

Supplementary Information

Role of the Lewis acid bulkiness on the stereoselectivity of Diels-Alder reactions between acyclic dienes and α,β -enals

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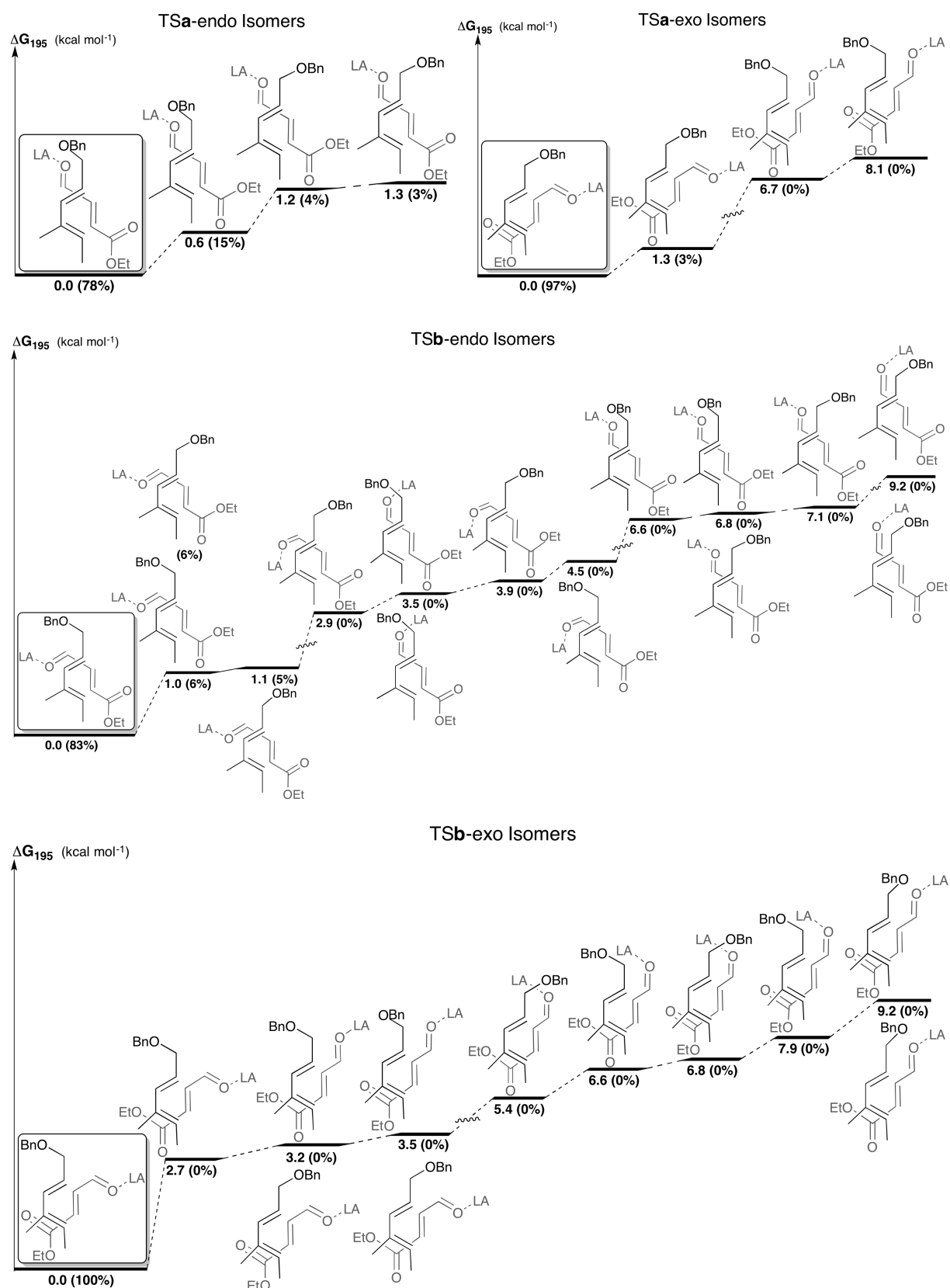


Figure S1. Energetic analysis for the endo/exo-TS structures coordinated to the Lewis acid $B(C_6F_5)_3$ (a) and $AlCl_3$ (b). ΔG_{195} : Relative free energies at 195.15 K with respect to the most stable structure (in kcal mol⁻¹). Isomer population estimated via standard Boltzmann distribution analysis (in parentheses). Calculations were obtained at the PCM(DCM)-B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/def2-SVP level. Dienophile lies behind the diene and it is shown in colour grey for clarity.

Table S1. Energy barriers (and its contributions) and overall reaction energies relative to the isolated reactants, and reactant complexes (in parentheses) for **a**– (B(C₆F₅)₃) and **b**–catalysed (AlCl₃), and non–catalysed Diels-Alder reactions between diene **1** and α,β –enal **2**. Endo:exo ratios were estimated as a function of the TSs free energy differences at 195.15 K by standard Boltzmann distribution analysis. All data (in kcal mol^{–1}) were computed at the PCM(DCM)-B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/def2-SVP level.

