.90942300	3.10809200	-1.39374600	C	1.44018600	3.30167600	-0.67459300
C	-3.83429700	0.19028500	-1.05053400	C	-3.94732700	-0.31689600	-1.18729600
C	1.59103800	-2.94436800	-1.53076700	C	1.90049500	-2.76101800	-0.62449600
C	-3.67022500	1.54210300	-1.75241100	C	-3.92563700	1.03459600	-1.90462700
H	-4.63174800	2.05950100	-1.78857300	H	-4.94900000	1.36287700	-2.10212900
H	-2.96279700	2.16406000	-1.20629200	H	-3.43329700	1.78036700	-1.28521100
H	-3.31525700	1.40837800	-2.77484100	H	-3.39548200	0.96333000	-2.85357600
C	-4.76911300	-0.70677900	-1.87692400	C	-4.58155800	-1.37050500	-2.10852600
H	-5.02752200	-1.62326000	-1.34493100	H	-4.75649800	-2.31651100	-1.59380200
H	-5.69788000	-0.16960500	-2.08401900	H	-5.54710900	-1.00370300	-2.46485400
H	-4.30554400	-0.96507900	-2.83029800	H	-3.94466100	-1.54590400	-2.97661100
C	-4.42322200	0.41667100	0.34667200	C	-4.75980200	-0.19057100	0.10669200
H	-4.49002300	-0.51141900	0.91636300	H	-4.75014600	-1.11438600	0.68853100
H	-3.83341600	1.13857600	0.91436200	H	-4.38804700	0.62861600	0.72651700
H	-5.43352700	0.81861800	0.24458600	H	-5.79893200	0.03115600	-0.14545100
C	0.46910600	-3.03103000	-2.57051400	C	1.04513400	-3.01814000	-1.87027200
H	0.26378700	-4.08086700	-2.79429300	H	0.96800300	-4.09645000	-2.03325300
H	-0.44139700	-2.56741200	-2.19621300	H	0.04662900	-2.60185300	-1.74756000
H	0.75474800	-2.52997000	-3.49457900	H	1.49570700	-2.56569700	-2.75211700
C	1.23886300	-3.83191000	-0.33476000	C	1.39844200	-3.62859100	0.53358600
H	1.96748700	-3.73988300	0.47299100	H	1.94406800	-3.42254800	1.45846800
H	0.24107800	-3.60977100	0.04300600	H	0.33027400	-3.49117700	0.69564100
H	1.24121600	-4.87393800	-0.66134100	H	1.56422600	-4.67967900	0.28867300
C	2.91322400	-3.41681700	-2.15468600	C	3.36625300	-3.11334100	-0.91790700
H	2.77226200	-4.41435900	-2.57746800	H	3.41054900	-4.14694000	-1.27194500
H	3.22022800	-2.74874100	-2.96025100	H	3.79349000	-2.47512100	-1.69268700
H	3.71434100	-3.47611800	-1.41595300	H	3.98578400	-3.04362600	-0.02084400
C	1.47503000	4.30220500	-2.26427200	C	1.03712000	4.26212300	-1.80401600
H	0.87495000	5.02197600	-1.70850700	H	0.24374800	4.94860500	-1.50333800
H	2.36563600	4.82069300	-2.62438800	H	1.90288100	4.86490600	-2.08636700
H	0.92100800	3.98866100	-3.15585700	H	0.71913000	3.69724200	-2.68100700
C	2.93201300	2.26270300	-2.15827200	C	2.75038400	2.60355100	-1.04288900
H	3.81227700	2.87277100	-2.37252400	H	3.54231100	3.34899600	-1.14563300
H	3.23598600	1.40097700	-1.56843800	H	3.04051000	1.89938500	-0.26558200
H	2.53233900	1.90202400	-3.10657100	H	2.69193100	2.06001900	-1.98420700

C	2.55409200	3.62577900	-0.10123700	C	1.63882800	4.07664800	0.63499600
H	1.85702600	4.21155000	0.49910700	H	0.73068500	4.58913400	0.95876800
H	2.93385700	2.80065600	0.50274000	H	1.98011300	3.41592100	1.43577900
H	3.39864700	4.26689300	-0.36118100	H	2.41233300	4.83145200	0.48109600
H	0.09085300	-0.23637300	0.22355100	Cl	4.21337300	-0.24395100	-2.92982100
Cl	0.04734500	0.10144000	4.78522100	H	-0.16476200	-0.09232200	0.70612500
<b>[L(HCl)], 33Cl, E<sub>0</sub>=-2191.674374 au</b>				<b>[L(HCl)], 34Cl, E<sub>0</sub>=-2191.670497 au</b>			
N	-0.00097700	-0.27743400	1.33008700	N	-0.05755000	0.00957200	1.24320600
C	-1.42217800	-0.20426600	1.84473700	C	0.32561200	-1.28340700	1.85708900
H	-1.77484600	0.78952000	1.60477400	H	-0.48624800	-1.98250800	1.65865700
H	-1.35631000	-0.31126200	2.92949500	H	0.43195000	-1.17229900	2.94632000
C	0.83046100	0.94768300	1.66568800	C	-1.40402100	0.44009900	1.67895600
H	1.78898200	0.78298300	1.19507800	H	-1.54903300	1.43671200	1.28077700
H	0.94121100	0.91747100	2.75343200	H	-1.43391400	0.51002300	2.77745200
C	0.69883300	-1.52978900	1.82605400	C	0.95007300	1.04490500	1.58421500
H	0.08397200	-2.36459600	1.50666800	H	1.92176000	0.60715100	1.38646400
H	0.70064500	-1.44773300	2.91590200	H	0.89064400	1.27579600	2.65883300
C	-2.24520400	-1.27021500	1.18070000	C	1.59817800	-1.85375800	1.28418600
C	-2.58658200	-2.41910400	1.90047500	C	2.76174100	-1.88725200	2.05050500
C	-2.61754800	-1.16889900	-0.17030400	C	1.61249900	-2.39408500	-0.01986100
C	-3.25407100	-3.47370000	1.28835500	C	3.93265700	-2.46109800	1.56223900
H	-2.30337600	-2.48026400	2.94522700	H	2.73971400	-1.47283800	3.05271500
C	-3.26025100	-2.24460100	-0.78731700	C	2.79980200	-2.94213600	-0.51103200
C	-3.57385500	-3.38995700	-0.06475900	C	3.94559300	-2.99223500	0.27820300
H	-3.50759600	-4.35931100	1.85829000	H	4.82398000	-2.48912600	2.17759100
H	-3.48994700	-2.18264200	-1.84070300	H	2.84158300	-3.32802500	-1.51721600
H	-4.07253800	-4.21515100	-0.55959400	H	4.85281500	-3.42729600	-0.12458600
C	2.08941200	-1.58630800	1.26418800	C	0.79617300	2.31457300	0.78526700
C	3.18533800	-1.44264800	2.11719100	C	0.07661300	3.39365400	1.30859000
C	2.29311000	-1.65739300	-0.12146800	C	1.35046800	2.43106200	-0.49914000
C	4.47193400	-1.34324700	1.59749200	C	-0.14431800	4.54527100	0.56163900
H	3.00884200	-1.36238500	3.18398600	H	-0.32143100	3.31983400	2.31506700
C	3.58054300	-1.50720000	-0.64091000	C	1.08196700	3.56784100	-1.26692400
C	4.66477000	-1.35370900	0.21757400	C	0.34162400	4.61993100	-0.74153800
H	5.31643500	-1.22415400	2.26533600	H	-0.70864300	5.36803000	0.98460600
H	3.72958200	-1.49445000	-1.71005500	H	1.44212400	3.60594300	-2.28471700
H	5.66058000	-1.23813900	-0.19386700	H	0.14424100	5.49610300	-1.34831900
C	0.20257600	2.23274400	1.22428300	C	-2.51882100	-0.46353500	1.21294800
C	-0.48681600	2.97137400	2.19622900	C	-3.03825500	-1.42305600	2.08777600
C	0.28476400	2.72875800	-0.08545900	C	-3.04454800	-0.37863700	-0.08660500
C	-1.11662700	4.16638500	1.87717600	C	-4.02591900	-2.31396600	1.68438300
H	-0.52251300	2.57582100	3.20653900	H	-2.64583300	-1.47417900	3.09792600
C	-0.36480600	3.92630900	-0.40059100	C	-4.01857900	-1.29331100	-0.49684800
C	-1.06164100	4.63718400	0.56769000	C	-4.50673300	-2.25484200	0.37853800
H	-1.64955400	4.71972400	2.64076300	H	-4.40711600	-3.05478300	2.37740900
H	-0.34170900	4.27897400	-1.42018800	H	-4.36286400	-1.26059200	-1.52021400
H	-1.55903600	5.56091400	0.29598300	H	-5.26189900	-2.95594200	0.04184300
N	-2.28525700	0.04981900	-0.88185300	N	0.37140600	-2.35897900	-0.72262800
N	1.01321700	1.99150200	-1.11637100	N	-2.50861300	0.61562900	-0.97986700
N	1.10761200	-1.83234300	-0.93238100	N	2.16998900	1.35421900	-0.98008900
O	-1.80895200	-0.29974300	-2.21455700	O	0.15318100	-1.01568400	-1.24110000
H	-0.89397400	-0.60658300	-2.07875400	H	-0.02093900	-0.48678700	-0.39871800
O	1.08370500	-0.81053700	-1.98303400	O	1.71531800	0.99023000	-2.29656100
H	1.17832900	0.04344000	-1.50371800	H	1.27089900	0.14197300	-2.10874800
O	0.27124700	2.14385000	-2.35595700	O	-2.26927400	-0.01497800	-2.25836900
H	-0.38798400	1.43320100	-2.33446600	H	-1.35831600	-0.33656400	-2.14351300
C	-3.46690900	0.97682100	-1.09447900	C	-0.00560600	-3.35779600	-1.75155200
C	1.00056100	-3.17066900	-1.61716000	C	3.64387900	1.61023600	-1.04422800
C	2.40163600	2.54865900	-1.41636500	C	-3.35773700	1.82038500	-1.25092800
H	-0.06567000	-0.36347900	0.31268500	C	4.30112700	0.27494300	-1.40717400
C	-4.65149400	0.29334800	-1.79765400	H	5.38956700	0.37720100	-1.39980800
H	-5.11924400	-0.46795000	-1.17274700	H	4.01507000	-0.49087400	-0.68784500
H	-5.40820600	1.04740900	-2.02554300	H	3.98876100	-0.04870500	-2.39997200
H	-4.33589700	-0.16015300	-2.73842900	C	4.02856100	2.67833600	-2.08263000
C	-3.90435900	1.49515300	0.27986400	H	3.70048900	3.67409100	-1.77971000
H	-4.17996700	0.68449600	0.95646400	H	5.11551400	2.70626700	-2.19512400

H	-3.12195700	2.10070000	0.73969600	H	3.58908900	2.43716400	-3.05139300
H	-4.78341100	2.12992700	0.15109900	C	4.11854100	2.04429900	0.34793200
C	-3.00407500	2.16094900	-1.94634100	H	3.63407300	2.96662500	0.67328200
H	-3.80877400	2.89807500	-1.99465500	H	3.92854000	1.26579700	1.08926300
H	-2.13543200	2.63878500	-1.50347000	H	5.19590900	2.22229800	0.31701200
H	-2.76337600	1.85100100	-2.96254200	C	-2.51868600	2.75452100	-2.12945300
C	2.36697400	4.02980900	-1.82323700	H	-3.03485200	3.70992400	-2.25719200
H	2.06067300	4.67403400	-0.99886800	H	-1.55230700	2.93733300	-1.66195200
H	3.37120200	4.33261400	-2.12758600	H	-2.34900400	2.31307500	-3.11063200
H	1.69660600	4.18714000	-2.66867700	C	-3.66249200	2.51455400	0.08138800
C	3.26714200	2.37709600	-0.16486700	H	-4.16314800	1.84544800	0.78411100
H	2.85078500	2.90100400	0.69683000	H	-2.75283000	2.90332800	0.54037900
H	3.40952800	1.32498600	0.08420600	H	-4.32759100	3.36034600	-0.10698300
H	4.25294300	2.80228200	-0.36385300	C	-4.67673800	1.47265700	-1.96309500
C	3.00142500	1.73105600	-2.56688800	H	-5.18558800	2.39418300	-2.25711300
H	4.01869400	2.08092000	-2.75549600	H	-4.48209000	0.88789100	-2.86279200
H	3.04804700	0.67149200	-2.32261400	H	-5.35083100	0.91193000	-1.31265600
H	2.41678600	1.84982900	-3.47738800	C	0.62442800	-3.09532700	-3.13180500
C	-0.29426200	-3.18992700	-2.43248400	H	1.71219500	-3.16850400	-3.12215700
H	-0.44806300	-4.19460800	-2.83219700	H	0.24708800	-3.82507100	-3.85241500
H	-1.14607100	-2.94040700	-1.80545600	H	0.35768500	-2.10037500	-3.48943400
H	-0.25221000	-2.49584600	-3.27165200	C	-1.53730300	-3.30290600	-1.87691800
C	2.18268100	-3.48654400	-2.54804100	H	-1.87837400	-4.07500600	-2.57160200
H	3.10365200	-3.67297600	-1.99549600	H	-1.99772800	-3.47523400	-0.90311100
H	1.95230700	-4.38841700	-3.11943400	H	-1.88350400	-2.34016900	-2.24224300
H	2.34489800	-2.67192100	-3.25565300	C	0.35687300	-4.75507100	-1.22222100
C	0.90479500	-4.22257900	-0.50526000	H	1.42682300	-4.95450500	-1.21938100
H	1.78333100	-4.21375100	0.14182700	H	-0.01660000	-4.88059000	-0.20337800
H	0.01202800	-4.06687900	0.10329500	H	-0.12393900	-5.50310900	-1.85557700
H	0.83379300	-5.21258600	-0.96008700	Cl	0.01335300	0.44576000	5.41224600
Cl	0.23270600	-0.01799400	4.82076300	H	0.02676500	0.58198100	6.69309100
<b>[L(HCl)], 35Cl, E<sub>g</sub>=-2191.662726 au</b>				<b>[L(HBr)], 23Br, E<sub>g</sub>=-4305.617584 au</b>			
O	-1.09161400	1.06423800	-0.78262600	N	-0.00024200	-0.00010600	-1.23946900
O	2.93860800	-1.10090200	-2.12320700	C	0.45494500	1.37126500	-1.70498500
O	-3.29838900	-0.54435600	-0.91529500	H	-0.27562800	2.05418900	-1.29683800
N	-0.97155100	2.47490600	-0.64247500	H	0.37853700	1.35816400	-2.79452700
N	2.90989400	-0.29245200	-0.94705600	C	-1.41556500	-0.29163500	-1.70478200
N	-2.85725500	-1.41661700	0.15049800	H	-1.64175000	-1.26560800	-1.29623500
N	-0.02450300	-0.36659800	2.01679200	H	-1.36627700	-0.35157000	-2.79432200
C	-1.15940500	0.67781900	1.92684000	C	0.95986900	-1.07993700	-1.70504400
C	-0.60214400	2.06974400	1.83808600	H	1.91691400	-0.78784800	-1.29831800
C	-0.08223100	2.59814400	3.02914100	H	0.98545300	-1.00822300	-2.79468400
C	0.58516300	3.81194000	3.07773700	C	1.83467000	1.76891900	-1.25929100
C	0.76953100	4.51598100	1.88993600	C	2.96356600	1.35457100	-1.97681000
C	0.26103900	4.01670800	0.70120900	C	2.00842400	2.56856600	-0.11643100
C	-0.46997400	2.81763100	0.64211500	C	4.24578600	1.63948600	-1.52808200
C	-2.26175400	3.13423800	-1.07774900	H	2.83268700	0.79027200	-2.89355600
C	-3.41247000	2.79858800	-0.11501900	C	3.30260000	2.81061700	0.35763400
C	-2.07095700	4.65519000	-1.13179600	C	4.41036600	2.34523500	-0.33644200
C	-2.56183800	2.63689500	-2.49782100	H	5.10721800	1.29962700	-2.08991000
C	1.12937200	-0.05984000	1.09413500	H	3.41394500	3.35105000	1.28620400
C	2.32775600	-0.94268300	1.29835700	H	5.40564200	2.54614000	0.04274300
C	2.61275600	-1.62614000	2.48121900	C	0.61560200	-2.47331200	-1.25749800
C	3.64424500	-2.55934100	2.53126800	C	-0.30902300	-3.24445900	-1.97257900
C	4.38955600	-2.82374600	1.38347100	C	1.22356200	-3.02266300	-0.11534400
C	4.15475700	-2.10261400	0.21784200	C	-0.70228700	-4.49710600	-1.52218900
C	3.16407400	-1.11937500	0.18347500	H	-0.73416600	-2.84972500	-2.88877600
C	3.82210400	0.89064400	-1.13095700	C	0.78737200	-4.26432200	0.36028100
C	5.26196800	0.45392600	-1.44468200	C	-0.17074800	-4.99166600	-0.33139100
C	3.25417600	1.71333900	-2.29201600	H	-1.42838700	-5.07368000	-2.08215200
C	3.79983300	1.74525900	0.14236100	H	1.20160800	-4.63027500	1.28828000
C	-0.58407400	-1.80227600	1.92669900	H	-0.49337900	-5.95389100	0.04907300
C	-0.63567400	-2.37531800	0.53935500	C	-2.44961500	0.70458400	-1.25893300
C	0.45275600	-3.13331300	0.09137300	C	-2.65369900	1.89047000	-1.97515900
C	0.50904300	-3.60526900	-1.21214100	C	-3.23033400	0.45444900	-0.11707500
C	-0.53641600	-3.32753300	-2.08527900	C	-3.54108800	2.85866800	-1.52601200