LA-reaction	$\Delta E^\ddagger(\text{ZPE})$	$\Delta E^\ddagger_{\text{strain}} \text{ [a]}$	$\Delta E^\ddagger_{\text{int}} \text{ [a]}$	$\Delta G^\ddagger_{(195)}$	endo:exo	$\Delta E_{\text{R}}(\text{ZPE})$	$\Delta G_{\text{R}(195)}$
a–endo	–9.5 (6.7)	33.2	–43.2	3.2 (8.1)	0:100	–38.6 (–22.4)	–25.3 (–20.4)
a–exo	–14.7 (4.4)	28.6	–46.1	–2.0 (5.6)		–37.4 (–18.3)	–24.2 (–16.6)
b–endo	–15.6 (1.3)	18.9	–36.2	–4.5 (2.2)	99:1	–36.5 (–19.6)	–25.7 (–19.0)
b–exo	–14.1 (4.2)	26.7	–43.1	–2.7 (4.4)		–33.8 (–15.5)	–22.6 (–15.5)
endo	3.9 (11.1)	27.3	–25.1	15.5 (12.9)	94:6	–30.7 (–23.5)	–19.3 (–21.9)
exo	4.9 (12.9)	29.9	–27.2	16.6 (14.6)		–31.2 (–23.1)	–19.1 (–21.1)

[a] The activation strain $\Delta E^\ddagger_{\text{strain}}$ and the TS interaction $\Delta E^\ddagger_{\text{int}}$ do not include ZPE-correction.

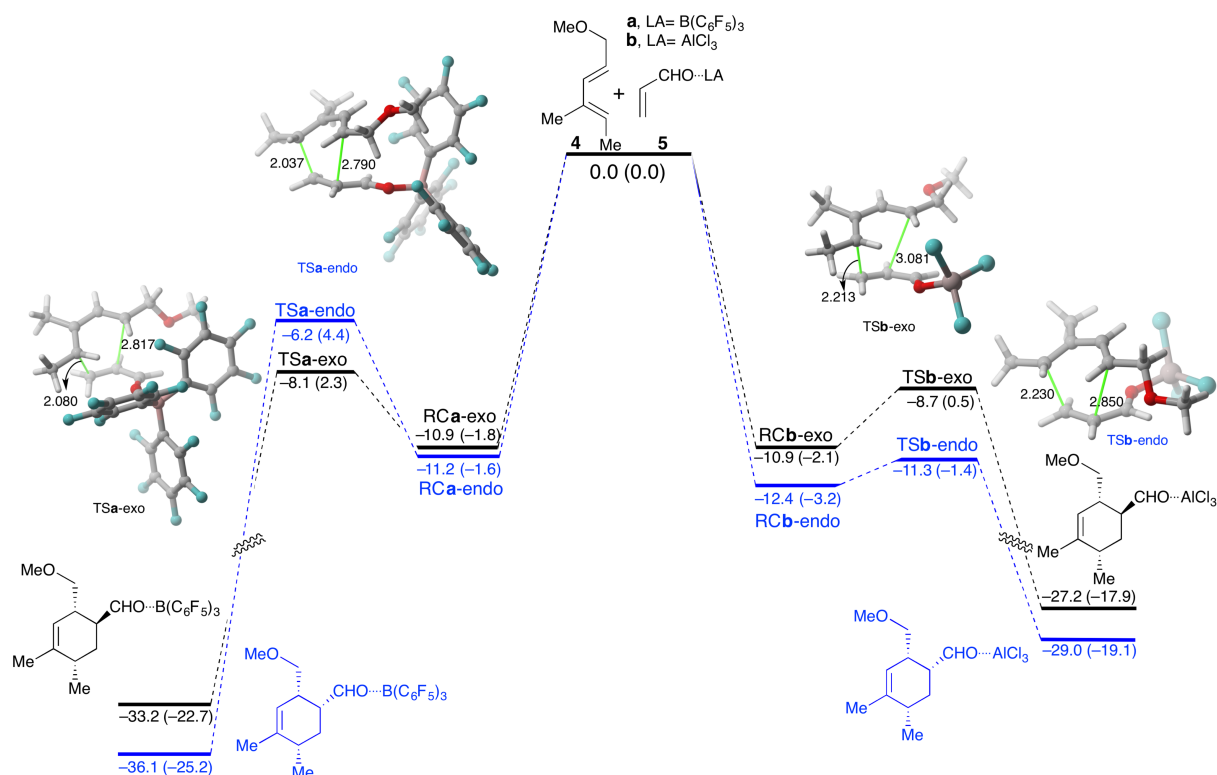


Figure S2. Comparison between the computed reaction profiles for the $\text{B}(\text{C}_6\text{F}_5)_3$ - (a, left side) and AlCl_3 -catalysed (b, right side) Diels-Alder reactions between diene **4** and acrolein **5**. Relative energies plus ZPE (in kcal mol⁻¹) together with free energies at 195.15 K (in parentheses) were obtained at the PCM(DCM)-B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/def2-SVP level. Transition states bond distances are given in angstroms.