C	-1.65037000	-2.62915800	-1.64049600	H	-2.09868600	2.05995100	-2.89123000
C	-1.72632300	-2.17233000	-0.32539800	C	-4.08679000	1.45430800	0.35729600
C	-4.07227100	-2.20092700	0.55400900	C	-4.23596400	2.64736300	-0.33536200
C	-3.68009100	-3.21152700	1.63742200	H	-3.67614300	3.77544000	-2.08682200
C	-4.70874600	-2.94849300	-0.62989000	H	-4.61162800	1.27972300	1.28507000
C	-5.06934800	-1.19169100	1.13736600	H	-4.90737600	3.40888800	0.04411400
H	0.34234400	-0.27557400	2.96442800	N	0.84920600	3.07756800	0.54923100
H	-1.78169500	0.37351200	1.10210200	N	-3.09328000	-0.80483000	0.54740700
H	-1.71860500	0.54763300	2.85524700	N	2.24478000	-2.27242100	0.54838800
H	-0.21580400	2.03049700	3.94657700	O	1.07376000	3.01217600	1.96187000
H	0.97028700	4.19156900	4.01581400	H	0.67608100	2.14593500	2.18799300
H	1.32747100	5.44481800	1.88410600	O	2.07829900	-2.43358000	1.96143800
H	0.44669300	4.53614800	-0.22721700	H	1.52621500	-1.65669500	2.18789700
H	-3.19963100	3.16835400	0.89184800	O	-3.15109500	-0.57941000	1.96028600
H	-3.59784000	1.72577500	-0.06859300	H	-2.20245900	-0.49171200	2.18820800
H	-4.33356400	3.27621800	-0.45825800	C	0.44311800	4.49093000	0.23984400
H	-1.90317200	5.09020300	-0.14601000	C	3.67144200	-2.62705400	0.23693700
H	-2.97981900	5.10187200	-1.54010500	C	-4.11406500	-1.86248800	0.23539900
H	-1.23878600	4.92108500	-1.78637800	H	-0.00058600	-0.00028500	-0.18041500
H	-1.69177000	2.77686400	-3.14120900	C	1.46502900	5.50857000	0.77461900
H	-3.40205700	3.20316400	-2.90631000	H	2.41933200	5.42715400	0.24903900
H	-2.82374500	1.58101200	-2.52501200	H	1.08697500	6.52343500	0.62783500
H	1.36778500	0.98395000	1.26946600	H	1.63441500	5.35225100	1.83951200
H	0.77530300	-0.14298800	0.07150300	C	-0.92101500	4.69810400	0.90871100
H	2.01661800	-1.46901200	3.37590000	H	-1.30186400	5.69809200	0.68421100
H	3.84790000	-3.09301200	3.45180400	H	-1.63583500	3.95821500	0.54349100
H	5.16760200	-3.57786700	1.40447900	H	-0.83473700	4.58881400	1.98874000
H	4.72484800	-2.29428300	-0.68014100	C	0.29769400	4.67160200	-1.27613600
H	5.26290400	-0.24105800	-2.28504600	H	1.22522500	4.45007400	-1.80742100
H	5.73494200	-0.02521700	-0.58399700	H	-0.50477800	4.05295600	-1.68105900
H	5.86432400	1.32469800	-1.71559600	H	0.03950400	5.71327100	-1.47810700
H	3.84009300	2.62885000	-2.41324300	C	-3.61283500	-3.14803900	0.90414800
H	2.21121900	1.97138500	-2.10509900	H	-4.28688000	-3.97814000	0.67605300
H	3.28805200	1.15010400	-3.22311800	H	-2.61309100	-3.39550300	0.54215100
H	2.80627800	2.16084900	0.32082100	H	-3.56519700	-3.02020800	1.98453400
H	4.48685700	2.58463700	0.01410400	C	-5.50713200	-1.48630500	0.76804900
H	4.12128900	1.18564500	1.02347700	H	-5.91247400	-0.61841500	0.24265800
H	-1.56261100	-1.74130500	2.38997900	H	-6.19708100	-2.32071200	0.61918400
H	0.06954100	-2.41029400	2.54730200	H	-5.45829000	-1.26257800	1.83326300
H	1.27962300	-3.32422700	0.76248200	C	-4.19523300	-2.07748500	-1.28089100
H	1.38279300	-4.14590500	-1.55181300	H	-4.46538000	-1.16279600	-1.81197500
H	-0.47902400	-3.63397000	-3.12182500	H	-3.25782800	-2.46365200	-1.68435600
H	-2.44533800	-2.37479500	-2.32442800	H	-4.96852400	-2.82109200	-1.48484900
H	-3.34867300	-2.71446600	2.55218300	C	4.53365800	-1.54990100	0.90584900
H	-2.89718200	-3.89091800	1.29662000	H	5.58955900	-1.71775500	0.67712100
H	-4.55625800	-3.81071100	1.89299300	H	4.24724800	-0.56043900	0.54439400
H	-4.05301600	-3.73912900	-0.99875200	H	4.39968000	-1.57312300	1.98627900
H	-4.92243400	-2.26019000	-1.44679000	C	3.89839900	-2.58958700	-1.27929700
H	-5.64616400	-3.41003900	-0.30963800	H	3.24152100	-3.28097400	-1.81051900
H	-5.94287400	-1.71430700	1.53484400	H	3.76385400	-1.58462200	-1.68252700
H	-5.39853200	-0.48884300	0.37374100	H	4.92911000	-2.88718500	-1.48330500
H	-4.60320400	-0.62609000	1.94849300	C	4.04273800	-4.02140100	0.76962900
H	-0.56991900	0.80331700	-1.61596300	H	3.49471800	-4.80669400	0.24376200
H	2.05731100	-0.89897300	-2.52289400	H	5.11055900	-4.20094900	0.62151900
H	-2.57996000	0.12108100	-0.95155700	H	3.82388400	-4.09118800	1.83469800
Cl	0.21120100	-0.05608200	-3.12692100	Br	-0.00294600	-0.00214700	2.01926300
<b>[L(HBr)], 24Br, E<sub>0</sub>=-4305.612844 au</b>				<b>[L(HBr)], 25Br, E<sub>0</sub>=-4305.611499 au</b>			
N	-0.06699800	0.16526000	-1.30458100	N	-0.49473700	0.37666900	1.65171900
C	1.05354600	-0.73644100	-1.82031100	C	0.78595500	1.11019300	2.02445500
H	1.96330600	-0.16896100	-1.66800700	H	1.57555400	0.41131500	1.78780100
H	0.86517700	-0.85706100	-2.88874500	H	0.73696400	1.25141100	3.10604200
C	0.20706000	1.58759100	-1.72267100	C	-0.56998000	-0.91894800	2.44636900
H	-0.63376800	2.17320900	-1.37772100	H	-1.50938300	-1.38481000	2.16198100
H	0.20094100	1.59221900	-2.81371000	H	-0.59231400	-0.62458800	3.49709700
C	-1.43234900	-0.34287600	-1.77785100	C	-1.72074500	1.22558700	1.87896300
H	-1.60914900	-1.22764900	-1.17635300	H	-1.52432500	2.16238800	1.37760000

H	-1.29782300	-0.61142900	-2.82666600	H	-1.76702300	1.40760900	2.95455900
C	1.16709700	-2.04592700	-1.10001900	C	1.00347800	2.41268700	1.31271000
C	0.28932400	-3.10036800	-1.36699500	C	0.42203500	3.59094100	1.79856700
C	2.14301900	-2.19926400	-0.10229500	C	1.80486900	2.46765500	0.15971500
C	0.31590700	-4.25808700	-0.60280000	C	0.54380700	4.78975900	1.10968800
H	-0.43392500	-3.00591400	-2.16886500	H	-0.14142000	3.56193200	2.72510100
C	2.13421900	-3.34622300	0.69177600	C	1.88030100	3.66858300	-0.55726700
C	1.22282400	-4.36371200	0.44946700	C	1.25064800	4.81422300	-0.09215900
H	-0.38247200	-5.06041100	-0.80755700	H	0.08113500	5.68987400	1.49569600
H	2.82163200	-3.40669800	1.52239600	H	2.43275700	3.67551800	-1.48508200
H	1.21944000	-5.24313300	1.08238000	H	1.32798900	5.73531600	-0.65809500
C	-2.56799300	0.63273600	-1.61144300	C	-3.00134100	0.61037300	1.39198700
C	-2.73460200	1.69952900	-2.50646400	C	-3.90072000	0.06338700	2.31183300
C	-3.47904800	0.49478400	-0.54980000	C	-3.31504100	0.59114000	0.02347200
C	-3.68976700	2.68151200	-2.28665500	C	-5.08876500	-0.52091800	1.89024100
H	-2.09160500	1.77037700	-3.37662600	H	-3.65872400	0.09112700	3.36918900
C	-4.40098700	1.51926000	-0.29821700	C	-4.49908600	-0.02059800	-0.39527600
C	-4.49844900	2.60859100	-1.15109200	C	-5.38010900	-0.56793100	0.52850200
H	-3.79470000	3.50397200	-2.98378900	H	-5.77369100	-0.94564600	2.61396500
H	-5.03147300	1.43716700	0.57562600	H	-4.69711100	-0.09309300	-1.45442000
H	-5.22446500	3.38799000	-0.95023400	H	-6.29425400	-1.03752300	0.18450400
C	1.50412900	2.15407700	-1.21844200	C	0.57655700	-1.83847700	2.15445500
C	2.47778100	2.55931700	-2.13519800	C	1.65882400	-1.95176900	3.02815600
C	1.74124500	2.31671800	0.15352600	C	0.55536400	-2.58584100	0.96377300
C	3.68179600	3.10385900	-1.70446200	C	2.72412800	-2.79226100	2.72316400
H	2.28914300	2.43866200	-3.19673300	H	1.66566900	-1.38111800	3.95081500
C	2.97637800	2.80753600	0.58252400	C	1.64212300	-3.40377500	0.65029000
C	3.93467800	3.21040000	-0.33913900	C	2.71527000	-3.50911900	1.52925200
H	4.42682400	3.41537700	-2.42644600	H	3.56183500	-2.87612800	3.40484400
H	3.17813100	2.85688900	1.64241500	H	1.66934500	-3.91806200	-0.29742100
H	4.88496100	3.59734900	0.00912200	H	3.55775500	-4.13766800	1.26713000
N	3.09889100	-1.14003800	0.08272800	N	2.51365100	1.29883100	-0.25208700
N	0.70671800	1.92202000	1.06453100	N	-0.59794000	-2.39918900	0.14476500
N	-3.42578300	-0.68617100	0.23679000	N	-2.34806000	1.11354600	-0.90355500
O	3.26631600	-0.90307600	1.48979100	O	2.52596700	1.30599100	-1.68205200
H	2.70639900	-0.12252400	1.64991300	H	2.30412900	0.37780400	-1.93632100
O	-3.55926700	-0.32992600	1.61206200	O	-2.26555600	0.19055500	-2.00370800
H	-2.66188900	-0.56412400	1.94906700	H	-1.53585000	-0.39182700	-1.71582900
O	1.34140700	1.18469600	2.12721800	O	-0.37705800	-1.25377700	-0.69813500
H	0.73938100	0.39321300	2.21177400	H	0.43209800	-1.43153000	-1.28756600
C	4.46534500	-1.39701500	-0.48928400	C	3.95582900	1.21632900	0.22407600
C	-4.40476100	-1.77523800	-0.08229000	C	-2.61746600	2.46479900	-1.50841200
C	-0.10045300	3.04466500	1.68212000	C	-1.30640400	-3.52412400	-0.52725100
C	-3.97961300	-2.99297800	0.74700500	H	-0.44893000	0.11063400	0.64455900
H	-4.60507800	-3.85360600	0.49506600	C	4.02049100	1.32331300	1.75306900
H	-2.93298800	-3.23572800	0.55412200	H	3.53635900	0.47382900	2.23868100
H	-4.08268700	-2.78647800	1.81155500	H	5.07030800	1.30939700	2.05341800
C	-5.84717100	-1.37039500	0.26292500	H	3.58416200	2.25221400	2.12573000
H	-6.20249800	-0.56492900	-0.38428100	C	4.47164900	-0.16224600	-0.19849900
H	-6.51621900	-2.22484400	0.13253600	H	3.82751800	-0.94931100	0.19690400
H	-5.90389200	-1.04210000	1.30102100	H	4.48580900	-0.26544200	-1.28187000
C	-4.30791800	-2.11757400	-1.57399300	H	5.48677400	-0.30719900	0.18148300
H	-4.56199900	-1.26657100	-2.20879600	C	4.81744200	2.32451100	-0.39972600
H	-3.30817800	-2.46980500	-1.83685300	H	5.86719500	2.15817200	-0.14596300
H	-5.01112900	-2.92270900	-1.79698300	H	4.71690900	2.31084300	-1.48431600
C	-1.18097500	2.39819300	2.55478300	H	4.53537000	3.31234900	-0.02744300
H	-1.83764300	3.17744000	2.95013700	C	-0.67462200	-4.01001800	-1.83893300
H	-1.78133400	1.69499100	1.97866400	H	0.30606100	-4.46049700	-1.69182700
H	-0.74237000	1.86001300	3.39405600	H	-1.32585900	-4.76343900	-2.29057900
C	-0.78459900	3.83711200	0.56186100	H	-0.55057400	-3.19285900	-2.54815100
H	-0.06919500	4.23300400	-0.16254200	C	-1.38565100	-4.66848700	0.49434600
H	-1.53233700	3.23061300	0.04744900	H	-0.41360400	-5.12476800	0.68246900
H	-1.30835600	4.68664600	1.00485000	H	-1.79029000	-4.31323400	1.44563600
C	0.76856200	3.98263700	2.53260600	H	-2.05270700	-5.44118900	0.10740100
H	0.12644700	4.68366800	3.07101600	C	-2.73166100	-3.02272400	-0.80660700
H	1.33674300	3.40830400	3.26494400	H	-3.33267700	-3.83037800	-1.23168800

H	1.45890600	4.56615400	1.92009500	H	-3.20342000	-2.68158600	0.11669500
C	5.19480900	-2.55065500	0.21924400	H	-2.73201400	-2.19370400	-1.51142400
H	4.71113900	-3.50998500	0.02810400	C	-1.37937000	2.81499200	-2.34161700
H	6.22235200	-2.61458900	-0.14771300	H	-1.46009300	3.83934000	-2.71452000
H	5.22305200	-2.37646200	1.29509000	H	-0.47657700	2.73424100	-1.73539800
C	5.26245100	-0.09977100	-0.32830300	H	-1.28008600	2.13931600	-3.18950300
H	6.25881600	-0.21629600	-0.76261400	C	-3.87337600	2.45958700	-2.39548800
H	4.75232600	0.71964000	-0.83324800	H	-4.78253600	2.32349100	-1.80534300
H	5.36722600	0.15663500	0.72516900	H	-3.95427300	3.41683000	-2.91607900
C	4.32241400	-1.71766000	-1.98229500	H	-3.81024400	1.66807200	-3.14188400
H	3.73534500	-2.62144900	-2.15182600	C	-2.78980800	3.49720300	-0.38958400
H	3.86054300	-0.88876900	-2.52382500	H	-3.57570100	3.21330500	0.31445200
H	5.31639100	-1.87720100	-2.40587800	H	-1.85601700	3.66347500	0.14805100
H	-0.07962100	0.11652100	-0.25963600	H	-3.07741400	4.45105900	-0.83658500
Br	-0.55224800	-1.23279000	1.85723800	Br	2.02029800	-1.72441600	-2.56733700
<b>[L(HBr)], 26Br, E<sub>0</sub>=-4305.613195 au</b>				<b>[L(HBr)], 27Br, E<sub>0</sub>=-4305.601638 au</b>			
O	-3.24437000	-0.82743200	-0.86868100	N	1.02016100	0.15427300	1.79474300
H	-2.78107400	0.03916200	-0.85548400	C	1.31030300	-1.16692600	2.40124300
O	-2.75801700	1.89299200	-2.56836600	H	0.35354500	-1.66663700	2.54986900
H	-2.92231400	0.96030100	-2.75313600	H	1.79337100	-1.03355400	3.38153900
O	4.11024800	-0.71539900	1.02639400	C	-0.00267700	0.89263100	2.56688800
H	3.59778000	-0.35711100	1.79042200	H	-0.04489000	1.88911700	2.14443000
N	-2.24904300	-1.78051400	-0.41779300	H	0.32535100	0.98652100	3.61473500
N	-2.47284700	1.89392000	-1.14911000	C	2.27315700	0.94607000	1.70935200
N	3.39959300	-0.17860700	-0.09700900	H	3.02073200	0.29281900	1.27398000
N	0.50251800	-0.18167800	0.36112500	H	2.60267000	1.21487000	2.72562100
H	1.40881700	0.13796000	0.77000200	C	2.17281200	-2.03836300	1.52323400
C	0.25526600	-1.55267400	1.01301500	C	3.49190500	-2.31655800	1.87578200
H	0.36547000	-2.28475500	0.22325500	C	1.63623900	-2.60865600	0.34901500
H	1.06769800	-1.66924000	1.72606900	C	4.28325500	-3.16119600	1.10154600
C	-1.06290100	-1.68027700	1.72292800	H	3.89661500	-1.87807300	2.78167900
C	-1.07137800	-1.62327300	3.11948900	C	2.44691800	-3.42966000	-0.43771100
H	-0.12941200	-1.49175500	3.63894200	C	3.75400100	-3.71941300	-0.05588100
C	-2.26761500	-1.65981100	3.82625100	H	5.30270400	-3.37641400	1.39845200
H	-2.25738100	-1.60235800	4.90788000	H	2.06562000	-3.84335500	-1.35806100
C	-3.47425000	-1.72862900	3.13472900	H	4.36232600	-4.36411100	-0.67930500
H	-4.41398300	-1.72599100	3.67491100	C	2.14130000	2.19328400	0.87223200
C	-3.47983500	-1.78837600	1.74550800	C	1.88432700	3.42613800	1.48024800
H	-4.41435200	-1.79578800	1.20445600	C	2.25552100	2.13982700	-0.52596000
C	-2.27975600	-1.79329000	1.03078400	C	1.68703000	4.57731900	0.72591100
C	-2.56348000	-3.07912600	-1.10172200	H	1.83093200	3.47689700	2.56268600
C	-2.49454600	-2.82366700	-2.61292200	C	2.00472800	3.28738700	-1.28349200
H	-1.57360100	-2.30255500	-2.87621000	C	1.72433500	4.49938100	-0.66402200
H	-3.33618400	-2.21627300	-2.94327500	H	1.48600800	5.52192300	1.21732400
H	-2.51889000	-3.77387200	-3.15106300	H	2.01196300	3.21224800	-2.36112600
C	-1.48952300	-4.09243200	-0.69053500	H	1.53589200	5.38109100	-1.26546600
H	-0.49817500	-3.78491200	-1.02465500	C	-1.37803800	0.26955400	2.53670800
H	-1.71402200	-5.05713900	-1.15046700	C	-1.79624300	-0.52470300	3.60873300
H	-1.46934000	-4.23618000	0.39133300	C	-2.26116500	0.46706500	1.46157800
C	-3.95558100	-3.63339600	-0.75350400	C	-3.03836400	-1.14867700	3.61021700
H	-4.16750100	-4.49853300	-1.38645500	H	-1.12553500	-0.66027900	4.45047200
H	-4.72675700	-2.88353200	-0.93533400	C	-3.50235500	-0.17486100	1.45831900
H	-4.01264800	-3.95945000	0.28570500	C	-3.88931500	-0.98060800	2.52157600
C	-0.51632800	0.86566000	0.77003500	H	-3.33516600	-1.76745700	4.44879400
H	-0.36761200	0.99038400	1.84165100	H	-4.15567100	-0.06633000	0.60511500
H	-1.49418600	0.45425600	0.58619600	H	-4.85368000	-1.47416100	2.49721700
C	-0.31725100	2.15210300	0.02727300	N	0.26756000	-2.30776300	0.08321600
C	0.82636300	2.91219700	0.29727100	N	-1.81577700	1.28396600	0.36021700
H	1.47219500	2.59263800	1.10876400	N	2.61691700	0.88617500	-1.12607900
C	1.13375600	4.02940700	-0.46643100	O	0.18387000	-0.96796500	-0.49122600
H	2.02842700	4.60104900	-0.25180900	H	0.43942200	-0.38666500	0.29814700
C	0.30085700	4.38826600	-1.52498700	O	1.68776200	0.61109300	-2.19124500
H	0.54843100	5.23697300	-2.15174700	H	1.17249500	-0.11979000	-1.80328200
C	-0.86654500	3.67537500	-1.76706400	O	-2.05415600	0.56167000	-0.87295100
H	-1.52159800	3.95610700	-2.57837600	H	-1.27354600	-0.02915800	-0.92426600
C	-1.20648900	2.57736800	-0.97107400	C	-0.63911600	-3.22795400	-0.64700800



C	-3.64508300	2.56668000	-0.43696200	C	4.00759400	0.78311700	-1.67502000
C	-3.79996100	4.03989600	-0.83517800	C	-2.42226200	2.64489600	0.20619600
H	-3.89608600	4.13936600	-1.91748100	C	4.20086000	-0.67663500	-2.09688000
H	-2.95976300	4.64628300	-0.49582600	H	5.22764900	-0.83670400	-2.43606100
H	-4.70805700	4.43851800	-0.37748600	H	4.00159100	-1.33899300	-1.25594500
C	-4.92375700	1.80548800	-0.81052400	H	3.52253600	-0.93452600	-2.91011500
H	-4.84956700	0.74767000	-0.55825300	C	4.25420700	1.70881100	-2.87855000
H	-5.14004000	1.90344500	-1.87404800	H	4.27191200	2.75967800	-2.58491500
H	-5.76158100	2.23084800	-0.25411700	H	5.22182700	1.47370500	-3.32924700
C	-3.40444600	2.44447400	1.07186900	H	3.47997500	1.56152400	-3.63262900
H	-2.49403500	2.95718800	1.38482800	C	4.99499200	1.11820000	-0.55054300
H	-3.35184800	1.40031800	1.38568900	H	4.85563600	2.13382100	-0.17583200
H	-4.24156200	2.90740000	1.59831900	H	4.89724400	0.41789000	0.28126300
C	0.69380200	-0.27907000	-1.13303000	H	6.01371400	1.03907200	-0.93668900
C	0.94832200	0.71871000	-1.47508300	C	-1.74490700	3.29587700	-1.00441700
H	-0.27147400	-0.56363100	-1.54689700	H	-2.02410100	4.35119400	-1.05844500
C	1.74296800	-1.29662600	-1.50183800	H	-0.66253900	3.22336500	-0.91119200
C	1.40403000	-2.32767800	-2.38297500	H	-2.04501100	2.80873900	-1.93120000
H	0.42376800	-2.32655700	-2.84068800	C	-2.08359400	3.44487800	1.47037700
C	2.28945300	-3.36229200	-2.65908800	H	-2.45223400	2.95290900	2.37290000
H	2.00376900	-4.15289300	-3.34250700	H	-1.00850600	3.60318800	1.55757500
C	3.52462000	-3.39342000	-2.01625800	H	-2.56201900	4.42431000	1.40509400
H	4.20800100	-4.21716400	-2.18640500	C	-3.94745000	2.62590500	0.00986000
C	3.88802000	-2.36140100	-1.16053200	H	-4.29478000	3.64402000	-0.18252500
H	4.83478100	-2.38046400	-0.64157600	H	-4.23598800	2.01320000	-0.84436200
C	3.02756200	-1.28305100	-0.93621700	H	-4.46624700	2.26067000	0.89777000
C	4.28153900	0.86078500	-0.75425200	C	-0.50044700	-3.14808900	-2.17754800
C	3.53973100	1.44851600	-1.95882800	H	0.49658100	-3.42163500	-2.52458900
H	2.62788600	1.96090500	-1.65218900	H	-1.21808000	-3.82502600	-2.64663800
H	3.29421300	0.68413500	-2.69897100	H	-0.71475100	-2.13959400	-2.53225500
H	4.18314000	2.18506800	-2.44513400	C	-2.06873600	-2.83840400	-0.24238900
C	5.62762500	0.27518800	-1.20766800	H	-2.79159900	-3.49509600	-0.73122900
H	5.50884300	-0.42286100	-2.03864600	H	-2.18746400	-2.91779100	0.83917900
H	6.11505800	-0.23602600	-0.37704500	H	-2.30262400	-1.81958900	-0.52943900
H	6.28062300	1.08484200	-1.54263000	C	-0.39600500	-4.65664500	-0.13347500
C	4.52668400	1.95638000	0.28829900	H	0.52968500	-5.09807300	-0.49770900
H	5.12246600	1.57672500	1.11674700	H	-0.37414400	-4.66845300	0.95863200
H	3.58587800	2.31987200	0.69807300	H	-1.22319500	-5.28788400	-0.46338400
H	5.06102800	2.78975400	-0.17505300	H	-3.43874800	-0.04054500	-1.65861100
Br	2.07773400	0.62200800	3.09641100	Br	-4.57731900	-0.59788000	-2.40388400
<b>[L(HBr)], 28Br, E<sub>0</sub>=-4305.604794 au</b>				<b>[L(HBr)], 29Br, E<sub>0</sub>=-4305.604688 au</b>			
N	-1.06523200	0.13606100	1.71150400	O	1.60720400	0.00815400	-1.71780000
C	-0.23219900	-0.76651800	2.60138400	O	-3.13261400	1.40634000	-2.46667400
H	-0.44971000	-1.77768400	2.28060200	O	2.01721100	2.63624900	-0.88434100
H	-0.60916300	-0.61952300	3.61514200	N	2.49038000	-1.13335200	-1.85091300
C	-2.50851000	-0.31030300	1.67868500	N	-2.48029300	0.20355600	-2.00536100
H	-3.03571600	0.43531500	1.09867300	N	1.42410900	2.53718600	0.43155500
H	-2.86226600	-0.26219300	2.70986700	N	-0.11735700	-0.50895200	1.31418900
C	-0.94725900	1.58475000	2.15243700	C	1.37605000	-0.69937000	1.07831100
H	0.11519400	1.78222000	2.21639800	C	1.67225600	-2.01942800	0.40249000
H	-1.38706700	1.62819400	3.15030400	C	1.42935800	-3.17546500	1.15821700
C	1.22680100	-0.44071700	2.50868000	C	1.57263100	-4.44783500	0.62129500
C	1.86243500	0.22982100	3.55763400	C	1.94734800	-4.59185300	-0.71025000
C	1.94294700	-0.75774100	1.34492700	C	2.19796100	-3.46031900	-1.47406600
C	3.19492800	0.60923400	3.44785300	C	2.10376300	-2.17244000	-0.93325500
H	1.30405700	0.46141800	4.45880300	C	3.91860200	-0.66711800	-1.80307200
C	3.26817800	-0.33313500	1.22209800	C	4.30294200	-0.05258800	-0.45096000
C	3.88709800	0.34066900	2.26946900	C	4.81445300	-1.88049800	-2.08699700
H	3.68270200	1.12507000	4.26628300	C	4.10289000	0.35594800	-2.93141000
H	3.80088800	-0.49884000	0.29161800	C	-0.90834200	-0.83425700	0.08657800
H	4.91554000	0.66215300	2.15552200	C	-2.40128400	-0.77962600	0.23433600
C	-1.63662600	2.52338500	1.20824200	C	-3.04709600	-1.22677400	1.39061500
C	-2.91314800	3.01304500	1.50272500	C	-4.42524100	-1.10289400	1.52190900
C	-1.02127800	2.87073700	-0.00307200	C	-5.17401300	-0.53666100	0.49150700
C	-3.60159300	3.79751500	0.58572800	C	-4.54735300	-0.12471100	-0.67773600
H	-3.37353000	2.76225700	2.45263900	C	-3.16465600	-0.26001100	-0.82526300

C	-1.74177900	3.61312400	-0.94278600	C	-2.43060000	-0.72862200	-3.18103300
C	-3.02021300	4.07271800	-0.65080800	C	-3.82903400	-1.01084900	-3.75398100
H	-4.59034800	4.17095900	0.82246300	C	-1.55468700	-0.05347100	-4.24314000
H	-1.29439000	3.81210900	-1.90514100	C	-1.77614200	-2.04527900	-2.74914600
H	-3.56265400	4.65231500	-1.38838500	C	-0.42220600	0.83096300	1.96876800
C	-2.68012400	-1.69507000	1.12671100	C	-0.87402200	1.94371400	1.05620500
C	-3.03655100	-2.72876000	1.99958900	C	-2.24489800	2.22301400	0.99772600
C	-2.45184900	-1.98201900	-0.22889800	C	-2.75109600	3.20863500	0.16120200
C	-3.14437300	-4.03981000	1.55574200	C	-1.88005000	3.92051400	-0.66266200
H	-3.21420300	-2.49745400	3.04462800	C	-0.51241600	3.67999200	-0.59607300
C	-2.53313800	-3.30947600	-0.66050300	C	0.00437000	2.73195100	0.29295700
C	-2.87685700	-4.32717100	0.21920100	C	2.14093400	3.54353300	1.29731700
H	-3.41443200	-4.82919100	2.24628100	C	1.49067700	3.56919500	2.68494300
H	-2.29855700	-3.53044800	-1.69064200	C	2.11308800	4.95855800	0.69538700
H	-2.93399800	-5.34784600	-0.14015900	C	3.59012100	3.06405900	1.43164600
N	1.24645100	-1.50076100	0.32484800	H	-0.34513200	-1.18866500	2.11472000
N	-2.06831500	-0.91562000	-1.12195900	H	1.72291500	0.17023000	0.54179500
N	0.32074900	2.41487800	-0.22595200	H	1.80393600	-0.69735000	2.08173300
O	1.27917100	-0.77179400	-0.91395700	H	1.09159900	-3.06213300	2.18423000
H	2.20813800	-0.77177100	-1.35548600	H	1.37171200	-5.31500600	1.23839500
O	0.36616100	1.85820000	-1.54869100	H	2.03327600	-5.57490100	-1.15809300
H	0.73913600	0.97210200	-1.38630600	H	2.47387600	-3.54851600	-2.51619600
O	-1.11918800	-1.46120200	-2.05011000	H	4.19389300	-0.77852000	0.35739400
H	-0.24737100	-1.15931200	-1.71646800	H	3.70044700	0.82452600	-0.22820900
C	1.68077100	-2.95321800	0.17991500	H	5.34782400	0.26598400	-0.47373600
C	1.39238000	3.47845700	-0.11820100	H	4.74225200	-2.63369800	-1.30246000
C	-3.18704800	-0.34897700	-1.97758100	H	5.85168100	-1.54306100	-2.13680100
C	2.73395700	2.77519100	-0.32895900	H	4.55767900	-2.34319900	-3.04167600
H	3.54854900	3.49148300	-0.19621500	H	3.75902700	-0.06199700	-3.88054100
H	2.85753500	1.97642500	0.39826900	H	5.16142000	0.60570400	-3.02848100
H	2.82009300	2.34032400	-1.32364700	H	3.56222700	1.28192400	-2.73735300
C	1.22498900	4.59535000	-1.15928600	H	-0.59298700	-1.83439500	-0.20025000
H	0.35221800	5.22027600	-0.95943400	H	-0.59694700	-0.14976800	-0.69557300
H	2.10595600	5.24081800	-1.13809800	H	-2.46932100	-1.64365100	2.21031300
H	1.14435400	4.16767000	-2.15926900	H	-4.90685200	-1.43760200	2.43272900
C	1.34065600	4.06523000	1.29732300	H	-6.24707100	-0.42287100	0.59494500
H	0.37416600	4.52249200	1.52137900	H	-5.11240400	0.33834400	-1.47377500
H	1.56222100	3.30327200	2.04835100	H	-4.33536600	-0.07940600	-4.00827800
H	2.10306000	4.84190000	1.38537300	H	-4.44248000	-1.56230700	-3.03915000
C	-2.55176400	0.69035900	-2.90704100	H	-3.74270000	-1.61495800	-4.66040600
H	-3.34002700	1.27093600	-3.39365400	H	-1.39228800	-0.72946400	-5.08544800
H	-1.90499900	1.36220900	-2.34730400	H	-0.58093200	0.21020700	-3.81874000
H	-1.94859700	0.20775800	-3.67375100	H	-2.01872500	0.86103700	-4.60902900
C	-4.21615600	0.33714000	-1.07637300	H	-0.74539600	-1.89664100	-2.42487300
H	-4.63707000	-0.34759000	-0.33604200	H	-1.76039900	-2.72608400	-3.60253100
H	-3.78802500	1.20714400	-0.57781900	H	-2.33209700	-2.53170600	-1.94618900
H	-5.04220400	0.69228500	-1.69587400	H	0.47182500	1.08395400	2.52558000
C	-3.87778600	-1.43655600	-2.81473300	H	-1.19807700	0.61218900	2.69959800
H	-4.57980400	-0.96420200	-3.50597300	H	-2.92416300	1.63694900	1.60319600
H	-3.14436400	-1.98829100	-3.40311900	H	-3.81713100	3.39398800	0.12859400
H	-4.43964500	-2.13776700	-2.19405700	H	-2.26111800	4.67742300	-1.33931300
C	3.20040300	-3.18091300	0.23412600	H	0.17413500	4.22084800	-1.23029400
H	3.62180500	-2.91770900	1.20586900	H	1.60118600	2.61483500	3.20162500
H	3.39415600	-4.24378400	0.06755000	H	0.43206400	3.82852000	2.63896400
H	3.71684900	-2.62039600	-0.54696500	H	1.99279800	4.32717500	3.28927800
C	1.15431700	-3.49864000	-1.14956400	H	1.10439500	5.37500500	0.69487700
H	1.34354000	-4.57426300	-1.17757900	H	2.49539600	4.95182100	-0.32533000
H	0.08652700	-3.32946900	-1.25569000	H	2.74491600	5.61827900	1.29459000
H	1.67040300	-3.04178600	-1.99402400	H	4.13386300	3.71954300	2.11568600
C	1.00797100	-3.70202200	1.33944000	H	4.09498500	3.07667000	0.46652600
H	1.32723200	-3.31004400	2.30896800	H	3.62042000	2.04839800	1.83125400
H	-0.07968800	-3.64411600	1.26262800	H	1.11280300	-0.00205500	-2.54577700
H	1.29427100	-4.75545400	1.30551900	H	-2.59542000	2.09946500	-2.06192600
H	-0.69983100	0.05215400	0.75012000	H	1.97789200	1.71586000	-1.19834100
Br	3.94019600	-0.50999300	-2.35439400	Br	-0.48776000	-1.97817100	4.02550800
<b>[L(HBr)], 30Br, E<sub>0</sub>=-4305.604259 au</b>				<b>[L(HBr)], 31Br, E<sub>0</sub>=-4305.602658 au</b>			

O	-2.73688800	-0.58450600	0.15911800	N	0.08264800	-0.14425400	0.97616600
H	-2.48416100	-0.32660700	-0.76451100	C	0.62418100	1.22556200	1.34158200
O	-1.24801000	3.31777300	-1.43453700	H	1.60942700	1.27461900	0.89471400
H	-1.38466800	2.51013900	-1.97865300	H	0.69673100	1.22320600	2.43333900
O	3.73494200	-2.48247400	0.72902800	C	1.00262500	-1.22104900	1.51066700
H	2.85203500	-2.83132000	0.89668800	H	0.54731200	-2.16338700	1.23594200
N	-2.65066200	-2.01636700	0.18984900	H	0.97754700	-1.10634000	2.59733500
N	-1.35061200	2.79301900	-0.10672400	C	-1.33633400	-0.35159000	1.48170600
N	3.49197200	-1.11690400	0.29494400	H	-1.89380000	0.51320300	1.15077100
N	0.84175800	-0.17980700	0.38827800	H	-1.26099100	-0.35051600	2.57234700
H	1.71477700	-0.42920000	0.88215200	C	-0.26482700	2.32911700	0.85571900
C	0.15252100	-1.48386600	0.03213700	C	-1.15454100	2.92860800	1.75299700
H	-0.57290900	-1.25884600	-0.74390500	C	-0.23051400	2.76219200	-0.47669800
H	0.92235600	-2.11434100	-0.41090300	C	-2.02804100	3.92180600	1.32418400
C	-0.45980200	-2.15052800	1.23012500	H	-1.15454800	2.58935400	2.78443500
C	0.36734700	-2.55015900	2.27952200	C	-1.12684800	3.74391100	-0.90545000
H	1.43309000	-2.34050800	2.22986000	C	-2.02453500	4.31781500	-0.01119700
C	-0.13507500	-3.20441000	3.39894900	H	-2.71522600	4.37732200	2.02680100
H	0.52612800	-3.50934400	4.20054500	H	-1.14076400	4.06087900	-1.93978900
C	-1.49986100	-3.45940100	3.46280800	H	-2.71740300	5.07504700	-0.35847300
H	-1.92098600	-3.96081600	4.32643100	C	-1.91324700	-1.61894000	0.92670400
C	-2.34171900	-3.05518800	2.43201800	C	-1.91724200	-2.78203700	1.70334200
H	-3.39864900	-3.23938600	2.52597000	C	-2.39998500	-1.66578400	-0.38834900
C	-1.85022800	-2.40337200	1.29207500	C	-2.34162600	-3.99161500	1.16548600
C	-3.97472000	-2.62287400	-0.12585800	H	-1.56559300	-2.72640000	2.72759900
C	-4.31412000	-2.17392900	-1.55875400	C	-2.78018500	-2.89226800	-0.93815100
H	-3.49661800	-2.41123200	-2.24047300	C	-2.74638400	-4.04863100	-0.16696400
H	-4.48713300	-1.09987500	-1.61230500	H	-2.33555200	-4.88743300	1.77453700
H	-5.22036500	-2.68376400	-1.89419200	H	-3.08506200	-2.93507800	-1.97370000
C	-3.82164100	-4.15053800	-0.13941200	H	-3.04423700	-4.99405500	-0.60512700
H	-2.99173200	-4.43765000	-0.78897700	C	2.39686400	-1.08016300	0.97408900
H	-4.73617500	-4.59374100	-0.53871000	C	3.41310900	-0.73625700	1.87198900
H	-3.64723400	-4.57877200	0.84688500	C	2.70051000	-1.22748000	-0.38900400
C	-5.10525300	-2.15456800	0.80939900	C	4.71371900	-0.52353100	1.43162500
H	-6.07217400	-2.44118300	0.38876900	H	3.15602300	-0.60663000	2.91767200
H	-5.07828600	-1.06788600	0.89641000	C	4.00525300	-0.98603300	-0.82780000
H	-5.04621100	-2.58262400	1.81073900	C	5.00401300	-0.63812200	0.07410100
C	-0.04797500	0.69424300	1.27041800	H	5.48770400	-0.25073600	2.13869100
H	-0.07743900	0.20078300	2.23963900	H	4.21989800	-1.04992300	-1.88420200
H	-1.03177400	0.65630800	0.82094800	H	6.00991700	-0.45572000	-0.28625200
C	0.45725800	2.10113100	1.36316200	N	0.75919700	2.15965300	-1.33848500
C	1.57814300	2.40572100	2.14081900	N	1.63642400	-1.55590700	-1.31664400
H	2.00937100	1.63773100	2.77441800	N	-2.46942400	-0.42665100	-1.12052800
C	2.15520400	3.66899500	2.09611200	O	0.11805600	1.51540300	-2.46119300
H	3.02633400	3.89261700	2.70020300	H	-0.24155000	2.19679200	-3.05086800
C	1.61642700	4.63607900	1.24745100	O	-1.91828000	-0.65267500	-2.43638800
H	2.07816800	5.61433300	1.17849100	H	-1.19617700	-0.00767900	-2.46043200
C	0.47348700	4.36052500	0.50641600	O	1.89066700	-0.81947400	-2.53477800
H	0.05128700	5.10267500	-0.15574800	H	1.23558900	-0.10808200	-2.51943600
C	-0.14535700	3.10869100	0.59082800	C	1.89047200	3.04147000	-1.79489400
C	-2.62870600	3.27535300	0.52509500	C	-3.85115000	0.15274100	-1.28514500
C	-2.70138200	4.80924900	0.58473100	C	1.55862400	-3.01302500	-1.73060200
H	-2.53765000	5.23081500	-0.40810200	C	-3.68930800	1.47750600	-2.03738300
H	-1.96239900	5.22293600	1.27453200	H	-4.64834400	1.99907100	-2.07895300
H	-3.69037800	5.11948700	0.93096900	H	-2.97098000	2.11421400	-1.52335100
C	-3.78171800	2.73118800	-0.32542000	H	-3.34924900	1.30517800	-3.05909500
H	-3.74362200	1.64340300	-0.37193100	C	-4.80049300	-0.76892000	-2.06660600
H	-3.73374700	3.12130200	-1.34107000	H	-5.05607300	-1.66430700	-1.49851400
H	-4.73469900	3.03071100	0.11875100	H	-5.72945800	-0.23506700	-2.28123000
C	-2.72380500	2.68272800	1.93664200	H	-4.35033800	-1.06382900	-3.01576300
H	-1.90634300	3.01799700	2.57857800	C	-4.42128500	0.43293900	0.11011400
H	-2.73187400	1.59191000	1.90014600	H	-4.48438200	-0.47309600	0.71466400
H	-3.66028900	3.00961100	2.39423500	H	-3.82180600	1.17306200	0.64317400
C	1.33180300	0.51442700	-0.85995100	H	-5.43129400	0.83506100	0.00591200
H	1.83370500	1.42106200	-0.53257200	C	0.42340600	-3.13111200	-2.75265600
H	0.44759700	0.78686600	-1.43746800	H	0.21543700	-4.18724100	-2.94167900