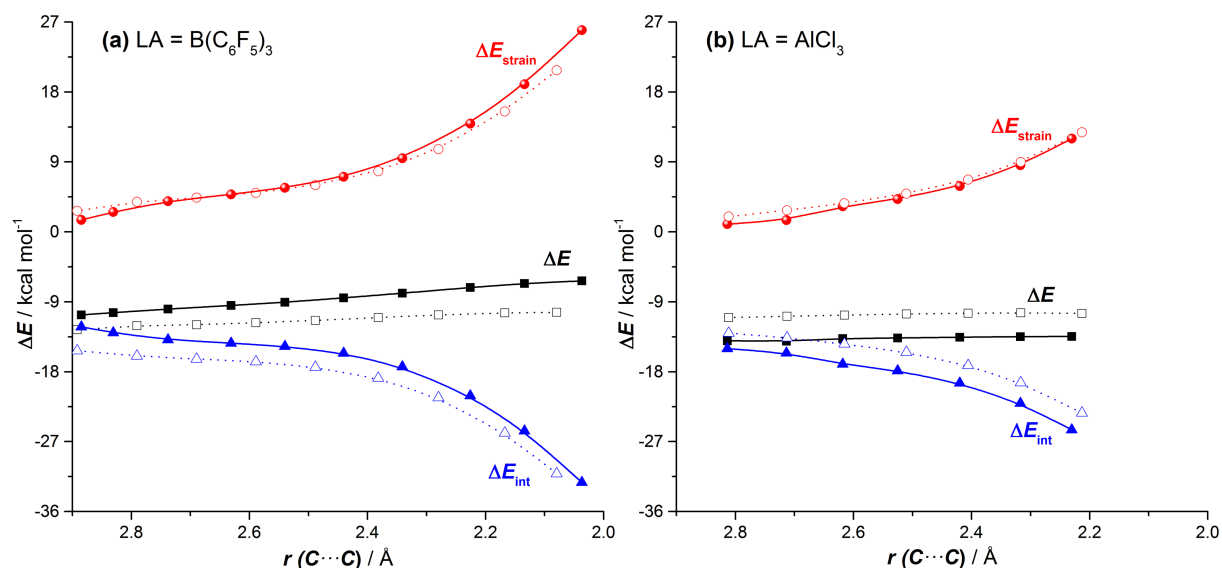


Figure S3. Activation-strain analysis of the endo- (solid lines) and exo-pathways (dotted lines) of the $\text{B}(\text{C}_6\text{F}_5)_3$ – (a) and AlCl_3 –catalysed (b) Diels-Alder cycloadditions between diene **4** and acrolein **5** along the reaction coordinate projected onto the forming shortest C...C bond distance. All energies were computed at the PCM(DCM)-B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/def2-SVP level.

Cartesian coordinates (in Å) and electronic energies (in a. u.) of all the stationary points discussed in the text. Calculations reported at B3LYP-D3BJ/def2-SVP level.

a-endo

1: E= -619.117986294

H	-3.99737200	-0.58915600	-0.02103500
C	-4.55438000	2.05371200	-0.01201100
C	-5.80558900	2.76989000	-2.79069600
H	-5.14059800	0.71116900	-3.18515200
H	-3.06931800	-0.41747400	-2.94241800
C	-2.59966800	-2.17681100	-1.70939100
H	-5.09899900	2.99502900	-0.15994600
H	-3.51731400	2.29992000	0.27431200
H	-5.00145400	1.53527600	0.85376600
H	-5.80273000	3.51748600	-1.98562000
H	-6.85454300	2.60321000	-3.09405100
H	-5.30182400	3.22046500	-3.66480000
H	-2.93626900	-2.88990700	-2.49587900
O	-2.91680800	-2.66583400	-0.43458400
H	-1.49589900	-2.09801800	-1.83389900
C	-2.30531000	-3.88804300	-0.11527300
H	-1.20276300	-3.77536600	-0.05647700
C	-3.92630400	-0.15501600	-1.02452300
C	-4.57562300	1.15615600	-1.22549200
C	-5.14549200	1.48154600	-2.40511100
C	-3.22715100	-0.83781500	-1.94273900
C	-2.84053300	-4.41326000	1.19388300
C	-2.05639400	-5.25802900	1.99031600
C	-4.13943500	-4.09556200	1.61202900
C	-2.56311600	-5.78634500	3.17995600
H	-1.03637500	-5.50185800	1.67896500
C	-4.64412700	-4.61754400	2.80535900
H	-4.74337700	-3.42870600	0.99512500
C	-3.85992200	-5.46641400	3.59166100
H	-1.93980600	-6.44301000	3.79194900
H	-5.65725700	-4.35911700	3.12376200
H	-4.25595300	-5.87374000	4.52506400
H	-2.49961000	-4.63145200	-0.91975600

2: E= -2665.51644229

C	-1.79199900	2.35131600	-3.34453700
C	-1.20471900	1.22183800	-2.90468500
C	-0.48800100	1.22138700	-1.65136100
H	-0.43917600	2.15125300	-1.06248000
O	0.06003500	0.19415000	-1.23420300
H	-1.25890400	0.29459000	-3.48168700
H	-1.74452700	3.28456800	-2.77581200
B	0.86837600	-0.01576800	0.16587300
C	1.32336900	1.44869900	0.70015600
C	1.96019900	2.35806900	-0.15038200
C	1.19836500	1.86556500	2.02866500
C	2.42625000	3.60716200	0.25301500
C	1.65691000	3.10634200	2.48254100
C	2.27322200	3.98240900	1.58938600
C	2.09042800	-0.96766900	-0.31077400
C	1.82963600	-2.10927200	-1.07852800
C	3.43325500	-0.75443200	0.01022000
C	2.82539000	-2.97114000	-1.53526300