C	2.24061000	-0.36343000	-1.68275000	H	-0.48232300	-2.65609400	-2.38100300
C	2.00520500	-0.41363700	-3.05985500	H	0.69708900	-2.65861000	-3.69520700
H	1.16329700	0.13732900	-3.46208200	C	1.22028200	-3.86121400	-0.50235000
C	2.79010600	-1.20552600	-3.88953200	H	1.95841400	-3.74400800	0.29341000
H	2.58444700	-1.23753000	-4.95251300	H	0.22702400	-3.62642200	-0.12007800
C	3.80453500	-1.98750700	-3.34413700	H	1.21826800	-4.91319500	-0.79527800
H	4.40052800	-2.63209100	-3.97943600	C	2.87214800	-3.50760400	-2.35566100
C	4.04449900	-1.95826100	-1.97559300	H	2.72465400	-4.51803500	-2.74420300
H	4.79509700	-2.59817600	-1.53566600	H	3.16970500	-2.86632800	-3.18616200
C	3.28722300	-1.13120200	-1.14413000	H	3.68251800	-3.54433500	-1.62561100
C	4.66636200	-0.31544200	0.79995200	C	1.44686800	4.20886600	-2.69623500
C	4.52667400	1.11727800	0.27766800	H	0.85701000	4.94777700	-2.15482000
H	3.61878700	1.59698700	0.64165400	H	2.33348600	4.71283900	-3.08563800
H	4.53561300	1.15078200	-0.81274600	H	0.87883400	3.86897200	-3.56910700
H	5.37388700	1.70440900	0.63761100	C	2.89894800	2.16857500	-2.54718900
C	6.01367000	-0.89840700	0.34759800	H	3.77835800	2.76805600	-2.79249900
H	6.14447100	-0.80930800	-0.73154400	H	3.20797800	1.32413000	-1.93540000
H	6.10317600	-1.94675100	0.63205900	H	2.48457700	1.78059900	-3.47826800
H	6.82209800	-0.34288500	0.82828300	C	2.55564800	3.59730600	-0.52894200
C	4.57747100	-0.32691400	2.33026800	H	1.86941800	4.20468500	0.06234600
H	4.71312600	-1.33508700	2.71996700	H	2.94128000	2.79024600	0.09540700
H	3.60562300	0.04595400	2.66208000	H	3.39859700	4.22647200	-0.82125100
H	5.35089800	0.31728800	2.75367200	H	0.08253800	-0.23965400	-0.04613600
Br	-1.69797200	0.34573900	-2.74809400	Br	0.11496000	0.24335100	4.66158800
<b>[L(HBr)], 32Br, E<sub>0</sub>=-4305.599687 au</b>				<b>[L(HBr)], 33Br, E<sub>0</sub>=-4305.601661 au</b>			
N	-0.90496400	-0.02907500	1.77175000	N	-0.07920000	0.27923500	1.04804700
C	-0.82694300	1.41003400	2.24534900	C	1.28660200	0.21286200	1.69598000
H	0.22743100	1.66181700	2.23956100	H	1.66291500	-0.78149000	1.49791200
H	-1.19671400	1.40756000	3.27212100	H	1.11940200	0.32720100	2.76938400
C	-0.01082600	-0.92536500	2.60388000	C	-0.93799400	-0.94430100	1.31226500
H	-0.20180500	-1.93277200	2.25577300	H	-1.84693600	-0.78443500	0.75057500
H	-0.36536600	-0.83409500	3.63191700	H	-1.15602700	-0.90838000	2.38375300
C	-2.33975500	-0.52686200	1.77463100	C	-0.82229600	1.53699100	1.46143500
H	-2.91586600	0.23848900	1.27171300	H	-0.18189000	2.36794100	1.18560800
H	-2.63540600	-0.57728600	2.82381600	H	-0.92186300	1.47308800	2.54822900
C	-1.63183700	2.33301100	1.37864700	C	2.16606100	1.27781900	1.10753100
C	-2.86810800	2.81678400	1.81408200	C	2.43833100	2.42873400	1.85304100
C	-1.15421400	2.68601400	0.10858400	C	2.65999500	1.17380900	-0.20359500
C	-3.64387700	3.62279800	0.98847700	C	3.15785500	3.48275800	1.30198100
H	-3.22510400	2.55559600	2.80479700	H	2.05974400	2.49185900	2.86708900
C	-1.96103700	3.45167500	-0.73455800	C	3.35458700	2.24922900	-0.76195500
C	-3.19342000	3.92352000	-0.29457400	C	3.59961700	3.39650700	-0.01626900
H	-4.59759700	4.00001000	1.33687500	H	3.35713700	4.37005500	1.89051600
H	-1.62279600	3.66134400	-1.73800800	H	3.67931400	2.18523900	-1.78990700
H	-3.80540400	4.52361600	-0.95763500	H	4.14020200	4.22141400	-0.46548000
C	-2.48197600	-1.85649900	1.09660900	C	-2.15741400	1.58251700	0.77810700
C	-2.53224600	-3.03434700	1.84860300	C	-3.32427500	1.43598000	1.53060900
C	-2.51988400	-1.92635100	-0.30405400	C	-2.23567300	1.64737500	-0.62047500
C	-2.55653900	-4.27506400	1.22423800	C	-4.55836200	1.32802600	0.89752400
H	-2.53489700	-2.97454000	2.93174100	H	-3.24311900	1.35915100	2.60930100
C	-2.47022100	-3.17733500	-0.92369500	C	-3.47049100	1.48902800	-1.25289700
C	-2.48989100	-4.34200700	-0.16595800	C	-4.62654500	1.33292800	-0.49424100
H	-2.59304600	-5.18140500	1.81590000	H	-5.45891400	1.20685200	1.48719100
H	-2.40727900	-3.22561400	-2.00053900	H	-3.52318700	1.47160300	-2.33100300
H	-2.45833900	-5.30449900	-0.66234300	H	-5.58092300	1.21089400	-0.99280700
C	1.43922800	-0.55491600	2.50518200	C	-0.26896400	-2.23084400	0.94202600
C	2.07523000	-0.00633400	3.62332400	C	0.32789700	-2.96131700	1.97903800
C	2.15684700	-0.72537300	1.30930900	C	-0.22651400	-2.73421800	-0.36676700
C	3.40537800	0.39008700	3.56210100	C	0.98870000	-4.15569000	1.72733500
H	1.51515100	0.11688500	4.54469400	H	0.26681500	-2.56044100	2.98624700
C	3.48672800	-0.30053400	1.24699000	C	0.45426800	-3.93057600	-0.61273100
C	4.10273000	0.25060900	2.36475100	C	1.05940700	-4.63333300	0.42103500
H	3.88727200	0.81498700	4.43446500	H	1.44889800	-4.70309600	2.54085900
H	4.03227300	-0.36520200	0.31002900	H	0.52834900	-4.28901000	-1.62790400
H	5.13372100	0.57561800	2.29067700	H	1.58369300	-5.55633400	0.20264400
N	0.16275000	2.23742600	-0.23551200	N	2.39640800	-0.04731900	-0.93978600

N	1.46029100	-1.27559500	0.17045000	N	-0.85912400	-2.00524200	-1.46447700
N	-2.60911800	-0.69295400	-1.03638800	N	-0.98199800	1.82553600	-1.32013600
O	0.07294600	1.51905300	-1.48743400	O	2.04715100	0.29840800	-2.31189100
H	0.74079800	0.79482500	-1.34783100	H	1.12111900	0.59885900	-2.26431300
O	-1.65519900	-0.74730500	-2.10895500	O	-0.85129700	0.79288700	-2.35287400
H	-1.11236000	0.04607300	-1.94682900	H	-0.99305800	-0.05649700	-1.87743300
O	1.69311500	-0.45394100	-0.97284400	O	-0.00531500	-2.16027000	-2.62930200
H	2.65076600	-0.47174600	-1.31934700	H	0.64468100	-1.44512600	-2.55188300
C	1.20043200	3.33625000	-0.34614500	C	3.59405300	-0.97349700	-1.03819300
C	-3.97167800	-0.40793300	-1.62640800	C	-0.82119300	3.15710100	-2.00644100
C	1.76273000	-2.72654400	-0.16079000	C	-2.21193900	-2.56924700	-1.88835400
C	-3.86768700	0.93650300	-2.34966300	H	0.08341700	0.35350000	0.04074400
H	-4.85505300	1.23985800	-2.70612700	C	4.83883800	-0.28929400	-1.62736100
H	-3.49209900	1.69907300	-1.67171300	H	5.24435600	0.47391900	-0.96256300
H	-3.19660800	0.86790000	-3.20498900	H	5.61485000	-1.04246900	-1.78122800
C	-4.43633000	-1.48424500	-2.61963600	H	4.61298100	0.16201000	-2.59463900
H	-4.67013800	-2.42829800	-2.12513700	C	3.90021200	-1.48974800	0.37196600
H	-5.34258900	-1.14157600	-3.12466100	H	4.10947100	-0.67803600	1.07070200
H	-3.67051000	-1.65507600	-3.37746700	H	3.07870000	-2.09625400	0.75614200
C	-4.97510700	-0.28613700	-0.47362900	H	4.78843900	-2.12325000	0.32776300
H	-5.03622700	-1.20327300	0.11560800	C	3.21551300	-2.15935600	-1.92837300
H	-4.71938200	0.54757900	0.18435200	H	4.02333800	-2.89413000	-1.90117100
H	-5.96758700	-0.08999100	-0.88477200	H	2.31091200	-2.63966600	-1.56781100
C	1.11574700	-3.01635900	-1.52000900	H	3.06939500	-1.85057200	-2.96274100
H	1.08297500	-4.09803400	-1.67505100	C	-2.13409700	-4.05185200	-2.28352400
H	0.10361300	-2.61732000	-1.56077700	H	-1.90307200	-4.69132800	-1.43138100
H	1.69088000	-2.56815800	-2.32878100	H	-3.10454700	-4.36031900	-2.67830500
C	1.10403700	-3.58934400	0.91957700	H	-1.38759400	-4.20970400	-3.06243900
H	1.49844000	-3.36153000	1.91366500	C	-3.18989700	-2.39596800	-0.72284300
H	0.02167700	-3.46963500	0.91443700	H	-2.85256700	-2.91362500	0.17637500
H	1.32308300	-4.64001000	0.71881900	H	-3.35937700	-1.34334100	-0.49363700
C	3.26246900	-3.05137000	-0.21900800	H	-4.15124800	-2.82691800	-1.00963200
H	3.38042100	-4.08734000	-0.54819500	C	-2.70624300	-1.75871000	-3.09274000
H	3.79283500	-2.41373400	-0.92851900	H	-3.70044600	-2.11353000	-3.37286100
H	3.73482700	-2.95901800	0.76161200	H	-2.77935700	-0.69847800	-2.85794500
C	0.95627200	4.28428400	-1.53020600	H	-2.03972700	-1.87838000	-3.94500200
H	0.11256400	4.95536600	-1.35969900	C	0.55078600	3.18330000	-2.68401100
H	1.84298800	4.90380200	-1.68022600	H	0.73432200	4.18518500	-3.07817700
H	0.78826700	3.71008200	-2.44197600	H	1.33594900	2.95036800	-1.96944100
C	2.56414500	2.66262600	-0.50574400	H	0.60337900	2.47962500	-3.51460700
H	3.34880200	3.42252100	-0.49178600	C	-1.90484900	3.44749000	-3.05784000
H	2.74581000	1.96735400	0.31150200	H	-2.87900900	3.63196200	-2.60481100
H	2.66136800	2.11461800	-1.44149200	H	-1.62574100	4.34380500	-3.61609000
C	1.18180100	4.11982500	0.97319300	H	-1.98650700	2.62127300	-3.76583100
H	0.22475500	4.61408100	1.15183600	C	-0.85315100	4.22262300	-0.90381100
H	1.41116300	3.46963700	1.82106800	H	-1.79486700	4.21151400	-0.35283500
H	1.95406900	4.89033200	0.93317200	H	-0.02833900	4.08396000	-0.20234500
H	-0.53459800	-0.07668300	0.80942900	H	-0.74393700	5.20796800	-1.36115200
Br	4.46594300	-0.15456800	-2.25984600	Br	-0.67695400	0.05140400	4.65939000
<b>[L(HBr)], 34Br, E<sub>0</sub>=-4305.591050 au</b>				<b>[L(HBr)], 35Br, E<sub>0</sub>=-4305.587969 au</b>			
N	0.05417600	-0.70915500	0.62340900	O	1.13065800	1.06410200	0.64359900
C	-0.32506100	-0.33545900	2.00548800	O	-3.03889600	-1.08528700	1.89902700
H	0.49069100	0.26389900	2.40861000	O	3.26075400	-0.66383900	0.78309900
H	-0.43598400	-1.23591000	2.62836500	N	1.08595500	2.48135100	0.50526300
C	1.39594800	-1.32854500	0.57583200	N	-2.94243700	-0.24374800	0.74918500
H	1.53781100	-1.67179300	-0.44139700	N	2.81592100	-1.48467700	-0.32084300
H	1.42109200	-2.21217200	1.23318900	N	0.03761400	-0.31188800	-2.18715200
C	-0.96080500	-1.63031200	0.05521000	C	1.19631400	0.70054800	-2.07328700
H	-1.92887500	-1.18794900	0.25999700	C	0.67238000	2.10464000	-1.97163500
H	-0.91102600	-2.59950300	0.57562700	C	0.15271000	2.65458800	-3.15269900
C	-1.59346000	0.47667000	2.06925100	C	-0.48038100	3.88739500	-3.18414200
C	-2.76053400	-0.07941900	2.58978200	C	-0.62654300	4.59067200	-1.99063500
C	-1.59998900	1.81995800	1.63595200	C	-0.11655600	4.06960500	-0.81166700
C	-3.92769200	0.67055700	2.70832800	C	0.57595200	2.84792400	-0.77053100
H	-2.74460200	-1.11130300	2.92395600	C	2.41892200	3.06949200	0.90894200
C	-2.78347000	2.55553500	1.73307100	C	3.53372000	2.65534700	-0.06533500

C	-3.93310900	1.99273400	2.28067400	C	2.31266500	4.59931800	0.94102700
H	-4.82200000	0.22474100	3.12705800	C	2.71385800	2.57643100	2.33124300
H	-2.81908400	3.57220800	1.37490800	C	-1.10764000	-0.00669400	-1.25321800
H	-4.83744300	2.58601400	2.34956300	C	-2.33142500	-0.84259900	-1.50450000
C	-0.80734500	-1.84747800	-1.42901500	C	-2.61651700	-1.47846700	-2.71386800
C	-0.09572900	-2.95133200	-1.90968700	C	-3.67344700	-2.37861400	-2.81249500
C	-1.35372300	-0.94119000	-2.35127600	C	-4.44509200	-2.65937800	-1.68639700
C	0.12563300	-3.13136800	-3.27039700	C	-4.21020700	-1.98310900	-0.49437200
H	0.29541000	-3.67287700	-1.20023300	C	-3.19312500	-1.03007500	-0.41122800
C	-1.08429400	-1.09604600	-3.71404300	C	-3.82815300	0.96075000	0.93869800
C	-0.35159600	-2.18400200	-4.17298400	C	-5.29212100	0.55826700	1.17726800
H	0.68352900	-3.99141800	-3.62157000	C	-3.28796800	1.72572900	2.15075500
H	-1.43780700	-0.34337800	-4.40364200	C	-3.72689700	1.85807300	-0.30095100
H	-0.15354100	-2.29189100	-5.23314000	C	0.56248000	-1.76335500	-2.14113200
C	2.51766700	-0.39706600	0.96347300	C	0.58196700	-2.38505900	-0.77451400
C	3.03743500	-0.44842800	2.26076500	C	-0.52871500	-3.13443200	-0.36861400
C	3.04919500	0.53614400	0.05847700	C	-0.61318300	-3.65103100	0.91645400
C	4.03160700	0.42814900	2.67926700	C	0.42498100	-3.42564900	1.81310000
H	2.64062300	-1.18361800	2.95291400	C	1.55902900	-2.73441200	1.40911800
C	4.02991400	1.43329500	0.49075400	C	1.66353800	-2.23411900	0.11207400
C	4.51849600	1.38311400	1.78996200	C	4.02021700	-2.27963000	-0.73716300
H	4.41307300	0.37523800	3.69220600	C	3.62292300	-3.24252600	-1.86142000
H	4.37910500	2.19060700	-0.19583500	C	4.62447100	-3.08213700	0.42739300
H	5.27886700	2.08776200	2.10692400	C	5.04572900	-1.27133800	-1.27069400
N	-0.35537800	2.32516100	1.15496200	H	-0.33036200	-0.18421000	-3.13008100
N	2.51257700	0.57920200	-1.27711800	H	1.80330800	0.37095700	-1.24661700
N	-2.16664300	0.12874400	-1.84431500	H	1.76140900	0.56829500	-2.99787000
O	-0.14171800	1.85260100	-0.20615000	H	0.25881800	2.09055300	-4.07601200
H	0.02822000	0.86821000	-0.06601400	H	-0.86738600	4.28367800	-4.11454500
O	-1.70305500	1.36390700	-2.42030200	H	-1.15478200	5.53652400	-1.97293000
H	-1.26046300	1.77009600	-1.65133800	H	-0.26883600	4.59006500	0.12250900
O	2.28463600	1.96423400	-1.62257800	H	3.32350000	3.01538800	-1.07628800
H	1.37380100	2.09155900	-1.30544100	H	3.66311500	1.57386600	-0.09046200
C	0.03171400	3.75319900	1.25332000	H	4.48374300	3.09189700	0.25273900
C	-3.64116300	0.02102800	-2.08309200	H	2.14808900	5.02687400	-0.04867900
C	3.35603900	0.00003800	-2.37226100	H	3.25247800	5.00219200	1.32396800
C	-4.29227400	1.16853100	-1.30461400	H	1.50960800	4.92085300	1.60680600
H	-5.38100400	1.10345300	-1.37946900	H	1.86732500	2.78344700	2.98782500
H	-4.00853600	1.11741900	-0.25454600	H	3.59684200	3.09264200	2.71509100
H	-3.97318900	2.13155900	-1.70304500	H	2.90647100	1.50609300	2.37155700
C	-4.02271500	0.11967400	-3.57026500	H	-1.31108600	1.05102000	-1.38244600
H	-3.69901500	-0.75913700	-4.13043500	H	-0.76093800	-0.14664200	-0.23397300
H	-5.10907700	0.19355900	-3.66638900	H	-2.00151300	-1.31090800	-3.59368800
H	-3.57724700	1.01045200	-4.01509500	H	-3.87617800	-2.87512800	-3.75376500
C	-4.12556000	-1.31642400	-1.51002000	H	-5.24356600	-3.38978300	-1.74464500
H	-3.64582700	-2.16596100	-1.99929500	H	-4.80138200	-2.18649800	0.38715600
H	-3.93817600	-1.37600500	-0.43617700	H	-5.34971000	-0.16364800	1.99264600
H	-5.20319100	-1.40147500	-1.66755400	H	-5.74341900	0.12350100	0.28219200
C	2.51568200	0.07239700	-3.65169600	H	-5.87834200	1.43817700	1.45385000
H	3.02540900	-0.45417000	-4.46312800	H	-3.84836500	2.65664000	2.27491000
H	1.54501900	-0.39275500	-3.48634700	H	-2.22941900	1.95310900	2.02146100
H	2.35543900	1.10740700	-3.95078500	H	-3.38445400	1.13556200	3.06053700
C	3.65026500	-1.46736100	-2.04068300	H	-2.71524500	2.25012800	-0.42159300
H	4.15093300	-1.57464500	-1.07632200	H	-4.39512500	2.71226900	-0.17155100
H	2.73639200	-2.06246200	-2.04031400	H	-4.02554200	1.33969800	-1.21472000
H	4.31198900	-1.87511100	-2.80818200	H	1.54795500	-1.70979300	-2.59007400
C	4.68057400	0.75813600	-2.56913500	H	-0.09706500	-2.33355200	-2.79058200
H	5.18550200	0.38260000	-3.46276900	H	-1.34987900	-3.28340100	-1.05729900
H	4.49386000	1.82398100	-2.70466800	H	-1.50232700	-4.18533900	1.22490300
H	5.35471000	0.61943200	-1.72164700	H	0.34645700	-3.76626900	2.83742500
C	-0.58848900	4.64089000	0.15871600	H	2.34732700	-2.51850100	2.11349400
H	-1.67658200	4.68306700	0.21376600	H	3.31629700	-2.70651300	-2.76274700
H	-0.20927500	5.66124800	0.25490700	H	2.82083300	-3.91654100	-1.55646200
H	-0.31613300	4.27266200	-0.83082800	H	4.48999700	-3.85116500	-2.12547600
C	1.56415300	3.80159600	1.13566300	H	3.94732000	-3.87124900	0.75890400
H	1.91254400	4.82884100	1.27146700	H	4.84106700	-2.42821100	1.27127400

H	2.01711300	3.17059200	1.90165500	H	5.55639400	-3.55182200	0.10302200
H	1.91090500	3.44999600	0.16803600	H	5.91348900	-1.79768600	-1.67575100
C	-0.33237700	4.25564900	2.66001600	H	5.37938700	-0.60384000	-0.47784800
H	-1.40173500	4.39335900	2.80862200	H	4.60267700	-0.66691400	-2.06662800
H	0.03018600	3.55559900	3.41616100	H	0.60964100	0.83431000	1.47885200
H	0.15753400	5.21740100	2.82390800	H	-2.16902500	-0.92703400	2.33856800
Br	-0.04431300	-4.22572600	3.02985300	H	2.56849200	0.02715700	0.82440700
H	-0.07063100	-5.39981700	3.84362200	Br	-0.19945400	-0.11040700	3.14526300
<b>[L(HI)], 23i, E<sub>0</sub> = -8650.991975 au</b>				<b>[L(HI)], 24i, E<sub>0</sub> = -8650.993781 au</b>			
N	-0.00175600	0.00001700	-1.89965900	N	0.03808000	0.57935300	-1.43768700
C	0.22860900	-1.42268400	-2.37445500	C	1.13623200	-0.30467300	-2.02876400
H	1.15543500	-1.73153900	-1.91570900	H	2.06258300	0.20219500	-1.78762500
H	0.38397100	-1.34964800	-3.45165500	H	0.97054500	-0.28330300	-3.10760800
C	1.11519600	0.91143600	-2.37337200	C	0.38487800	2.02210600	-1.69851500
H	0.92024200	1.86701500	-1.91129300	H	-0.46128000	2.61006500	-1.36822200
H	0.97288000	1.01283500	-3.45007100	H	0.47921900	2.13450200	-2.77951600
C	-1.34950800	0.51163200	-2.37333500	C	-1.33440200	0.16316300	-1.96564700
H	-2.07959100	-0.13663000	-1.91337500	H	-1.52327400	-0.79437500	-1.49297400
H	-1.36522800	0.34002100	-3.45042600	H	-1.20626700	0.03587600	-3.04179500
C	-0.91452100	-2.34267700	-2.07101400	C	1.18610600	-1.69867100	-1.48202500
C	-1.82081100	-2.65515500	-3.09033100	C	0.28051900	-2.67874400	-1.90155900
C	-1.13161600	-2.83824500	-0.77543800	C	2.16096200	-2.02822700	-0.52603100
C	-2.96087100	-3.40448800	-2.83446600	C	0.28410800	-3.94181700	-1.32864000
H	-1.63437500	-2.28331700	-4.09256200	H	-0.43856200	-2.44795800	-2.67900200
C	-2.30253200	-3.56099400	-0.51673000	C	2.12752600	-3.28493000	0.07921000
C	-3.20741800	-3.83775000	-1.53313300	C	1.19334000	-4.23154300	-0.31411800
H	-3.65631000	-3.63168700	-3.63307500	H	-0.43574500	-4.68509200	-1.64846700
H	-2.49488600	-3.88067500	0.49603300	H	2.81350900	-3.48936800	0.88749600
H	-4.10553700	-4.40152400	-1.30915500	H	1.16901100	-5.19663100	0.17695300
C	-1.57591300	1.96167700	-2.07062900	C	-2.45590500	1.11833900	-1.65782300
C	-1.39644300	2.90204300	-3.09121200	C	-2.59012700	2.32303900	-2.36360700
C	-1.89636700	2.39823000	-0.77529200	C	-3.39436900	0.81393100	-0.65591000
C	-1.47871700	4.26411800	-2.83695000	C	-3.53756900	3.26895800	-1.99976800
H	-1.16769800	2.55407000	-4.09325400	H	-1.93144100	2.52680300	-3.20041200
C	-1.94034000	3.77386400	-0.51825200	C	-4.30910200	1.79626400	-0.25341100
C	-1.73098500	4.69521300	-1.53597800	C	-4.37170700	3.01646900	-0.90934500
H	-1.33014700	4.97938200	-3.63654800	H	-3.61779000	4.19852400	-2.54994900
H	-2.12092300	4.10110800	0.49427100	H	-4.96323000	1.57515400	0.57758800
H	-1.77294000	5.75506600	-1.31331600	H	-5.09295600	3.76126000	-0.59332500
C	2.48399700	0.38095400	-2.07314500	C	1.64885700	2.45865000	-1.01227600
C	3.20617500	-0.24583200	-3.09476300	C	2.67105000	3.03582200	-1.76954900
C	3.02466100	0.44021700	-0.77879000	C	1.81585700	2.31489100	0.37258400
C	4.42645300	-0.85725600	-2.84225700	C	3.85290400	3.45627000	-1.17160300
H	2.78892000	-0.26936400	-4.09617200	H	2.53836400	3.14669900	-2.84046500
C	4.23744000	-0.21122800	-0.52347200	C	3.02941000	2.68092000	0.95794300
C	4.92796900	-0.85471100	-1.54207400	C	4.03534000	3.25945600	0.19458900
H	4.96972400	-1.34447100	-3.64257800	H	4.63604600	3.90386500	-1.77123200
H	4.61290100	-0.21836300	0.48839500	H	3.17672400	2.49552200	2.01138800
H	5.86646500	-1.34957700	-1.32079600	H	4.96820200	3.54498900	0.66568500
N	-0.18501600	-2.54167400	0.25980800	N	3.14755400	-1.03619600	-0.19072200
N	2.29630300	1.11032700	0.25862500	N	0.73364600	1.75118400	1.13754200
N	-2.10870500	1.43086300	0.26149600	N	-3.38636600	-0.48785500	-0.08640800
O	-0.95038500	-2.46206100	1.47024700	O	3.32733300	-1.02249800	1.23467900
H	-0.60141000	-1.68144900	1.95904900	H	2.73478900	-0.30429300	1.52166600
O	-1.65453800	2.05587600	1.47004600	O	-3.66000200	-0.37155300	1.30899200
H	-1.15078400	1.36455800	1.95836900	H	-2.84502400	-0.76116900	1.70729200
O	2.61261700	0.40688000	1.46797900	O	1.33464800	0.85822400	2.09557000
H	1.76312200	0.31769800	1.95848000	H	0.70789300	0.08124700	2.12356600
C	0.88725700	-3.60530800	0.48918000	C	4.50602100	-1.24114900	-0.80161800
C	-3.56477900	1.03218200	0.49486300	C	-4.34602100	-1.48882500	-0.67817300
C	2.68053600	2.57089000	0.48867100	C	-0.10580800	2.76670100	1.90451700
H	-0.00182500	-0.00039300	-0.86809800	C	-4.02182600	-2.83810600	-0.02767300
C	0.25842600	-4.94730400	0.89006200	H	-4.62934300	-3.62435600	-0.48384500
H	-0.30836300	-5.39045900	0.06757900	H	-2.96434300	-3.07714500	-0.15229200
H	1.04793800	-5.64864800	1.16983300	H	-4.23096400	-2.81293800	1.04084500
H	-0.40159000	-4.81432400	1.74649700	C	-5.80758000	-1.10016500	-0.40569500

C	1.73748100	-3.79636700	-0.77180500	H	-6.08616700	-0.18720900	-0.93763900
H	1.13905700	-4.06075100	-1.64640700	H	-6.47255200	-1.90003400	-0.74096100
H	2.34302600	-2.91352600	-0.98746100	H	-5.96108600	-0.94894100	0.66280200
H	2.43150700	-4.62006100	-0.59261700	C	-4.11516000	-1.59112600	-2.19069700
C	1.78954900	-3.07990500	1.60943500	H	-4.28325900	-0.64088600	-2.70105300
H	2.63118900	-3.76373600	1.74755100	H	-3.10770900	-1.94585900	-2.41711300
H	2.17881900	-2.09175500	1.36019300	H	-4.81832200	-2.31804300	-2.60227100
H	1.25167800	-3.00280700	2.55287000	C	-1.22174400	1.99586800	2.61274100
C	4.15729500	2.69851300	0.88870400	H	-1.88777300	2.70743100	3.10730100
H	4.82413700	2.42999500	0.06571300	H	-1.80907900	1.41058000	1.90681100
H	4.36907000	3.73312200	1.16837900	H	-0.82649100	1.31582900	3.36552600
H	4.37337800	2.06054000	1.74487900	C	-0.74127500	3.74153700	0.90754100
C	2.41947000	3.40402100	-0.77133700	H	0.00367300	4.26274600	0.30223900
H	2.94857600	3.02051100	-1.64649100	H	-1.45819600	3.23501900	0.25983100
H	1.35203900	3.48548800	-0.98717000	H	-1.29471400	4.49721300	1.46826300
H	2.78383200	4.41732900	-0.59051200	C	0.73089200	3.53938700	2.93312900
C	1.77444700	3.08772900	1.60978800	H	0.06596300	4.14793400	3.55006300
H	1.94513600	4.15847400	1.74925400	H	1.26255500	2.84717900	3.58618000
H	0.72418300	2.93021100	1.36036600	H	1.44960100	4.20914600	2.45703300
H	1.97704200	2.58224500	2.55254900	C	5.20995000	-2.49923500	-0.26597800
C	-3.55618200	-0.01171700	1.61522200	H	4.70330600	-3.41062200	-0.58751200
H	-4.56820500	-0.40019500	1.75648500	H	6.23449000	-2.53428000	-0.64490200
H	-2.89457100	-0.84183800	1.36391800	H	5.24498100	-2.47968100	0.82330200
H	-3.21824700	0.41610100	2.55763100	C	5.33235300	0.00306900	-0.46434100
C	-4.41356600	2.24633900	0.89799900	H	6.32833300	-0.07702800	-0.90755800
H	-4.51814900	2.95828800	0.07562200	H	4.84469500	0.89596400	-0.85458000
H	-5.41411900	1.91132400	1.18110700	H	5.43606100	0.11122000	0.61451600
H	-3.96658400	2.75259200	1.75280400	C	4.35403100	-1.34768600	-2.32408300
C	-4.15761800	0.39038100	-0.76457800	H	3.74266900	-2.20321800	-2.61507500
H	-4.09182700	1.04140800	-1.63910700	H	3.91652200	-0.43963600	-2.74561700
H	-3.69412700	-0.57426400	-0.98205400	H	5.34336500	-1.47447800	-2.76884600
H	-5.21695600	0.19850000	-0.58222700	H	0.03113200	0.48021500	-0.40103600
I	0.00400300	0.00045200	3.59791600	I	-0.67530800	-1.78602000	1.99885100
<b>[L(HI)], 25l, E<sub>0</sub>=-8650.993785 au</b>				<b>[L(HI)], 26l, E<sub>0</sub>=-8650.997403 au</b>			
N	-0.89369200	0.51487900	1.68203500	O	-3.45924000	-0.86792100	-0.62985800
C	0.18323500	1.51186400	2.09055200	H	-2.97744800	-0.02054900	-0.76000200
H	1.10946300	0.96370100	1.99225800	O	-3.09759900	1.54199300	-2.70456100
H	-0.00339600	1.72459900	3.14491700	H	-3.31040200	0.60063200	-2.72139200
C	-0.82292400	-0.69141200	2.60822500	O	4.05086100	-0.84515500	0.53927700
H	-1.62348700	-1.35341100	2.29097000	H	3.67085200	-0.35024400	1.30115700
H	-1.01925600	-0.30783000	3.61089300	N	-2.45386400	-1.78342400	-0.12540200
C	-2.27204000	1.12869700	1.69749400	N	-2.65406900	1.74646100	-1.34214400
H	-2.19331000	2.03909400	1.12085600	N	3.22457800	-0.43018100	-0.55710000
H	-2.47308300	1.39174200	2.73781200	N	0.40330500	-0.21081000	0.15622300
C	0.22649600	2.77273500	1.27952000	H	1.36725000	0.11177300	0.38663000
C	-0.61435100	3.84750700	1.59651900	C	0.18158600	-1.44881500	1.04469100
H	1.12296800	2.89723800	0.20496300	H	0.21481300	-2.30242800	0.37920500
C	-0.64748700	4.99041400	0.80982100	H	1.04693000	-1.47618900	1.70291200
H	-1.25791800	3.77923000	2.46705900	C	-1.07595500	-1.41774900	1.86865500
C	1.04676200	4.03031300	-0.61485500	C	-0.96036500	-1.16568500	3.23888300
C	0.16567100	5.06109800	-0.32092100	H	0.02624700	-1.00645300	3.65760300
H	-1.30955800	5.80884500	1.06482300	C	-2.08951600	-1.04805900	4.04052900
H	1.68551100	4.07636600	-1.48432600	H	-1.98034100	-0.83929700	5.09773600
H	0.12799600	5.93308400	-0.96341600	C	-3.35409700	-1.15758200	3.46870800
C	-3.35577400	0.23918600	1.15953000	H	-4.24191800	-1.03463800	4.07823100
C	-4.25192000	-0.36877200	2.04368500	C	-3.48381400	-1.41530700	2.10860400
C	-3.49502300	0.02554000	-0.22142200	H	-4.46199900	-1.45930500	1.65345700
C	-5.26489100	-1.19831200	1.57867800	C	-2.35274800	-1.57746400	1.30503500
H	-4.14595900	-0.19203500	3.10898700	C	-2.86950700	-3.15620300	-0.56951100
C	-4.50089400	-0.82868600	-0.67986000	C	-2.94812400	-3.13363800	-2.10163700
C	-5.38058500	-1.43158900	0.20993000	H	-2.05102700	-2.68685700	-2.53082900
H	-5.94866900	-1.66659200	2.27610400	H	-3.80880500	-2.55731200	-2.43833800
H	-4.55611000	-1.04107500	-1.73722700	H	-3.04159800	-4.15307900	-2.48248900
H	-6.15488200	-2.09043700	-0.16536000	C	-1.78536900	-4.13785500	-0.11116700
C	0.49822600	-1.39464100	2.53416800	H	-0.82438700	-3.92175000	-0.57876500
C	1.48169300	-1.20385500	3.50589000	H	-2.07680900	-5.15098600	-0.39607700



C	0.74644900	-2.24725900	1.44495400	H	-1.66330800	-4.11956200	0.97341900
C	2.71277300	-1.84160400	3.39447600	C	-4.23320800	-3.59643800	-0.01009100
H	1.28272700	-0.55414100	4.35156100	H	-4.52783700	-4.53742900	-0.48097500
C	1.99413500	-2.86128100	1.32461700	H	-5.00025600	-2.85281600	-0.23088900
C	2.96807800	-2.66118400	2.29784900	H	-4.19507100	-3.76109400	1.06731500
H	3.47320900	-1.68864500	4.15065600	C	-0.52614200	0.93933200	0.49907400
H	2.21847200	-3.45495000	0.45205100	H	-0.25524500	1.22121000	1.51642400
H	3.93706600	-3.13208200	2.18525700	H	-1.53050100	0.55116100	0.48907800
N	2.08548100	1.86679600	-0.02122900	C	-0.37454700	2.08457300	-0.45565500
N	-0.32544800	-2.37191000	0.51044700	C	0.81008000	2.82883300	-0.42981000
N	-2.52471600	0.61417000	-1.10505800	H	1.53163300	2.61690800	0.35220300
O	2.25969800	1.77140200	-1.43830600	C	1.06054300	3.80225300	-1.38665500
H	2.25485700	0.80596900	-1.62814500	H	1.98677300	4.36299200	-1.35701700
O	-2.17044700	-0.38509100	-2.07708400	C	0.12671200	4.02853100	-2.39621500
H	-1.38186800	-0.78872300	-1.66658500	H	0.32546000	4.75984700	-3.17084000
O	-0.20048100	-1.32320100	-0.46648400	C	-1.07817300	3.33703400	-2.39970700
H	0.67278100	-1.42836100	-0.95814200	H	-1.81121100	3.51760200	-3.17180300
C	3.45310300	2.11773600	0.59828300	C	-1.35734300	2.39051000	-1.40948500
C	-2.93926500	1.83054200	-1.89018900	C	-3.71924200	2.57142200	-0.62083400
C	-0.76621800	-3.68214700	-0.04502900	C	-3.87612100	3.97277600	-1.22405700
H	-0.69016900	0.17760000	0.71907200	H	-4.09018300	3.91163100	-2.29220800
C	3.31920100	2.35166800	2.10852000	H	-2.98656000	4.58518600	-1.07417300
H	2.95526300	1.46139200	2.62506400	H	-4.71559300	4.47652600	-0.73980800
H	4.31064700	2.57246200	2.50931700	C	-5.05241400	1.82051500	-0.73309400
C	2.67278200	3.19911200	2.34497500	H	-4.97814400	0.80895400	-0.33393800
H	4.27354700	0.84625500	0.36556500	H	-5.38638300	1.76990200	-1.76911700
H	3.75437500	-0.02444800	0.77011700	H	-5.80912700	2.35945500	-0.15924800
H	4.43739300	0.66632100	-0.69529000	C	-3.31395300	2.66757300	0.85424600
H	5.24536300	0.94047500	0.85778700	H	-2.35961900	3.17910500	0.98566800
C	4.14748000	3.32779100	-0.04413100	H	-3.25767500	1.68175800	1.31974100
H	5.17235100	3.40023200	0.32771500	H	-4.07251400	3.24317000	1.38848600
H	4.18002200	3.21083500	-1.12664000	C	0.41753500	-0.55111800	-1.31532000
H	3.63628900	4.26238600	0.19896600	H	0.65178400	0.36951000	-1.84021000
C	0.07795400	-4.22191900	-1.20688100	H	-0.59473500	-0.85996700	-1.56655300
H	1.09676600	-4.46599000	-0.90847400	C	1.39605100	-1.65506000	-1.62643000
H	-0.38548300	-5.13464700	-1.59121300	C	0.94086200	-2.78125800	-2.31848800
H	0.14206400	-3.50241100	-2.02211200	H	-0.07836700	-2.79845600	-2.68002000
C	-0.77060200	-4.67418800	1.12765100	C	1.76088000	-3.88338300	-2.52598600
H	0.23652600	-4.91885800	1.46620700	H	1.38429100	-4.74626800	-3.06193400
H	-1.33260700	-4.27332500	1.97522500	C	3.05059200	-3.88262600	-2.00078400
H	-1.25324300	-5.59887000	0.80569900	H	3.68729400	-4.75216300	-2.11426400
C	-2.21306800	-3.47935500	-0.51943700	C	3.52854900	-2.76030700	-1.33670200
H	-2.62422000	-4.42795300	-0.87326600	H	4.52041800	-2.75082900	-0.91026000
H	-2.83448800	-3.11018100	0.29843700	C	2.72954300	-1.62317700	-1.18905200
H	-2.26840400	-2.76128400	-1.33531200	C	4.05992600	0.46410000	-1.45384200
C	-1.68847400	2.30244900	-2.64041900	C	3.20670200	0.90688000	-2.64633900
H	-1.89071400	3.25552500	-3.13594400	H	2.34904400	1.49742800	-2.32499800
H	-0.85614500	2.43891000	-1.94909600	H	2.86086700	0.05737200	-3.23867700
H	-1.38917100	1.57330200	-3.39140200	H	3.81393700	1.53873800	-3.29811700
C	-4.07000300	1.51631000	-2.88346500	C	5.32629500	-0.24498400	-1.95687900
H	-5.00530400	1.28462000	-2.36872800	H	5.09257800	-1.04964800	-2.65656300
H	-4.24656400	2.38712800	-3.51929600	H	5.89051400	-0.65207100	-1.11756800
H	-3.79582100	0.67659300	-3.52158000	H	5.96020400	0.47651800	-2.47792700
C	-3.40120200	2.92644200	-0.92490100	C	4.45646400	1.68490000	-0.61831900
H	-4.20434400	2.58367800	-0.26798400	H	5.12411100	1.40097400	0.19354300
H	-2.57315000	3.30809500	-0.32747400	H	3.58097500	2.15624800	-0.17506900
H	-3.78883500	3.76427300	-1.50804800	H	4.96858100	2.41167900	-1.25392700
I	2.59102700	-1.55221200	-2.26891300	I	2.35529400	1.03985400	2.84428500
<b>[L(HI)], 27I, E<sub>0</sub>=-8650.980488 au</b>				<b>[L(HI)], 28I, E<sub>0</sub>=-8650.989537 au</b>			
N	1.51382500	0.21098700	1.76618800	N	-1.56944100	0.11449900	1.63939900
C	1.79282900	-1.09666400	2.40621000	C	-0.83699300	-0.72650900	2.66694000
H	0.83193000	-1.52234600	2.69376700	H	-0.95141800	-1.75352300	2.34327700
C	2.39856300	-0.95029400	3.31386400	H	-1.37091600	-0.58307100	3.60799000
H	0.63979300	1.05327000	2.61120300	C	-2.96494500	-0.41201200	1.39595100
H	0.60894700	2.02911400	2.14204100	H	-3.43444300	0.29482000	0.72492400
H	1.09704900	1.17424400	3.60656200	H	-3.47549400	-0.36815500	2.35933700