C	4.46239900	-1.59532500	-0.42342800
C	4.15604700	-2.70916300	-1.20359100
C	-0.24691000	-0.75413300	1.08709900
C	-0.01234500	-1.92731400	1.81011200
C	-1.52985300	-0.21890400	1.22382300
C	-0.99251800	-2.54623700	2.59092400
C	-2.54045800	-0.80039600	1.98622500
C	-2.26506900	-1.98078400	2.67793200
F	0.64430700	1.07165900	2.95122500
F	1.51423500	3.45526300	3.75749200
F	2.70945000	5.16520700	2.00457100
F	3.01374700	4.43254900	-0.61003900
F	2.14946400	2.03006700	-1.44516200
F	5.72710800	-1.34407800	-0.09254600
F	5.12162500	-3.51855100	-1.62439300
F	2.52091200	-4.04159000	-2.26604100
F	0.56567600	-2.43575400	-1.38484600
F	3.80694000	0.27860900	0.77908000
F	1.19080700	-2.51086700	1.80404100
F	-1.83871500	0.94749900	0.61134700
F	-0.71949000	-3.66239500	3.25990700
F	-3.20497700	-2.55660000	3.41799500
F	-3.74535500	-0.24032800	2.06950000
C	-2.53861600	2.37270200	-4.63847400
O	-2.66680000	1.41459900	-5.36146300
O	-3.03520400	3.58851500	-4.87362500
C	-3.78504700	3.75794200	-6.09628200
H	-3.13378700	3.48725300	-6.94251300
H	-4.62322400	3.04314300	-6.09060300
C	-4.25116500	5.19429600	-6.16243200
H	-4.89638400	5.43923600	-5.30526400
H	-3.39581100	5.88668900	-6.16343500
H	-4.82743400	5.35544700	-7.08603700

RC: E= -3284.68122989

H	-2.31138500	-0.31059100	0.43869600
C	-2.98964900	2.25646900	0.45290700
C	-4.08344100	3.14394600	-2.22040300
H	-3.44834400	1.09601400	-2.80099700
H	-1.87233400	-0.43096800	-2.60093500
C	-1.21363800	-2.05922900	-1.28742400
H	-3.78849900	3.01019800	0.42141400
H	-2.03007200	2.79477900	0.55529000
H	-3.09775800	1.65774200	1.36851800
H	-3.37777100	3.97802200	-2.07138900
H	-4.93522700	3.32162900	-1.54106200
H	-4.46260000	3.21702300	-3.24900300
H	-1.67058800	-2.82743900	-1.95025300
O	-1.35055200	-2.42249800	0.05809100
H	-0.14291700	-2.00768600	-1.57691100
C	-0.76811800	-3.66461300	0.39025100
H	0.32569100	-3.56226000	0.50642300
C	-0.53268900	2.31739800	-2.54662800
C	0.21244800	1.24847300	-2.17627000
C	0.84975800	1.21475700	-0.89498000
H	0.77175700	2.09588700	-0.24027900
O	1.50584300	0.22633200	-0.51769800
H	0.35712000	0.40716600	-2.85497200
H	-0.65394100	3.18973600	-1.90133300
B	2.36325400	0.06858000	0.83789300
C	-2.37924400	0.04945200	-0.58869000
C	-2.97185500	1.37476600	-0.77111200

C	-3.45056500	1.80442000	-1.96851100
C	-1.85575000	-0.73737800	-1.55065600
C	2.79754700	1.56033500	1.32735100
C	3.33014000	2.48551200	0.42350800
C	2.74899100	1.99263300	2.65611400
C	3.76121100	3.76215800	0.77761500
C	3.17601900	3.26139000	3.06078400
C	3.68383800	4.15210300	2.11589500
C	3.60261400	-0.84802300	0.32342900
C	3.35437400	-2.01091200	-0.41262900
C	4.94952100	-0.58469200	0.58252500
C	4.35594500	-2.85097800	-0.89393000
C	5.98831800	-1.39928400	0.12095100
C	5.68965000	-2.53870400	-0.62436200
C	1.36158400	-0.69299300	1.86721700
C	1.70962400	-1.81477100	2.62620600
C	0.07637900	-0.20664500	2.09966200
C	0.84177300	-2.41062000	3.54392000
C	-0.83829300	-0.79182600	2.96836200
C	-0.44590200	-1.90276100	3.71127300
F	2.30368700	1.18966000	3.62927100
F	3.10642500	3.62294200	4.33911000
F	4.08959900	5.36175600	2.48430300
F	4.24770500	4.60024500	-0.13537000
F	3.44908600	2.14901900	-0.87651700
F	7.25623800	-1.09847100	0.39252900
F	6.66434500	-3.32422900	-1.07002300
F	4.05464300	-3.94662700	-1.58941400
F	2.08707900	-2.39344700	-0.66223800
F	5.31983300	0.47459400	1.31575800
F	2.92925900	-2.36123900	2.53214100
F	-0.32985200	0.92558900	1.47951300
F	1.23101500	-3.47153800	4.24759900
F	-1.28536100	-2.47035700	4.56496500
F	-2.07800000	-0.30726400	3.08272500
C	-1.38938400	-4.21529600	1.64830200
C	-0.66146400	-5.09090400	2.46341500
C	-2.70777400	-3.89543700	1.99724800
C	-1.24405600	-5.64964900	3.60239800
H	0.37797400	-5.32209300	2.21593900
C	-3.29064100	-4.45475200	3.13614700
H	-3.26468400	-3.19667400	1.37160600
C	-2.56299300	-5.33626600	3.93966400
H	-0.65906900	-6.31956600	4.23667100
H	-4.31754000	-4.19304000	3.40308500
H	-3.01730100	-5.76613900	4.83543900
H	-0.93311200	-4.38435100	-0.43875300
C	-1.16625400	2.35125700	-3.88824700
O	-1.24763500	1.39434100	-4.62647300
O	-1.62942700	3.57270300	-4.17589500
C	-2.29618600	3.72999000	-5.44297500
H	-1.59020900	3.46573900	-6.24611200
H	-3.12605200	3.00677300	-5.49242500
C	-2.77286200	5.16119300	-5.54385600
H	-3.48343000	5.39779600	-4.73748000
H	-1.92731600	5.86236100	-5.47746900
H	-3.27855500	5.31933800	-6.50845400