C	2.79401900	0.91005800	1.49010600	C	-1.59863200	1.57371300	2.06044500
H	3.44116600	0.18687400	1.00700900	H	-0.57136000	1.83106900	2.28433300
H	3.26032500	1.20437400	2.44386000	H	-2.19076900	1.60643700	2.97652000
C	2.48657100	-2.06608900	1.48231900	C	0.60096600	-0.32470400	2.78919200
C	3.81843500	-2.41817000	1.69153700	C	1.03331400	0.39839800	3.90459900
C	1.77643200	-2.65329400	0.41333000	C	1.50403900	-0.62553200	1.75888100
C	4.45458100	-3.35181900	0.87734100	C	2.34630500	0.84601900	3.99070100
H	4.35735000	-1.96629100	2.51742700	H	0.33161100	0.61732100	4.70278900
C	2.43154300	-3.56515700	-0.41694600	C	2.80986900	-0.13543100	1.83116000
C	3.75440800	-3.92647300	-0.17666000	C	3.22574800	0.59119900	2.94134300
H	5.48689700	-3.62299800	1.06321600	H	2.67493400	1.40318100	4.85976300
H	1.91545300	-3.99453600	-1.26137600	H	3.49194700	-0.29290800	1.00286200
H	4.24055700	-4.64083000	-0.83065700	H	4.24253600	0.96353400	2.97748000
C	2.64028200	2.12142000	0.60528600	C	-2.18034000	2.45920300	0.99988200
C	2.53384800	3.39705500	1.16846600	C	-3.51085600	2.88217200	1.08241200
C	2.58368100	1.99227500	-0.79146600	C	-1.40287900	2.82296400	-0.10902500
C	2.31957400	4.52081500	0.37824700	C	-4.08809100	3.61465300	0.05264600
H	2.61301800	3.50403700	2.24520900	H	-4.09969600	2.62026600	1.95526300
C	2.31573900	3.11587500	-1.57844800	C	-2.00564400	3.51207600	-1.16497900
C	2.18650100	4.37286500	-1.00009100	C	-3.33631000	3.90432200	-1.08471600
H	2.23691900	5.49971300	0.83552100	H	-5.11970000	3.93653300	0.12523500
H	2.18974000	2.98788500	-2.64366500	H	-1.42429400	3.72331500	-2.05008100
H	1.98260500	5.23498400	-1.62446100	H	-3.78652000	4.44331300	-1.90990900
C	-0.76531700	0.52499600	2.77676800	C	-2.97730900	-1.81200300	0.85606200
C	-1.10084400	-0.18657600	3.93267000	C	-3.41011900	-2.85063300	1.68751500
C	-1.75675200	0.73058800	1.80227900	C	-2.53022600	-2.10579500	-0.44248800
C	-2.37052900	-0.72271700	4.11380300	C	-3.38234500	-4.17181800	1.26185200
H	-0.34386900	-0.32765800	4.69677200	H	-3.75752900	-2.61419700	2.68778500
C	-3.02693000	0.17598200	1.97974400	C	-2.47754900	-3.44172300	-0.85173700
C	-3.33381200	-0.54892800	3.12408300	C	-2.89974200	-4.46362300	-0.01186000
H	-2.60268900	-1.27875000	5.01442000	H	-3.71470000	-4.96443800	1.92075000
H	-3.76842200	0.28810300	1.20247000	H	-2.07792500	-3.66488400	-1.82925100
H	-4.32314700	-0.97558800	3.23973000	H	-2.84988500	-5.49086800	-0.35305300
N	0.40777000	-2.27083200	0.29522700	N	1.01235600	-1.42086400	0.66200600
N	-1.39787600	1.46042000	0.61210500	N	-2.06986900	-1.03317700	-1.29085300
N	2.79314900	0.68917700	-1.35778400	N	-0.02013700	2.43978700	-0.11144300
O	0.33907900	-0.95915600	-0.34170700	O	1.20564000	-0.71037900	-0.57401500
H	0.72136300	-0.35831600	0.37829400	H	2.17701900	-0.68551800	-0.86888800
O	1.72844000	0.42633300	-2.29101800	O	0.26284400	1.88267400	-1.40481300
H	1.21781300	-0.24687900	-1.80487800	H	0.66176800	1.02374300	-1.17809900
O	-1.83519500	0.70055400	-0.54070600	O	-0.96438400	-1.54123700	-2.05298300
H	-1.10412600	0.05853800	-0.65628200	H	-0.17123300	-1.18286700	-1.60379000
C	-0.63936200	-3.16019300	-0.26492600	C	1.52912600	-2.85266500	0.62038800
C	4.09939100	0.46577100	-2.05751600	C	0.96117300	3.56393700	0.14863300
C	-1.93271300	2.85064800	0.45639800	C	-3.07251300	-0.53942300	-2.31893700
C	4.15026100	-1.02217000	-2.41779800	C	2.35709500	2.93991800	0.14870500
H	5.11749400	-1.26753800	-2.86414600	H	3.09885400	3.69875100	0.40940600
H	4.01189200	-1.62894700	-1.52434300	H	2.41167500	2.14042600	0.88366800
H	3.36528300	-1.27161000	-3.13163300	H	2.62276500	2.52454100	-0.82217200
C	4.25812900	1.31414900	-3.33078200	C	0.89028400	4.66963600	-0.91500000
H	4.37591000	2.37417100	-3.09986700	H	-0.03798300	5.24147500	-0.85632800
H	5.14879300	0.99237600	-3.87657000	H	1.71833100	5.36578800	-0.76407400
H	3.39203200	1.18410300	-3.98095900	H	0.98975900	4.23928000	-1.91211300
C	5.23239900	0.78592200	-1.07486400	C	0.66287200	4.14636100	1.53517700
H	5.20182200	1.82536100	-0.74322800	H	-0.35219000	4.54338100	1.60884400
H	5.19095000	0.13439300	-0.19982900	H	0.81677700	3.39985800	2.31798700
H	6.19114700	0.61933000	-1.57108200	H	1.35467400	4.96874000	1.72808600
C	-1.35965400	3.39941100	-0.85446500	C	-2.35661000	0.52016600	-3.16294500
H	-1.58248200	4.46635700	-0.93573700	H	-3.08964600	1.05003000	-3.77695300
H	-0.27963400	3.26358500	-0.87616700	H	-1.83991600	1.23462800	-2.52609500
H	-1.78919800	2.88739800	-1.71447800	H	-1.61846900	0.06103000	-3.81782300
C	-1.40575500	3.68390700	1.63138800	C	-4.26132900	0.10165800	-1.59950700
H	-1.69908000	3.25943900	2.59377500	H	-4.75461300	-0.59498900	-0.91723500
H	-0.32001600	3.77476500	1.59180600	H	-3.96032400	1.00041800	-1.06064500
H	-1.82811600	4.68886800	1.56701000	H	-5.00012500	0.40286300	-2.34491000
C	-3.46876600	2.92192400	0.42977000	C	-3.57009400	-1.67400300	-3.22762100

H	-3.77541000	3.94948900	0.21949600	H	-4.18119400	-1.24940800	-4.02758100
H	-3.88491700	2.28733900	-0.35291200	H	-2.72816600	-2.19335400	-3.68577700
H	-3.90556100	2.63441300	1.38757000	H	-4.18398600	-2.39573900	-2.68469800
C	-0.68944500	-3.16482000	-1.80293100	C	3.02941700	-3.00378800	0.91885400
H	0.23574800	-3.52738900	-2.25243900	H	3.28019800	-2.70050100	1.93666400
H	-1.50401200	-3.80899200	-2.14168600	H	3.29593400	-4.05843700	0.81287600
H	-0.87849200	-2.16166700	-2.18595300	H	3.63954800	-2.43675400	0.21369300
C	-1.97855300	-2.65189700	0.28935300	C	1.24412200	-3.44499300	-0.76172300
H	-2.79851000	-3.27604900	-0.07225100	H	1.48223400	-4.51072200	-0.73289500
H	-1.96580700	-2.67429300	1.37999000	H	0.20034100	-3.32807100	-1.03872800
H	-2.17749600	-1.63192900	-0.01972400	H	1.86685600	-2.98117300	-1.52697600
C	-0.42488700	-4.57580100	0.29518200	C	0.71677900	-3.61390200	1.67780500
H	0.41752000	-5.09811100	-0.15422000	H	0.86073000	-3.19084000	2.67567000
H	-0.26626600	-4.53643300	1.37527900	H	-0.34638700	-3.61121600	1.42945400
H	-1.32552000	-5.16268100	0.10540000	H	1.05327900	-4.65218900	1.71438400
H	-3.37619100	0.11088600	-1.16690600	I	4.22790800	-0.27747600	-1.78922900
I	-4.77201100	-0.49088900	-1.84696800	H	-1.05670400	0.03809900	0.74727200
<b>[L(HI)], 29I, E<sub>0</sub>=-8650.988978 au</b>				<b>[L(HI)], 30I, E<sub>0</sub>=-8650.987680 au</b>			
O	1.94558500	1.25022400	-1.06539700	O	-3.25360500	-1.39914700	0.68950700
O	-2.36452600	3.66977600	-0.47184300	H	-3.11127300	-0.90663100	-0.14657900
O	2.53479900	2.05264400	1.53627000	O	-1.90936800	3.33786500	-1.53687500
N	2.68967100	0.49958300	-2.05720900	H	-1.98071300	2.50718500	-2.05186500
N	-1.96084900	2.45940700	-1.14763300	O	4.13982800	-1.81414500	1.03366700
N	1.70350500	1.09655800	2.23472800	H	3.33013000	-2.12590100	1.45210400
N	-0.33570400	-1.05063700	0.31622600	N	-2.15365700	-2.31971100	0.67000500
C	1.14448900	-1.30089000	0.03848300	N	-1.75780800	2.82812400	-0.21111900
C	1.39428500	-1.60926400	-1.42019300	N	3.72445000	-0.61171600	0.33012300
C	0.88965400	-2.82846400	-1.89418700	N	0.93902000	-0.00934300	0.40638900
C	0.96508200	-3.18593000	-3.23353500	H	1.81566900	0.02802700	0.94473700
C	1.53832500	-2.30603100	-4.14522100	C	0.48932400	-1.46242400	0.38829300
C	2.05161700	-1.09712000	-3.69582100	H	-0.29711200	-1.53720900	-0.36151300
C	2.02557100	-0.74467300	-2.34125600	H	1.34850400	-2.04926000	0.07104500
C	4.13521800	0.43069600	-1.64896100	C	-0.03659500	-1.85779400	1.73670300
C	4.35209400	-0.34729800	-0.34461700	C	0.77199000	-1.78134900	2.87549500
C	4.90860100	-0.25083800	-2.78591300	H	1.83008500	-1.55023000	2.77837800
C	4.63800300	1.87312000	-1.50667400	C	0.22832200	-1.93481700	4.14455300
C	-0.92969400	-0.11742600	-0.69358500	H	0.86233900	-1.86987500	5.02054400
C	-2.40628500	0.12247600	-0.57613600	C	-1.14461100	-2.14143000	4.28144600
C	-3.29835600	-0.89910200	-0.23951400	H	-1.58332200	-2.22460700	5.26885300
C	-4.65181200	-0.62996600	-0.07502600	C	-1.95175200	-2.25215800	3.15531900
C	-5.12865700	0.66730000	-0.25561800	H	-3.01723000	-2.39866900	3.25791500
C	-4.25733600	1.68297200	-0.62847900	C	-1.40060400	-2.15874200	1.87299100
C	-2.89782500	1.41809000	-0.81099600	C	-2.62236700	-3.70176900	0.33852800
C	-1.81913200	2.81198400	-2.60016800	C	-3.22426100	-3.64334400	-1.06975800
C	-3.11668700	3.39604300	-3.18220800	H	-2.51741000	-3.20522100	-1.77484600
C	-0.69000800	3.84480500	-2.69582900	H	-4.12629300	-3.03180500	-1.08215700
C	-1.42293800	1.55602000	-3.38389200	H	-3.48670600	-4.65196400	-1.39912800
C	-0.58698700	-0.70019700	1.77847100	C	-1.38467700	-4.60792700	0.32628100
C	-0.72514000	0.76455900	2.10749900	H	-0.64113700	-4.23576300	-0.38264200
C	-2.01810300	1.27436100	2.27809300	H	-1.67710700	-5.61283800	0.01461800
C	-2.23929300	2.61661300	2.55525000	H	-0.92315800	-4.68314400	1.31331900
C	-1.15228000	3.48583100	2.63983700	C	-3.67069500	-4.23790000	1.32728400
C	0.14074200	2.99288000	2.50612800	H	-4.10103000	-5.16573500	0.94246700
C	0.36755300	1.62977400	2.28973300	H	-4.47663000	-3.51149600	1.44493800
C	2.36677300	0.85206600	3.56820800	H	-3.23704700	-4.45641000	2.30524100
C	1.48334800	-0.07555400	4.40963600	C	-0.13200500	0.88239800	1.01540800
C	2.61859100	2.15661700	4.34257500	H	-0.31094100	0.50808800	2.01957100
C	3.69887900	0.15138400	3.28100300	H	-1.02280800	0.74049400	0.40612300
H	-0.78072700	-2.01339300	0.24870900	C	0.27284000	2.32617800	1.00927500
H	1.67966900	-0.44524200	0.42047800	C	1.44530200	2.74673900	1.64426700
H	1.38144400	-2.17530900	0.64638100	H	2.01053200	2.04103800	2.24407000
H	0.40557400	-3.49859100	-1.19015500	C	1.90454800	4.04955700	1.50276100
H	0.56006700	-4.13672700	-3.55756500	H	2.81837100	4.36162600	1.99404100
H	1.57800400	-2.55004100	-5.20026200	C	1.18945500	4.94412000	0.70440900
H	2.48808900	-0.39156100	-4.38978000	H	1.55544700	5.95420500	0.56118700
H	4.01548900	-1.38153800	-0.44146800	C	-0.00642500	4.55475200	0.11613100

H	3.83427100	0.12130700	0.48863900	H	-0.57160600	5.23995700	-0.49959300
H	5.41642800	-0.36576500	-0.09854200	C	-0.50238300	3.25838300	0.30208100
H	4.60929300	-1.29061600	-2.91743900	C	-2.97474800	3.16750600	0.60277400
H	5.97255000	-0.23429800	-2.54132900	C	-3.15998400	4.68517900	0.75558100
H	4.76524000	0.27746100	-3.73024300	H	-3.16815000	5.16174300	-0.22615400
H	4.41485700	2.44228400	-2.41220500	H	-2.36657200	5.13063100	1.36018100
H	5.71997600	1.86973500	-1.35994800	H	-4.11373100	4.89616200	1.24577600
H	4.19147900	2.38082800	-0.65210900	C	-4.18242500	2.56343400	-0.12161900
H	-0.69022500	-0.55246200	-1.66059800	H	-4.02368500	1.50168700	-0.31059400
H	-0.40192300	0.82681900	-0.61243100	H	-4.34595200	3.05380800	-1.08018000
H	-2.93500200	-1.90801100	-0.06903100	H	-5.07743100	2.68805600	0.49306800
H	-5.32496600	-1.43100100	0.20527800	C	-2.83370300	2.50401100	1.97853600
H	-6.18057200	0.88692300	-0.11348100	H	-1.95706800	2.86505900	2.52087200
H	-4.60995100	2.69734600	-0.74702900	H	-2.77911700	1.41761100	1.88339700
H	-3.44866000	4.25386000	-2.59692800	H	-3.71458900	2.74210200	2.57875400
H	-3.91243700	2.64907500	-3.19655800	C	1.32558300	0.46148200	-0.97645700
H	-2.94566800	3.72541400	-4.20992400	H	1.73001400	1.46340700	-0.85270300
H	-0.46871100	4.06774800	-3.74180300	H	0.39512900	0.52710800	-1.54420600
H	0.21921500	3.45667800	-2.22623500	C	2.28999900	-0.46888500	-1.66046800
H	-0.96116800	4.76881600	-2.18774000	C	1.98472800	-0.85798000	-2.96804800
H	-0.45553000	1.16762400	-3.06279900	H	1.06925600	-0.49193100	-3.41880900
H	-1.34175600	1.81336000	-4.44178000	C	2.80548900	-1.74145900	-3.65892300
H	-2.16962600	0.76588200	-3.29079100	H	2.54807900	-2.03743900	-4.66852600
H	0.21503500	-1.18063400	2.32503900	C	3.92814000	-2.27512700	-3.03197300
H	-1.50319700	-1.22717900	2.03708700	H	4.55591700	-2.99010500	-3.55055200
H	-2.86249100	0.60641700	2.16735400	C	4.23977200	-1.90519300	-1.72885200
H	-3.25079400	2.98454200	2.67059900	H	5.08024200	-2.35204500	-1.21884800
H	-1.30840100	4.54142800	2.83285800	C	3.44376300	-0.98312900	-1.04687300
H	0.99214500	3.65433500	2.56677400	C	4.83478500	0.39095600	0.53460600
H	1.38413200	-1.06282500	3.95639600	C	4.48522900	1.65535000	-0.25573100
H	0.48920800	0.34151900	4.57657300	H	3.55970100	2.11078400	0.09550000
H	1.95426600	-0.21152600	5.38510700	H	4.40026800	1.45135200	-1.32415400
H	1.68402800	2.62063700	4.66231200	H	5.28438000	2.38645900	-0.11821400
H	3.17765300	2.86651100	3.73301900	C	6.20158700	-0.14135100	0.07779500
H	3.20417400	1.93725700	5.23833100	H	6.23957200	-0.27155100	-1.00432400
H	4.18444400	-0.11789800	4.22165700	H	6.43276000	-1.09135000	0.56007200
H	4.36826200	0.80294300	2.72075800	H	6.97531700	0.57860300	0.35379800
H	3.53355900	-0.76194300	2.70593100	C	4.87678200	0.70421100	2.03440500
H	1.60624400	1.99922600	-1.56939600	H	5.16709300	-0.17572700	2.60720900
H	-1.82814600	3.64575000	0.33100500	H	3.90028800	1.04269100	2.38712100
H	2.44021300	1.76929400	0.61011400	H	5.60036500	1.49877700	2.22790700
I	-1.37694400	-4.18167900	0.94772900	I	-2.11137600	-0.07408900	-2.46099500
<b>[L(HI)], 311, E<sub>0</sub>=-8650.990227 au</b>				<b>[L(HI)], 321, E<sub>0</sub>=-8650.984674 au</b>			
N	0.68316000	-0.00604000	-0.21808300	N	-1.40208100	-0.01211900	1.75877300
C	1.23448900	0.47104300	1.11236100	C	-1.39962300	1.42937800	2.23123600
H	0.92105300	1.50384500	1.20203800	H	-0.35619200	1.69084300	2.36472000
H	2.32170700	0.41423500	1.01471700	H	-1.90277200	1.42831700	3.19965200
C	1.21759600	0.85905900	-1.33972300	C	-0.60607700	-0.89572200	2.69720900
H	0.80945300	0.44646600	-2.25287900	H	-0.74574200	-1.90658800	2.33526300
H	2.29990500	0.71206500	-1.32907900	H	-1.08240000	-0.80212400	3.67453500
C	0.99902900	-1.47113900	-0.47280400	C	-2.82150000	-0.52561100	1.58911700
H	0.68979500	-1.99703700	0.41942200	H	-3.33870000	0.23031400	1.01313000
H	2.08500700	-1.52636100	-0.57694900	H	-3.24346700	-0.57106200	2.59440000
C	0.74740600	-0.36365000	2.25731000	C	-2.09022000	2.33891800	1.25833300
C	1.58207400	-1.35762900	2.77796000	C	-3.37618300	2.81643000	1.52280100
C	-0.52776700	-0.17417100	2.80716300	C	-1.45345800	2.68206700	0.05726200
C	1.14253000	-2.18097000	3.80850900	C	-4.04345600	3.60576400	0.59276300
H	2.57359100	-1.47828400	2.35214500	H	-3.85786500	2.56254200	2.46121200
C	-0.97132100	-1.02074500	3.82567400	C	-2.14838800	3.43122700	-0.89329400
C	-0.14270600	-2.02214800	4.32111900	C	-3.43153500	3.89605000	-0.62409600
H	1.79676300	-2.94919100	4.20228200	H	-5.03754500	3.97779300	0.80865000
H	-1.96790600	-0.91450800	4.23288800	H	-1.68284400	3.63330400	-1.84606900
H	-0.50156100	-2.67445700	5.10833600	H	-3.95622200	4.48280300	-1.36883000
C	0.26907000	-1.96785200	-1.68386300	C	-2.86681700	-1.86211900	0.91163700
C	0.93217700	-2.05205800	-2.91227200	C	-3.01104900	-3.03234100	1.66344100
C	-1.09227400	-2.29849300	-1.60904600	C	-2.71931100	-1.94643600	-0.48092100