TS: E= -3284.67122118

H	-4.00835700	-0.55939100	0.01540000
C	-4.97428700	1.91913400	-0.04930900
C	-5.35740400	2.94576800	-2.78967300

H	-4.74092100	0.91547500	-3.35742000
H	-3.62270600	-0.73757300	-3.04409800
C	-2.74008200	-2.22184800	-1.70755200
H	-6.00952500	2.29445500	-0.10680300
H	-4.32453700	2.81206900	-0.00837400
H	-4.84020500	1.36595200	0.88890300
H	-4.94159500	3.76835600	-2.18817800
H	-6.42358700	2.84983800	-2.52417600
H	-5.30661100	3.24483900	-3.84421300
H	-3.11423600	-3.01090400	-2.39755400
O	-2.89112000	-2.60784200	-0.37375200
H	-1.67065800	-2.07248800	-1.96603200
C	-2.24201400	-3.82289300	-0.04921600
H	-1.15148700	-3.67034000	0.02120100
C	-2.68742900	1.99140700	-2.97268800
C	-1.82926200	0.88575300	-2.71801300
C	-1.11065400	0.83028600	-1.51808500
H	-1.25224700	1.64691000	-0.79767700
O	-0.29802400	-0.09506100	-1.21874700
H	-1.59987100	0.18036400	-3.51684200
H	-2.56317000	2.86985700	-2.33333100
B	0.62491300	-0.12982400	0.06305300
C	-4.08417500	-0.20425700	-1.01176200
C	-4.62144000	1.07724700	-1.23979600
C	-4.63909600	1.63913500	-2.54406800
C	-3.47345800	-0.95996300	-1.98787500
C	0.99222100	1.41399100	0.46374800
C	1.39985700	2.32192200	-0.51983700
C	0.99614600	1.91720800	1.76755800
C	1.75316100	3.64486300	-0.25970800
C	1.34797700	3.23461600	2.07797700
C	1.72757800	4.10503400	1.05762600
C	1.91888200	-0.97114400	-0.46548700
C	1.74305300	-2.16263200	-1.17417600
C	3.24921500	-0.60346900	-0.25244500
C	2.79113200	-2.93068900	-1.67644600
C	4.33442400	-1.34104000	-0.73672500
C	4.10411700	-2.51174800	-1.45661500
C	-0.22425600	-0.90458000	1.23001400
C	0.25689500	-1.98085000	1.98382200
C	-1.50101900	-0.47746800	1.59379900
C	-0.47551900	-2.58750500	3.00804200
C	-2.28507600	-1.07468100	2.57422200
C	-1.76019800	-2.13710000	3.30414900
F	0.67723100	1.14133200	2.81191300
F	1.32884300	3.66203700	3.33902300
F	2.06183700	5.36141400	1.33532900
F	2.12113500	4.46319800	-1.24498500
F	1.47228100	1.92528100	-1.80369500
F	5.58319300	-0.93736200	-0.50988800
F	5.12353500	-3.22672900	-1.92364800
F	2.55384300	-4.05998000	-2.34452200
F	0.50345800	-2.65819700	-1.37196500
F	3.56135100	0.49110900	0.45689200
F	1.48202300	-2.48279300	1.77515000
F	-2.04713000	0.60904800	0.99802400
F	0.03587500	-3.61501200	3.68471100
F	-2.47814500	-2.72390400	4.25248000
F	-3.53322800	-0.64890800	2.79767000
C	-2.78860200	-4.38473700	1.23701200
C	-1.99847000	-5.24747100	2.00718800
C	-4.08941100	-4.08844200	1.66220100
C	-2.50384800	-5.81729900	3.17669800