C	0.24114200	-2.40160200	-4.06669000	C	-2.94943400	-4.27962800	1.05494100
H	1.99151900	-1.82321200	-2.95148200	H	-3.15563900	-2.96113300	2.73619800
C	-1.79133800	-2.60212000	-2.77949300	C	-2.58628400	-3.20377500	-1.07501600
C	-1.12899200	-2.64848200	-4.00115400	C	-2.70192700	-4.36062300	-0.31387600
H	0.76320400	-2.45943400	-5.01402800	H	-3.06025200	-5.17992300	1.64656600
H	-2.85490100	-2.78448500	-2.72758800	H	-2.38331000	-3.26348600	-2.13383800
H	-1.68251200	-2.88584400	-4.90212400	H	-2.60357700	-5.32801800	-0.79162000
C	0.86158800	2.30424500	-1.15164000	C	0.84299600	-0.51487700	2.77256400
C	1.89915700	3.20672400	-0.89407500	C	1.33245800	0.05538500	3.95202700
C	-0.46491900	2.76421500	-1.17519700	C	1.70659500	-0.70180000	1.68032400
C	1.63367800	4.54762700	-0.64502200	C	2.65874300	0.45704700	4.05226500
H	2.91627500	2.83101100	-0.86240600	H	0.66093900	0.19078700	4.79369200
C	-0.72542000	4.10895600	-0.89789400	C	3.03257900	-0.27336500	1.77998500
C	0.31410800	4.99363000	-0.63572700	C	3.50265300	0.29966000	2.95585600
H	2.44772400	5.23226800	-0.44039900	H	3.02548400	0.89906000	4.97083400
H	-1.75112900	4.44511600	-0.86662400	H	3.69499600	-0.35262700	0.92368300
H	0.09084100	6.03290500	-0.42366300	H	4.53423900	0.62702200	3.00597500
N	-1.31451900	0.91661600	2.28144900	N	-0.09942100	2.24161400	-0.10716500
N	-1.53505200	1.81722000	-1.41688900	N	1.16243500	-1.27333800	0.47147500
N	-1.71034900	-2.29274900	-0.30755700	N	-2.70974200	-0.72118100	-1.23252700
O	-2.55859300	0.41921000	1.74072400	O	-0.01749300	1.52806200	-1.36319000
H	-3.12762300	0.13431000	2.47313500	H	0.63581300	0.81481800	-1.14459600
O	-2.96658100	-1.58777500	-0.41166400	O	-1.62189600	-0.79033600	-2.16849800
H	-2.84590000	-0.87476400	0.23268800	H	-1.11117500	0.01145700	-1.95495000
O	-2.64510800	2.20559600	-0.57590500	O	1.53386900	-0.46350800	-0.64522200
H	-2.64267700	1.54816500	0.13361500	H	2.51522400	-0.49623800	-0.86942400
C	-1.55271000	2.08564500	3.20000200	C	0.93507000	3.35023400	-0.07966200
C	-1.98338400	-3.65100800	0.28643900	C	-3.98202500	-0.44402700	-2.00219600
C	-2.08345200	1.79971500	-2.83169200	C	1.50934700	-2.72685400	0.20107300
C	-2.58236500	-3.41362500	1.67622600	C	-3.77480300	0.88155600	-2.73812500
H	-2.68977000	-4.36582000	2.20082200	H	-4.70837200	1.18499200	-3.21802800
H	-1.92820500	-2.76809200	2.26011800	H	-3.47460100	1.65726800	-2.03806600
H	-3.56756800	-2.95199500	1.60117600	H	-3.00675000	0.78613300	-3.50464400
C	-2.95613600	-4.49095500	-0.55589000	C	-4.32224400	-1.54126900	-3.02252800
H	-2.50932500	-4.80441100	-1.50027200	H	-4.62483300	-2.47281100	-2.54182600
H	-3.22958500	-5.39264800	-0.00258300	H	-5.15305000	-1.20613300	-3.64795800
H	-3.86781600	-3.92764500	-0.76078700	H	-3.46656000	-1.73274200	-3.67151400
C	-0.64626500	-4.38637500	0.43357400	C	-5.12471600	-0.29016800	-0.99185100
H	-0.14190500	-4.51256600	-0.52557600	H	-5.26510100	-1.19148100	-0.39167400
H	0.02255800	-3.86291500	1.11918800	H	-4.95169200	0.56066600	-0.32880500
H	-0.83247300	-5.38049500	0.84545700	H	-6.05542600	-0.10426700	-1.53194800
C	-3.23656400	0.79126800	-2.85518400	C	1.04264900	-3.03907800	-1.22536800
H	-3.54073200	0.61408000	-3.88980500	H	1.03302300	-4.12295400	-1.36673100
H	-2.93201100	-0.15467200	-2.41182300	H	0.04318900	-2.64507800	-1.40119100
H	-4.09568600	1.16895100	-2.30221900	H	1.71523900	-2.60171500	-1.96184700
C	-0.98340000	1.32868400	-3.78573100	C	0.72001700	-3.57680600	1.20099100
H	-0.10004900	1.96867300	-3.74201800	H	0.98323500	-3.33329600	2.23390400
H	-0.70010000	0.29562900	-3.58473400	H	-0.35296800	-3.46193600	1.05510200
H	-1.36709900	1.36975900	-4.80724100	H	0.96572400	-4.62911000	1.04514600
C	-2.59359800	3.18072500	-3.27079400	C	3.00473500	-3.04495000	0.34146900
H	-3.08536000	3.08750300	-4.24194400	H	3.16756500	-4.08494800	0.04666900
H	-3.32349200	3.56685800	-2.55832600	H	3.62210400	-2.42004200	-0.30626700
H	-1.78083000	3.90156200	-3.37472900	H	3.34846100	-2.93374200	1.37215200
C	-2.39318100	1.73979400	4.44336800	C	0.83423400	4.30351000	-1.27989600
H	-1.86135200	1.08523400	5.13303900	H	-0.03286500	4.96319000	-1.21585400
H	-2.63095900	2.66154900	4.97763700	H	1.72518000	4.93420500	-1.30984200
H	-3.35269800	1.27964000	4.18305600	H	0.79352200	3.73477500	-2.20944400
C	-2.25450700	3.18478300	2.39760300	C	2.31255700	2.68704800	-0.06997700
H	-2.33665400	4.08160700	3.01550400	H	3.08474700	3.45021000	0.04905500
H	-1.68930800	3.42600600	1.50043200	H	2.39379800	1.98516000	0.75772000
H	-3.26017000	2.88886000	2.09714700	H	2.53032400	2.15101900	-0.99229100
C	-0.17196100	2.59024900	3.63925500	C	0.74440200	4.12578500	1.23055900
H	0.38664500	1.83199800	4.18913700	H	-0.23339500	4.60767700	1.29238400
H	0.41781400	2.91036600	2.77920600	H	0.87722600	3.47445500	2.09793000
H	-0.30430900	3.45373300	4.29397900	H	1.50581200	4.90587700	1.28814400
H	-0.33701100	0.11355400	-0.21673400	H	-0.91988500	-0.05538500	0.84778400

I	4.64252200	-0.42601400	-0.19311100	I	4.65043900	-0.10434100	-1.76188900
[L(HI)], 33I, E <sub>0</sub> =-8650.989080 au				[L(HI)], 34I, E <sub>0</sub> =-8650.972358 au			
N	-0.75749700	-0.16654700	0.26093900	N	-0.64266000	0.02403400	-0.14200700
C	-1.22295900	0.58622600	-0.97195500	C	-1.02440700	-0.36608900	-1.51818200
H	-0.93430100	1.61445400	-0.80805400	H	-0.75361400	0.46249900	-2.17164500
H	-2.31322800	0.51057000	-0.95888900	H	-2.11260800	-0.51889700	-1.58427700
C	-1.37143900	0.44147000	1.50903900	C	-1.19667600	1.34431700	0.22421700
H	-0.94982000	-0.10359100	2.34661900	H	-0.96483200	1.49354800	1.27137500
H	-2.44457900	0.25111100	1.43550400	H	-2.29419900	1.32784700	0.12511600
C	-1.01261100	-1.65643300	0.19297500	C	-1.09422000	-1.01138200	0.81891700
H	-0.70654100	-1.96694800	-0.79672300	H	-0.78302400	-1.96718400	0.41361400
H	-2.09157700	-1.78922300	0.29288400	H	-2.19454800	-1.00713900	0.87568900
C	-0.66402900	0.04185000	-2.24932500	C	-0.31663100	-1.60750200	-1.99757900
C	-1.49030300	-0.80828000	-2.99732300	C	-1.01797900	-2.80130700	-2.15593900
C	0.61831700	0.35058800	-2.72774400	C	1.05560400	-1.56132800	-2.32460500
C	-1.04931100	-1.37605500	-4.18456200	C	-0.39485900	-3.94492700	-2.64841700
H	-2.48603200	-1.01868900	-2.61900000	H	-2.07334900	-2.82566400	-1.90632500
C	1.05904400	-0.23831800	-3.91682800	C	1.67798400	-2.72139600	-2.79148100
C	0.23745100	-1.09567300	-4.63701300	C	0.95650600	-3.89875800	-2.96909600
H	-1.70101100	-2.03466600	-4.74549100	H	-0.95915000	-4.86087200	-2.77659800
H	2.06378700	-0.03835600	-4.25588700	H	2.73336000	-2.71680900	-3.01351200
H	0.60518900	-1.54105700	-5.55397900	H	1.46154100	-4.78405200	-3.33749600
C	-0.22888700	-2.34512500	1.27211000	C	-0.51954700	-0.83636900	2.20175000
C	-0.89361900	-2.80405400	2.41314700	C	-1.24312000	-0.15431600	3.18510200
C	1.16772900	-2.47204900	1.18945600	C	0.75417500	-1.33272500	2.52043200
C	-0.18710200	-3.34874000	3.47919700	C	-0.70154300	0.08746900	4.44256100
H	-1.97296700	-2.71089400	2.45922600	H	-2.24277300	0.19730100	2.95260900
C	1.87398900	-2.99092100	2.27687200	C	1.31606200	-1.04259300	3.76690400
C	1.20237000	-3.42334800	3.41460500	C	0.59430200	-0.33898000	4.72354600
H	-0.71508700	-3.69652400	4.35871300	H	-1.27721100	0.62186400	5.18903500
H	2.95212200	-3.03104800	2.22968900	H	2.33018600	-1.35660400	3.96696600
H	1.76628800	-3.82331500	4.24914400	H	1.04255700	-0.12423000	5.68673300
C	-1.06867500	1.91003500	1.55965400	C	-0.65002300	2.48936700	-0.59139100
C	-2.10159200	2.83560100	1.39892600	C	-1.39039600	2.98086400	-1.67111100
C	0.25796600	2.35547000	1.64648600	C	0.59613500	3.06995400	-0.30474400
C	-1.81633300	4.19343800	1.29768600	C	-0.89952800	3.99516700	-2.48482400
H	-3.11979700	2.47299400	1.30837500	H	-2.36279600	2.54659100	-1.87831700
C	0.54286300	3.71400800	1.49512700	C	1.09807600	4.07084300	-1.14127100
C	-0.49257200	4.62776500	1.32401000	C	0.35935800	4.53095800	-2.22381400
H	-2.62172800	4.90564200	1.16587100	H	-1.48730000	4.35468500	-3.32122300
H	1.56856400	4.05060300	1.49571500	H	2.08780500	4.45912300	-0.95002000
H	-0.26290000	5.68037600	1.20776800	H	0.76545400	5.30777800	-2.86160400
N	1.49422900	1.25170000	-1.98147800	N	1.68940400	-0.29175300	-2.17366000
N	1.26152200	1.33162500	1.84057600	N	1.34772200	2.56264100	0.81377000
N	1.82408200	-2.02423900	-0.02324200	N	1.43880500	-2.11662700	1.53099900
O	2.84696900	0.73934000	-2.11323800	O	1.98584300	-0.06993000	-0.76471100
H	2.93191700	0.08753700	-1.40035300	H	1.06734000	0.06343100	-0.37194200
O	3.04840100	-1.32060400	0.33784000	O	2.77412100	-1.59905500	1.38527300
H	2.75181500	-0.44215400	0.63862300	H	2.70695200	-1.15954200	0.51671900
O	2.31146500	1.48379600	0.82896000	O	2.71865000	2.38943400	0.38977600
H	1.83167500	1.49350600	-0.02956500	H	2.69956700	1.47706100	0.05301000
C	1.55204900	2.66936900	-2.54375300	C	2.84336400	0.14006200	-2.99904100
C	2.25234900	-3.15493500	-0.94045600	C	1.52890500	-3.58939500	1.78705700
C	1.94022000	1.35570400	3.18624400	C	1.38750700	3.40834500	2.05071400
H	0.25552400	-0.05211700	0.35019300	C	2.13223500	-4.21307500	0.52463500
C	1.97674200	2.70056500	-4.01984400	H	2.15759900	-5.30197400	0.61830900
H	1.22727700	2.25122000	-4.67160900	H	1.53375900	-3.94888200	-0.34593700
H	2.10319700	3.74135200	-4.32558600	H	3.14918000	-3.85361800	0.36781200
H	2.92899900	2.18917000	-4.16323500	C	2.39812600	-3.93978400	3.00710600
C	0.16569000	3.30158900	-2.39148000	H	1.92379500	-3.63739400	3.94224900
H	-0.60312700	2.73821900	-2.92247200	H	2.55437100	-5.02087300	3.04809700
H	-0.11685900	3.40285400	-1.34301000	C	3.37193100	-3.45480300	2.92776700
C	0.19300000	4.30517700	-2.82057700	C	0.10849500	-4.13143400	1.98830700
H	2.56903200	3.46571400	-1.71707300	H	-0.38374700	-3.67309400	2.84788200
H	2.58055400	4.49843700	-2.07211600	H	-0.50568800	-3.96677200	1.10091500
H	2.30708200	3.47440300	-0.66077100	H	0.16037700	-5.20823600	2.16468400

H	3.56946800	3.04953400	-1.82112100	C	2.14510900	2.59709200	3.10726700
C	2.65017700	2.68318500	3.49843000	H	2.09984800	3.10794800	4.07289800
H	1.94529800	3.49620200	3.67277300	H	1.69713000	1.60990600	3.21109400
H	3.24451500	2.56169600	4.40665300	H	3.18956100	2.47374700	2.82391000
H	3.32653500	2.95918100	2.68788600	C	-0.04939000	3.64708300	2.52844400
C	0.85034700	1.07902000	4.22908700	H	-0.66013900	4.12592800	1.76043600
H	0.06218000	1.83322100	4.20589400	H	-0.52320200	2.71409900	2.83566300
H	0.40573100	0.09362400	4.07759100	H	-0.02529800	4.30889900	3.39709900
H	1.30022200	1.09550100	5.22370200	C	2.08559200	4.76091500	1.82520900
C	2.96619500	0.22090000	3.22540000	H	2.20706500	5.27205600	2.78358500
H	3.37601000	0.14652300	4.23499000	H	3.07412500	4.61236500	1.38934900
H	2.49808700	-0.72840500	2.97872400	H	1.50201700	5.41184900	1.17128800
H	3.79286500	0.40123600	2.53848500	C	4.19265500	-0.43139200	-2.52615100
C	3.02341100	-2.55494800	-2.11832800	H	4.24097400	-1.51826900	-2.59760600
H	3.22382700	-3.34277500	-2.84792500	H	4.99977500	-0.02034000	-3.13749300
H	2.43931900	-1.78215300	-2.60895500	H	4.38173700	-0.15412300	-1.48868100
H	3.97642700	-2.13521400	-1.79867800	C	2.88927900	1.67509900	-2.92091100
C	3.14512600	-4.19307000	-0.24075700	H	3.68307300	2.05402600	-3.57000500
H	2.60349300	-4.76057500	0.51651100	H	1.93623600	2.09403900	-3.24688400
H	3.51255600	-4.90113900	-0.98689100	H	3.07894500	2.02734200	-1.91088100
H	4.00958300	-3.71388900	0.22114400	C	2.55514200	-0.23234800	-4.46262400
C	0.98299400	-3.83045300	-1.47073700	H	2.63529200	-1.29908300	-4.66317800
H	0.35551600	-4.21708800	-0.66595800	H	1.55132800	0.09371700	-4.74421900
H	0.40015600	-3.14494900	-2.08786200	H	3.27294000	0.28568100	-5.10156600
H	1.27241300	-4.67643000	-2.09738900	I	-5.03314200	-0.20190900	-0.38005500
I	-4.66717800	-0.58607100	-0.02328800	H	-6.65535400	-0.28998000	-0.50394400
<b>[L(HI), 35I, E<sub>0</sub>=-8650.972242 au</b>							
O	1.17119100	1.06651700	0.52235000				
O	-3.18160200	-1.10000900	1.63022100				
O	3.23586200	-0.76940000	0.61680500				
N	1.19821200	2.48894000	0.40554100				
N	-2.99084300	-0.21245300	0.52600900				
N	2.79010000	-1.51932500	-0.53580200				
N	0.05470100	-0.21167600	-2.36989000				
C	1.22834200	0.77374500	-2.21136900				
C	0.72746500	2.18302000	-2.06960100				
C	0.19805400	2.77197700	-3.22691500				
C	-0.40965300	4.01811300	-3.21459200				
C	-0.51636300	4.69617300	-2.00253000				
C	0.00525300	4.13566000	-0.84660800				
C	0.66785700	2.89777100	-0.85043500				
C	2.57097600	3.00257400	0.77173100				
C	3.63690200	2.53743900	-0.23357300				
C	2.53937300	4.53574100	0.80941600				
C	2.88113700	2.48963500	2.18345300				
C	-1.08769000	0.06679800	-1.42434000				
C	-2.32859900	-0.72252700	-1.73899000				
C	-2.60148500	-1.29289700	-2.98376600				
C	-3.67651800	-2.16064600	-3.15067800				
C	-4.48043000	-2.47670300	-2.05730600				
C	-4.25847300	-1.86309800	-0.82978400				
C	-3.22173100	-0.93998400	-0.67716500				
C	-3.85194200	1.01225700	0.72612000				
C	-5.33830900	0.64616700	0.86080400				
C	-3.36238100	1.70076300	2.00296500				
C	-3.65287800	1.96605600	-0.45816700				
C	0.55521600	-1.67301700	-2.39215700				
C	0.54896200	-2.36311700	-1.05914300				
C	-0.57809300	-3.11398000	-0.70397900				
C	-0.68316200	-3.69753600	0.55075500				
C	0.34978500	-3.53746700	1.46753400				
C	1.49817500	-2.84254900	1.11214000				
C	1.62312100	-2.27488500	-0.15507300				
C	3.98735100	-2.30913500	-0.98373300				
C	3.58873300	-3.20178800	-2.16411200				
C	4.56572500	-3.18434600	0.14083300				

C	5.03431800	-1.28950500	-1.44948400				
H	-0.31129300	-0.03407400	-3.30544100				
H	1.82048000	0.40747800	-1.38912200				
H	1.80230200	0.66097900	-3.13308900				
H	0.27569800	2.23062700	-4.16656500				
H	-0.80619000	4.44522500	-4.12718300				
H	-1.02139700	5.65341600	-1.95273700				
H	-0.11135300	4.63744100	0.10308200				
H	3.41783400	2.90987300	-1.23815000				
H	3.71404500	1.45124200	-0.26168900				
H	4.61493100	2.92739600	0.05891400				
H	2.36386100	4.97312300	-0.17421700				
H	3.50869600	4.89245000	1.16325000				
H	1.77356600	4.89331400	1.50012800				
H	2.06843500	2.74189600	2.86640000				
H	3.80279300	2.95443300	2.54109300				
H	3.01578300	1.41012300	2.21658200				
H	-1.26317800	1.13510700	-1.48957500				
H	-0.75232600	-0.14425500	-0.41324000				
H	-1.96342000	-1.09966300	-3.84145600				
H	-3.86797300	-2.60570400	-4.11958400				
H	-5.29386000	-3.18407400	-2.16814300				
H	-4.87553200	-2.09272800	0.02705900				
H	-5.46671000	-0.10871600	1.63725800				
H	-5.74946000	0.26726500	-0.07780700				
H	-5.91230200	1.53182000	1.14421800				
H	-3.90517600	2.63972300	2.14246500				
H	-2.29337600	1.90704400	1.94431600				
H	-3.52518700	1.07114600	2.87605500				
H	-2.62592000	2.33389300	-0.49923800				
H	-4.30434900	2.83217200	-0.32328500				
H	-3.91141300	1.50387800	-1.41330700				
H	1.54627800	-1.61353700	-2.82745500				
H	-0.10616400	-2.19828700	-3.07649600				
H	-1.39469000	-3.21174500	-1.40730400				
H	-1.58302800	-4.23417200	0.82208900				
H	0.25649200	-3.93128600	2.47124400				
H	2.28153400	-2.67642100	1.83525000				
H	3.30391300	-2.61213400	-3.03874200				
H	2.77159700	-3.87771000	-1.90707900				
H	4.44893800	-3.81016200	-2.45019100				
H	3.87330700	-3.98022400	0.42059600				
H	4.78249400	-2.58204000	1.02223200				
H	5.49422500	-3.64961700	-0.19922700				
H	5.89727300	-1.80684800	-1.87571700				
H	5.37122800	-0.67408200	-0.61690400				
H	4.60983200	-0.63337500	-2.21397900				
H	0.65995200	0.86083000	1.35934700				
H	-2.33729900	-1.00141000	2.12622500				
H	2.56639000	-0.05967200	0.68139000				
I	-0.20345800	-0.22244300	3.24449500				
<b>L, 36a, E<sub>0</sub>=-1730.840272 au</b>				<b>L, 36b, E<sub>0</sub>=-1730.835542 au</b>			
N	-0.05825200	-0.03241400	1.57383100	N	0.10796300	0.06652000	1.62203200
C	0.32990400	-1.34811000	2.13230000	C	-1.04410100	-0.74238200	2.06936600
H	-0.48082500	-2.04092300	1.90837300	H	-1.93609300	-0.23126900	1.72512500
H	0.43772700	-1.27728300	3.22612900	H	-1.07695600	-0.77201500	3.17128500
C	-1.40513200	0.37245600	2.03026900	C	-0.08071100	1.48734900	1.97614100
H	-1.55304300	1.38780400	1.68354500	H	0.80892500	2.01258700	1.64875500
H	-1.43128400	0.38641300	3.13232900	H	-0.11890600	1.58359400	3.07440500
C	0.94500200	0.98995800	1.96108600	C	1.37153000	-0.42173400	2.22155200
H	1.91866800	0.56387700	1.74780900	H	1.43704700	-1.48829800	2.01198700
H	0.88005800	1.17188800	3.04604600	H	1.35143000	-0.27553200	3.31382700
C	1.60236800	-1.89299000	1.53403100	C	-1.01347500	-2.15129400	1.53152400
C	2.76740800	-1.95959400	2.29587300	C	-0.54026600	-3.19282400	2.33460100
C	1.61463800	-2.37842000	0.20837200	C	-1.41730800	-2.44175100	0.21855500
C	3.93723800	-2.51347300	1.78269500	C	-0.42033800	-4.48892000	1.84600700