H	-0.97056600	-5.45822300	1.70069500
C	-4.59421400	-4.65721400	2.83369800
H	-4.69672400	-3.40178500	1.07124400
C	-3.80598600	-5.52661900	3.59132400
H	-1.87078800	-6.47636300	3.77498500
H	-5.60763200	-4.41256700	3.16123000
H	-4.19902100	-5.96352400	4.51221600
H	-2.40855000	-4.55514500	-0.86685200
C	-2.87922800	2.29866300	-4.42721800
O	-3.05292000	1.45479700	-5.27636800
O	-2.84729500	3.61389600	-4.66529200
C	-3.01927200	4.02911100	-6.03627400
H	-2.23433300	3.55584800	-6.64645500
H	-3.98661200	3.64614700	-6.39936800
C	-2.94576800	5.53877900	-6.07556800
H	-3.73861700	5.98885000	-5.45883600
H	-1.97334400	5.89403200	-5.70259300
H	-3.06989600	5.89224100	-7.11046400

P: E= -3284.73663597

H	-3.84268600	-0.64250800	-0.74031200
C	-4.05637000	1.88432900	0.08892300
C	-1.23381700	3.03299100	-0.23718100
H	-2.50546200	3.00110900	-1.93832600
H	-2.37629000	-0.71565200	-3.05107700
C	-1.74202500	-2.15483400	-1.62249300
H	-4.49418400	2.79381800	-0.35687900
H	-3.62504100	2.18245300	1.05899800
H	-4.86869300	1.17102500	0.28834500
H	-0.69028700	2.37731100	0.45677500
H	-1.94321200	3.62214400	0.36077200
H	-0.51016800	3.73367800	-0.67820300
H	-2.68034200	-2.69038100	-1.38931400
O	-0.89389700	-2.11912600	-0.49111800
H	-1.23801300	-2.68303700	-2.45252100
C	-0.46952600	-3.35052000	0.06521900
H	0.61100700	-3.26930200	0.25288200
C	-0.95504400	1.57064700	-2.31933700
C	-0.69246300	0.08002100	-1.99497300
C	-0.03833500	-0.02128800	-0.65629900
H	-0.64592700	0.09912500	0.24462000
O	1.19745100	-0.05826400	-0.57470900
H	0.00954100	-0.32019100	-2.73911300
H	-0.00095800	2.11436900	-2.24666900
B	2.10987200	-0.03321200	0.72497000
C	-3.02978300	-0.01947700	-1.12940500
C	-3.00878500	1.28674100	-0.81252500
C	-1.95877900	2.24888800	-1.34690700
C	-2.01651600	-0.70607300	-2.00941100
C	2.29195700	1.55481200	1.08437700
C	2.19058100	2.57587800	0.13784700
C	2.55160200	1.99124800	2.38898500
C	2.25850000	3.93451000	0.45384500
C	2.64952000	3.33504200	2.74800800
C	2.48950300	4.31997200	1.77140500
C	3.48536000	-0.71738000	0.18500000
C	3.46482600	-1.76994400	-0.73708200
C	4.75921100	-0.31073100	0.58945900
C	4.61299500	-2.36219100	-1.25884000
C	5.93851300	-0.87658300	0.09407800
C	5.86456700	-1.90697200	-0.84081500
C	1.34412600	-0.85234500	1.92649200

C	1.75741600	-2.09718200	2.41758500
C	0.26112500	-0.29897700	2.62092300
C	1.18481500	-2.71779800	3.53138400
C	-0.34642500	-0.88136700	3.72983300
C	0.13739900	-2.09793400	4.20525700
F	2.72718200	1.10214200	3.37463700
F	2.89002800	3.68686500	4.00892600
F	2.56060800	5.60698100	2.09556100
F	2.08124700	4.85562200	-0.49578300
F	1.99279300	2.29915900	-1.16740600
F	7.12587700	-0.44180700	0.51126500
F	6.97362200	-2.45879700	-1.32319700
F	4.52748700	-3.36336000	-2.13460800
F	2.29474800	-2.30269000	-1.13869000
F	4.91566900	0.65607700	1.50378400
F	2.74257000	-2.78918000	1.82775300
F	-0.25993700	0.88760900	2.23183300
F	1.61967700	-3.90901700	3.93582800
F	-0.41613200	-2.67254600	5.26575400
F	-1.38912200	-0.30226600	4.32239100
C	-1.20650000	-3.67574300	1.34478000
C	-0.84899100	-4.81723100	2.07565900
C	-2.21479500	-2.84025400	1.83608400
C	-1.49324400	-5.11974100	3.27508100
H	-0.04321600	-5.46245500	1.71434300
C	-2.86220400	-3.14379600	3.03775900
H	-2.47538600	-1.93577100	1.28547100
C	-2.50559300	-4.28424200	3.75830000
H	-1.19394400	-6.00286700	3.84370800
H	-3.63487400	-2.47306800	3.42011600
H	-2.99910700	-4.51270900	4.70520400
H	-0.60016600	-4.15791700	-0.67761000
C	-1.34987600	1.70102200	-3.78711000
O	-1.36695700	0.79885700	-4.59091300
O	-1.63851900	2.97017000	-4.09672500
C	-1.98205300	3.24805500	-5.46874200
H	-1.14466500	2.93177700	-6.11044600
H	-2.85260700	2.63240300	-5.74508300
C	-2.26516800	4.72901000	-5.58424200
H	-3.10679300	5.02146400	-4.93787900
H	-1.38394500	5.32101700	-5.29429000
H	-2.52457200	4.98038200	-6.62397900

a-exo

1: E= -619.116373508

H	-4.22041200	-0.52162700	-1.43185400
C	-4.47433200	-3.12231400	-0.81518900
C	-1.69507700	-4.13087800	0.21606100
H	-1.31687900	-1.96659800	0.14046600
H	-2.37862400	-0.05012900	0.98827200
C	-3.31094800	1.63815000	-0.07545100
H	-4.25230300	-4.19471100	-0.74530600
H	-4.80724900	-2.91298000	-1.84669100
H	-5.33584400	-2.90930300	-0.15892900
H	-1.36985100	-4.26287000	1.26358400
H	-0.82963200	-4.41011200	-0.41065400
H	-2.49873300	-4.85486000	0.02401100
H	-3.95271000	1.78480700	-0.96871800
O	-2.08957300	2.33158200	-0.21555700
H	-3.87137200	2.04993000	0.79325200
C	-2.23524600	3.72122100	-0.32476300