H	2.74845500	-1.58796400	3.31483500	H	-0.24901100	-2.97336300	3.35625600
C	2.80094300	-2.90615100	-0.30690100	C	-1.25862900	-3.73667200	-0.28185900
C	3.94789600	-2.99036200	0.47762600	C	-0.76527700	-4.75534600	0.52383500
H	4.82924300	-2.56785900	2.39521500	H	-0.04506300	-5.27917200	2.48554300
H	2.84081600	-3.24968500	-1.32834400	H	-1.49962900	-3.93015400	-1.31647300
H	4.85409300	-3.40898700	0.05566000	H	-0.65051500	-5.75428300	0.11907300
C	0.79157500	2.29310800	1.21738600	C	2.58496500	0.25826100	1.64100200
C	0.07040500	3.34894200	1.78395000	C	3.27493300	1.22419300	2.37225700
C	1.34979200	2.46474800	-0.05928100	C	3.02582000	-0.07356300	0.34275000
C	-0.14766700	4.53198800	1.08696900	C	4.38813300	1.87127400	1.84468800
H	-0.33150900	3.23280500	2.78494700	H	2.93153800	1.46827600	3.37178300
C	1.08387500	3.63367000	-0.77806100	C	4.13112000	0.59775400	-0.18703700
C	0.34255400	4.66265400	-0.21008300	C	4.81224200	1.55522200	0.55895800
H	-0.71299200	5.33592700	1.54338200	H	4.91378100	2.61684200	2.42926700
H	1.44716800	3.71543700	-1.79213000	H	4.46435100	0.38259100	-1.18949100
H	0.14767100	5.56439900	-0.77897000	H	5.66795300	2.06026200	0.12604200
C	-2.51955000	-0.50844400	1.52070700	C	-1.31808900	2.14240300	1.41049600
C	-3.04125500	-1.50807200	2.34794500	C	-2.35410400	2.45793300	2.29802600
C	-3.04395100	-0.36185100	0.22595100	C	-1.48275700	2.45564500	0.04930400
C	-4.03018000	-2.37727600	1.90259400	C	-3.53809500	3.04500100	1.87031800
H	-2.65040200	-1.60869800	3.35503400	H	-2.22514900	2.21708100	3.34790300
C	-4.01925700	-1.25451100	-0.22749600	C	-2.68270000	3.03732500	-0.37754900
C	-4.51014900	-2.25535200	0.60089900	C	-3.70230600	3.32978000	0.51783500
H	-4.41295500	-3.14933800	2.55965000	H	-4.32515400	3.26636800	2.58145600
H	-4.36230600	-1.17308500	-1.24850600	H	-2.81499000	3.22134000	-1.43339400
H	-5.26644000	-2.93817900	0.23093700	H	-4.62214500	3.77694000	0.15865400
N	0.37299400	-2.31336600	-0.49130500	N	-1.94319000	-1.36303900	-0.58294200
N	-2.50580900	0.67154900	-0.62038800	N	-0.45931100	2.10061400	-0.89987300
N	2.17050100	1.40951700	-0.58409400	N	2.27072300	-1.08714300	-0.32652000
O	0.15624000	-0.94943400	-0.95370200	O	-1.26476700	-1.38358200	-1.87516000
H	-0.02074400	-0.45697700	-0.09132300	H	-0.33579100	-1.18846800	-1.61968300
O	1.71854300	1.10273900	-1.91599600	O	1.08253300	-0.45790600	-0.88602500
H	1.27640000	0.24578000	-1.76701500	H	0.57598800	-0.16703900	-0.07332600
O	-2.26641100	0.09882700	-1.92595200	O	-1.12468800	1.63671200	-2.09417500
H	-1.35529400	-0.22712200	-1.82662200	H	-1.10661800	0.66993000	-2.01474200
C	-0.00457100	-3.26797300	-1.56167700	C	-3.41753900	-1.41785800	-0.85977700
C	3.64466700	1.66858300	-0.63450400	C	2.86440800	-1.97668000	-1.35370100
C	-3.35411700	1.88799900	-0.83790600	C	0.47319500	3.19370000	-1.34703800
C	4.30289100	0.35005300	-1.05261700	C	-3.85912700	-2.68063600	-1.62092100
H	5.39126400	0.45206100	-1.03885600	H	-3.77272500	-3.57930400	-1.00869100
H	4.01575000	-0.44567300	-0.36700900	H	-4.90726100	-2.57611100	-1.91163400
H	3.99262500	0.06885500	-2.05890700	H	-3.26653200	-2.80762300	-2.52806900
C	4.03115800	2.77982600	-1.62581700	C	-4.13704300	-1.34683300	0.49310700
H	3.70292200	3.76194100	-1.28144200	H	-3.85544100	-2.17334100	1.14827700
H	5.11830000	2.81221300	-1.73498700	H	-3.92651000	-0.40246900	0.99825000
H	3.59355000	2.58018800	-2.60480100	H	-5.21448900	-1.40460600	0.32400400
C	4.11660700	2.04325900	0.77567900	C	-3.78620300	-0.17923500	-1.68206100
H	3.63097100	2.95061100	1.13919900	H	-4.87217800	-0.13333600	-1.79659400
H	3.92625600	1.23358000	1.48278800	H	-3.44930900	0.72544500	-1.18181800
H	5.19385100	2.22317500	0.75423700	H	-3.33722700	-0.21479400	-2.67409700
C	-2.51370900	2.85957700	-1.67339000	C	-0.27173400	4.34964600	-2.03593000
H	-3.02807400	3.82077200	-1.75708200	H	-0.91278800	4.88976700	-1.33601000
H	-1.54679400	3.01895300	-1.19860600	H	0.45293300	5.05887500	-2.44392700
H	-2.34540400	2.46305000	-2.67378700	H	-0.88201800	3.97463500	-2.85819900
C	-3.65900100	2.52203300	0.52398000	C	1.24141200	3.72839000	-0.13459300
H	-4.15971700	1.82219100	1.19610400	H	0.57070400	4.09869400	0.64366200
H	-2.74930400	2.89022300	0.99960100	H	1.90044300	2.96614600	0.28218100
H	-4.32421100	3.37529200	0.37367700	H	1.86632100	4.56414000	-0.45728800
C	-4.67296600	1.57405600	-1.56582500	C	1.47135700	2.55754900	-2.32270700
H	-5.17946200	2.50863000	-1.81991200	H	2.25505000	3.27945200	-2.56794400
H	-4.47846400	1.02889100	-2.49007300	H	1.92092400	1.67627400	-1.86834000
H	-5.34929400	0.98709700	-0.94138700	H	0.97343800	2.25495200	-3.24297400
C	0.62555500	-2.94805700	-2.92970100	C	1.88437000	-3.14965700	-1.52364800
H	1.71328700	-3.02172800	-2.92356500	H	2.32876300	-3.91302000	-2.16729500
H	0.24800300	-3.64712200	-3.67997200	H	1.65518200	-3.59121200	-0.55390500
H	0.35884100	-1.93910600	-3.24570300	H	0.94875300	-2.83123300	-1.97967600

C	-1.53607000	-3.20613600	-1.68486900	C	3.07720100	-1.31197000	-2.72842600
H	-1.87779800	-3.94732500	-2.41208700	H	3.89535400	-0.59195800	-2.73442300
H	-1.99701200	-3.41969000	-0.71954000	H	3.31217800	-2.07886600	-3.47074600
H	-1.88080600	-2.22818500	-2.00886100	H	2.16952900	-0.79724200	-3.04318900
C	0.35657900	-4.68656800	-1.09165300	C	4.17601000	-2.54041000	-0.78842200
H	1.42629900	-4.88709600	-1.09733900	H	4.95822000	-1.78807800	-0.69655100
H	-0.01704300	-4.85475800	-0.07902300	H	4.00464900	-2.97734400	0.19812700
H	-0.12492700	-5.40675400	-1.75596900	H	4.53977900	-3.32649400	-1.45329200
<b>L, 36c, E<sub>0</sub>=-1730.823127 au</b>				<b>L, 36d, E<sub>0</sub>=-1730.822443 au</b>			
N	-0.05681100	-0.05148300	1.56877800	N	-0.84754500	0.23268300	-0.43449400
C	0.50829800	1.21633400	2.03155200	C	-1.84590900	0.50797400	-1.46000600
H	1.55597800	1.22603400	1.74334100	H	-2.00387700	-0.42758000	-1.99999900
H	0.46305000	1.29745200	3.13499600	H	-1.49921100	1.24351000	-2.20540200
C	0.76861900	-1.19201900	1.97935300	C	-0.51973400	1.30898900	0.50306500
H	0.27006500	-2.08505900	1.62186400	H	0.06940200	0.85598500	1.29649100
H	0.79842200	-1.26375700	3.08419300	H	-1.45332600	1.66773000	0.94208600
C	-1.43437400	-0.22405100	2.05220000	C	0.29161200	-0.54510200	-0.90059600
H	-1.98663400	0.67140600	1.78372500	H	1.13689400	0.08013800	-1.21070400
H	-1.45148600	-0.31764900	3.15534500	H	-0.03055500	-1.07520800	-1.79937500
C	-0.18926600	2.40970400	1.42592900	C	-3.16526900	1.00447500	-0.90080300
C	-1.14197800	3.11616800	2.16411300	C	-3.66310300	2.23228200	-1.35092000
C	0.08006900	2.82289700	0.11262400	C	-3.89699000	0.31304400	0.08017700
C	-1.84085400	4.18714000	1.61663800	C	-4.80410100	2.80775200	-0.80428500
H	-1.34086600	2.80934000	3.18509900	H	-3.12305100	2.75289100	-2.13354500
C	-0.64345700	3.88051100	-0.44481000	C	-5.00700400	0.92345500	0.67412500
C	-1.59992600	4.56265100	0.29919500	C	-5.45926700	2.16328200	0.24119300
H	-2.57775100	4.71557000	2.20991300	H	-5.15932800	3.76399200	-1.17016500
H	-0.47169300	4.17507900	-1.47149600	H	-5.50018600	0.41764200	1.49131900
H	-2.15319300	5.37896700	-0.14973200	H	-6.32456000	2.61719600	0.71020400
C	-2.10293300	-1.43077200	1.44146900	C	0.74151700	-1.57375300	0.12673100
C	-2.20368800	-2.62584100	2.15905500	C	-0.24173800	-2.10343800	0.96975100
C	-2.56303500	-1.39641300	0.11777700	C	2.05825400	-2.03903300	0.26824600
C	-2.69661400	-3.78399400	1.56751000	C	0.05924400	-3.03219600	1.95550700
H	-1.86249800	-2.64852400	3.18859100	H	-1.25190900	-1.75137800	0.80822500
C	-3.00854800	-2.57307000	-0.49073400	C	2.36538700	-2.95685500	1.28078600
C	-3.07561400	-3.76143800	0.22752700	C	1.37878900	-3.44759100	2.12371300
H	-2.75793800	-4.70291700	2.13884500	H	-0.72733300	-3.42366800	2.59077800
H	-3.28119500	-2.55458300	-1.53585400	H	3.39579800	-3.25141100	1.41286800
H	-3.42318700	-4.66634800	-0.25748600	H	1.63943600	-4.15562100	2.90193600
C	2.19418600	-1.17107300	1.48079600	C	0.23275600	2.48182400	-0.10793400
C	3.21039600	-0.84849600	2.38832800	C	-0.48386500	3.50598500	-0.73715300
C	2.55114900	-1.46669300	0.15385600	C	1.63541000	2.54490200	-0.13252900
C	4.54596600	-0.79039100	2.00976100	C	0.15704100	4.52108500	-1.43735600
H	2.93347600	-0.62701200	3.41371300	H	-1.56397100	3.49954300	-0.66991000
C	3.89694500	-1.39357400	-0.22607900	C	2.28095500	3.54288900	-0.87063500
C	4.88789300	-1.05965500	0.68730400	C	1.54758200	4.52190600	-1.52794900
H	5.30798500	-0.52971800	2.73503600	H	-0.42378000	5.29987300	-1.91833800
H	4.14735800	-1.56464500	-1.26256800	H	3.35976700	3.52696200	-0.93316800
H	5.92222300	-1.00902500	0.36625800	H	2.05964600	5.29159200	-2.09414000
N	1.11791200	2.13162000	-0.60738900	N	-3.47590700	-1.00601000	0.47539000
N	1.52674400	-1.76429600	-0.81450600	N	2.37425600	1.55458400	0.60302500
N	-2.52617100	-0.13211500	-0.56424300	N	3.10936500	-1.54012100	-0.59510100
O	0.55672400	1.45973400	-1.74652300	O	-3.48568800	-1.05705400	1.92317000
H	0.22273300	1.22236600	-2.37175300	H	-2.54978600	-0.95601100	2.13498200
O	-1.78362500	-0.29883300	-1.78747300	O	4.33659900	-1.49859200	0.16951400
H	-0.94033200	0.12341100	-1.56245500	H	4.42797500	-0.54926400	0.34901100
O	1.87265700	-1.05720000	-2.02789500	O	3.49500700	1.13704400	-0.21241600
H	1.35445300	-0.24158600	-1.95431100	H	3.14279200	0.31595300	-0.62483100
C	2.34990300	2.89612100	-0.97669600	C	-4.30251800	-2.15211100	-0.02426400
C	-3.83739700	0.50369700	-0.88431000	C	3.42198000	-2.35356800	-1.82979900
C	1.34254000	-3.20191600	-1.20165100	C	2.90952200	1.97473300	1.94002000
C	-3.52126800	1.90045700	-1.43016400	C	4.03475500	3.01639100	1.82467900
H	-4.44627200	2.45616600	-1.60497700	H	3.66071200	3.96499500	1.43554100
H	-2.90947000	2.44943000	-0.71616800	H	4.46347400	3.20423700	2.81234400
H	-2.97769100	1.82757300	-2.37272600	H	4.82732200	2.65477900	1.16892500
C	-4.67281900	-0.27413200	-1.91722000	C	3.42665100	0.71199000	2.64160200

H	-5.06556900	-1.20384200	-1.50336600	H	2.68052400	-0.08297800	2.59494600
H	-5.52461700	0.33327300	-2.23442900	H	4.34789300	0.34621100	2.18872500
H	-4.06821500	-0.50187800	-2.79656600	H	3.64397600	0.93296200	3.68948800
C	-4.61947100	0.64053200	0.42784400	C	1.75736300	2.56119300	2.76654600
H	-4.83696700	-0.33253700	0.87143100	H	1.32041700	3.43945500	2.29038700
H	-4.06248200	1.23824800	1.15229900	H	0.96972000	1.82527800	2.93380100
H	-5.56929800	1.14289500	0.23009800	H	2.14641600	2.86301100	3.74122900
C	0.19593600	-3.24075000	-2.21960300	C	4.46459100	-1.56082100	-2.62653700
H	-0.10378300	-4.27712500	-2.39800300	H	5.39453400	-1.46869100	-2.06721300
H	-0.65891500	-2.68126700	-1.84273100	H	4.67549200	-2.06931900	-3.57017500
H	0.50355600	-2.79790500	-3.16624900	H	4.09215000	-0.55829900	-2.85244600
C	0.93481000	-3.99417000	0.04432100	C	3.96637200	-3.74258700	-1.46626200
H	1.67434200	-3.90447900	0.84314800	H	4.24776300	-4.27357300	-2.37880800
H	-0.03848800	-3.67167200	0.41324400	H	4.84790700	-3.65747500	-0.83126900
H	0.85731600	-5.05149500	-0.21967900	H	3.21366100	-4.33874500	-0.94699400
C	2.60806600	-3.82300400	-1.81834400	C	2.15292100	-2.50317500	-2.67110000
H	2.37644600	-4.82287700	-2.19450900	H	1.36564400	-3.02768600	-2.12769600
H	2.96166100	-3.21870500	-2.65492600	H	1.77849100	-1.53272700	-2.99785300
H	3.41090800	-3.91857200	-1.08449600	H	2.39280400	-3.08825000	-3.56130800
C	2.13001800	4.00474400	-2.02489600	C	-3.59099100	-3.44114700	0.40620000
H	1.55037800	4.83917600	-1.63033900	H	-4.13211600	-4.30914200	0.02221900
H	3.09938000	4.39608400	-2.34079700	H	-2.57188400	-3.46696400	0.01777400
H	1.64021000	3.62342700	-2.92680200	H	-3.55018900	-3.51351000	1.49296900
C	3.37152100	1.88593000	-1.50816500	C	-5.74083500	-2.15216500	0.52235500
H	4.32271700	2.39156200	-1.69211700	H	-6.24433800	-3.07520400	0.22442700
H	3.52928300	1.09124700	-0.78229000	H	-5.73595300	-2.10326500	1.61219900
H	3.04140500	1.42940700	-2.44085100	H	-6.32127500	-1.31525500	0.13154900
C	2.88630600	3.51383900	0.32131700	C	-4.32855900	-2.07683100	-1.55471700
H	2.18680900	4.23300900	0.75022100	H	-4.79320600	-1.15477300	-1.90778100
H	3.08973900	2.73676400	1.05982100	H	-3.31930000	-2.14197500	-1.96480600
H	3.82261500	4.03397000	0.10833600	H	-4.90692300	-2.91776300	-1.94349400
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H	-1.61121100	3.16571000	-2.92581100				
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H	1.88119200	-0.40378500	1.01174400				
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C	-0.08474200	-1.59292700	-0.21049900				
H	-0.78578400	-1.61589700	-1.05038000				
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H	-2.48544700	-2.72268600	4.47954100				
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C	-2.17815700	-2.11530300	1.14813500				
C	-3.44845400	-3.17561500	-0.72840900				
C	-4.08031700	-2.73138700	-2.05322600				
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C	-2.24517100	-4.08121400	-1.01760800				
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H	-2.59624500	-4.97543600	-1.53713800				
H	-1.74741200	-4.39821700	-0.10028900				
C	-4.47796200	-3.94296400	0.11673900				
H	-4.87770700	-4.77948200	-0.46181900				

H	-5.30642100	-3.29173200	0.39684700
H	-4.02449300	-4.34891200	1.02258600
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H	-1.10222200	0.40112300	1.05451500
H	-1.29749600	0.72105600	-0.66560300
C	-0.09883600	2.15257600	0.36097000
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H	-3.46488100	5.22563000	-1.11631800
H	-2.85873100	5.09193800	0.54625700
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C	-4.29349200	2.57019000	-1.36856400
H	-4.05915100	1.51988200	-1.56704800
H	-4.29992700	3.09988600	-2.32126100
H	-5.29274600	2.63015700	-0.93130500
C	-3.29164700	2.43650300	0.92420800
H	-2.54835900	2.82578100	1.62105300
H	-3.12673300	1.36527400	0.81077700
H	-4.27817300	2.57516700	1.37131100
C	1.24108100	0.10908200	-1.32954000
H	1.68046200	1.09457300	-1.17330000
H	0.53564200	0.17527200	-2.17317800
C	2.33046300	-0.87414900	-1.68132000
C	2.18387000	-1.68658400	-2.80524500
H	1.27765000	-1.60128900	-3.39544200
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H	3.04398000	-3.20006900	-4.07035900
C	4.32971800	-2.68615700	-2.42123900
H	5.10909100	-3.38801400	-2.69531700
C	4.48640100	-1.89534800	-1.28640200
H	5.37979000	-2.00617000	-0.69323100
C	3.50662500	-0.97389500	-0.90478100
C	4.88290000	0.36700600	0.78266300
C	5.75521200	0.88716700	-0.36790700
H	5.19014500	1.59485300	-0.97902900
H	6.12063300	0.09294000	-1.01766200
H	6.62076400	1.40754000	0.04813700
C	5.62297500	-0.68902600	1.62813700
H	6.04996700	-1.49307000	1.02859300
H	4.93615800	-1.12854200	2.35136600
H	6.44423400	-0.21578500	2.17252800
C	4.53509600	1.55907100	1.69146300
H	3.88910600	1.24028300	2.50912400
H	4.01784900	2.32679400	1.11489100
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