H	-2.90704300	3.97427300	-1.17462700
H	-2.72101500	4.13789700	0.58377900
C	-3.53490700	-0.79939700	-0.61908400
C	-3.29729900	-2.24860600	-0.45564100
C	-2.10168600	-2.71162500	-0.03438600
C	-3.03046800	0.18498200	0.13984500
C	-0.89461700	4.38324300	-0.53363800
C	-0.78428800	5.77770800	-0.43598100
C	0.24274600	3.63024300	-0.84631300
C	0.44068600	6.41036600	-0.65271300
H	-1.66666400	6.37458600	-0.18546700
C	1.47077400	4.26375200	-1.05952900
H	0.15117300	2.54604400	-0.91460000
C	1.57457000	5.65341400	-0.96556800
H	0.51256000	7.49795000	-0.57280100
H	2.35300800	3.66520300	-1.30066000
H	2.53520700	6.14673300	-1.13238700

2: E= -2665.51668480

C	-0.55745000	-1.64459200	-1.95906100
C	-0.61168700	-0.30459700	-1.81869000
C	0.15676800	0.37087700	-0.78954800
O	0.88179100	-0.27448500	-0.02233900
B	1.86536400	0.21055800	1.15935300
H	-1.24082800	0.29385000	-2.48189300
H	0.06717500	-2.25585400	-1.30116300
H	0.09721100	1.46632400	-0.69540800
C	1.40910900	1.70145500	1.60724600
C	2.29715300	2.75900900	1.82304100
C	0.06842500	1.98203100	1.88749700
C	1.88464600	4.01749800	2.27088400
C	-0.39117300	3.22109100	2.32907200
C	0.53270400	4.24970000	2.52474400
C	1.60343000	-0.93576500	2.27927200
C	1.54408300	-2.28785600	1.92247600
C	1.45114500	-0.67004400	3.64235400
C	1.31024000	-3.31459600	2.83602700
C	1.22057200	-1.66840100	4.59305000
C	1.14700400	-2.99989300	4.18610000
C	3.31815200	0.12577100	0.43918300
C	4.42524000	-0.53306500	0.98061300
C	3.53600900	0.74446900	-0.79449700
C	5.66140500	-0.59667100	0.33106200
C	4.74729400	0.70479900	-1.48153200
C	5.82261900	0.02396200	-0.90815400
F	2.53931000	1.45039300	-1.37364400
F	4.88944700	1.31086700	-2.65788700
F	6.99148100	-0.02746000	-1.53559400
F	6.68627400	-1.23546900	0.88752100
F	4.35589900	-1.12727100	2.17685400
F	3.61157800	2.60398600	1.63011400
F	2.76910900	4.99151000	2.46213000
F	0.12603600	5.44023900	2.94735000
F	-1.68339900	3.42855900	2.56868700
F	-0.85650100	1.01220500	1.73078300
F	1.53786200	0.58138200	4.11396800
F	1.74336200	-2.66419600	0.64512000
F	1.07820500	-1.35935400	5.87933000
F	1.25595500	-4.58414400	2.43708000
F	0.92772200	-3.96197800	5.07527900
C	-1.35524100	-2.32674100	-3.02111800
O	-2.07872500	-1.75375300	-3.80101500

O	-1.15529100	-3.64462800	-2.98350000
C	-1.86537100	-4.43933900	-3.95680100
H	-2.94480200	-4.25702200	-3.83263800
H	-1.59042000	-4.08342700	-4.96256000
C	-1.49474200	-5.88793500	-3.73496900
H	-1.77599200	-6.21572700	-2.72287200
H	-2.02175800	-6.52230200	-4.46368800
H	-0.41237700	-6.04112500	-3.86111600

RC: E= -3284.69288901

H	-4.32447600	-0.56761000	-1.31516400
C	-4.23268000	-3.16801100	-1.07770100
C	-1.74632300	-4.06171800	0.52584000
H	-1.58733800	-1.88732500	0.81346400
H	-2.38382700	0.03371000	0.99820000
C	-3.36300100	1.66410000	-0.08043600
H	-3.90614600	-4.21420500	-1.03015300
H	-4.33218300	-2.87564700	-2.13602300
H	-5.24090200	-3.11069000	-0.63327000
H	-2.23944400	-4.50258700	1.41150700
H	-0.66434700	-4.10613900	0.71125600
H	-1.97185600	-4.70675700	-0.33535400
H	-4.05763700	1.79038600	-0.93414200
O	-2.14206800	2.34542800	-0.32546000
H	-3.84878900	2.10319500	0.81513000
C	-2.27469000	3.75259200	-0.39202100
H	-2.98846800	4.02013100	-1.19960200
H	-2.69896300	4.13836200	0.55488200
C	-0.63366900	-1.72934200	-1.84086900
C	-0.68963500	-0.38344600	-1.67704700
C	0.08749200	0.26137600	-0.65806600
O	0.90522300	-0.39325400	0.02541700
B	1.89617500	0.11618000	1.14819000
C	-3.60587500	-0.80389200	-0.52118400
C	-3.29415500	-2.22711700	-0.36856100
C	-2.19268100	-2.64816700	0.31335700
C	-3.06490400	0.22012500	0.16778900
H	-1.37307000	0.22542900	-2.26754400
H	0.06431600	-2.33610900	-1.26294400
H	-0.06576300	1.32821300	-0.45939200
C	1.29819900	1.53034200	1.69718800
C	1.96318600	2.75931600	1.71644800
C	-0.01232400	1.56119300	2.17625500
C	1.36311100	3.93783700	2.16845900
C	-0.67068400	2.71769200	2.57894500
C	0.03461600	3.91936200	2.58858900
C	1.82786400	-1.07817500	2.25580000
C	1.63800800	-2.42091200	1.91639400
C	1.94860300	-0.82507000	3.62507800
C	1.51219400	-3.44064400	2.86154100
C	1.84237600	-1.81546200	4.60328400
C	1.61053600	-3.13629300	4.21809700
C	3.32433800	0.23094400	0.37596400
C	4.52714300	-0.28613500	0.86386900
C	3.42162200	0.90122700	-0.84611500
C	5.74266000	-0.15690700	0.18321000
C	4.60727100	1.06086600	-1.55737500
C	5.78337400	0.51955100	-1.03575900
F	2.32662000	1.48120300	-1.38304100
F	4.62712100	1.73027100	-2.70998700
F	6.93139900	0.65453600	-1.69069400
F	6.86073100	-0.66841000	0.69231400

F	4.57759600	-0.92648300	2.03790800
F	3.23258600	2.86651800	1.30905800
F	2.04403500	5.08071500	2.18439000
F	-0.56530700	5.04193300	2.97596100
F	-1.95958400	2.69097400	2.92858000
F	-0.71858300	0.41079300	2.23458200
F	2.19243200	0.41767900	4.06452200
F	1.56997600	-2.81600800	0.62975400
F	1.95820600	-1.51235100	5.89439300
F	1.29168400	-4.69874700	2.47219300
F	1.49592800	-4.09433000	5.13265100
C	-0.93137200	4.39022800	-0.64298700
C	-0.61155800	5.61209600	-0.03592200
C	0.01586300	3.78322500	-1.47803600
C	0.63409700	6.20613600	-0.24483100
H	-1.33321800	6.08920000	0.63095200
C	1.27347800	4.36204100	-1.66793700
H	-0.22979800	2.84681500	-1.97964500
C	1.58601200	5.57456700	-1.04929200
H	0.87435800	7.14841600	0.25177300
H	2.01423100	3.85282600	-2.28704900
H	2.57261100	6.02236100	-1.18661800
C	-1.48967800	-2.40605200	-2.84459200
O	-2.32580200	-1.85152800	-3.52341800
O	-1.22455400	-3.71877700	-2.89554800
C	-1.96921200	-4.50051900	-3.84721900
H	-3.04318900	-4.39359600	-3.63040500
H	-1.79860900	-4.08499100	-4.85321200
C	-1.50481500	-5.93518400	-3.73206400
H	-1.69397100	-6.33120400	-2.72249500
H	-2.04523200	-6.56329000	-4.45649600
H	-0.42689400	-6.01700400	-3.93751900

TS: E= -3284.68280089

H	-4.69124900	-0.51926000	-1.45517200
C	-4.22527300	-3.15633300	-1.50374300
C	-1.45476500	-3.82263200	-0.65609700
H	-1.39294700	-1.70632900	-0.10467100
H	-2.12435800	0.11187600	0.14468500
C	-3.39222600	1.72987700	-0.59723400
H	-3.78630700	-3.71995000	-2.34152900
H	-5.18633800	-2.74007200	-1.83264700
H	-4.41753500	-3.89359600	-0.70512600
H	-1.92999400	-4.31839200	0.20794200
H	-0.36978400	-3.85506100	-0.49809800
H	-1.69300000	-4.40764100	-1.55464300
H	-4.19878300	1.86485200	-1.34504800
O	-2.27943600	2.53470800	-0.90170800
H	-3.80713500	2.02001900	0.39317800
C	-2.55221700	3.92326200	-0.92174400
H	-3.38381800	4.12609700	-1.62914700
H	-2.88308800	4.26220100	0.07787500
C	-1.05945500	-1.55803800	-2.39294900
C	-1.08348500	-0.14257200	-2.28966300
C	-0.18941000	0.50531100	-1.42703300
O	0.48952700	-0.17515000	-0.59618300
B	1.57417700	0.33090200	0.38376000
C	-3.73227200	-0.74395200	-0.97689700
C	-3.29464100	-2.08815700	-1.01096900
C	-1.93636100	-2.39895500	-0.75342900
C	-2.96511500	0.29878600	-0.51917800
H	-1.70428400	0.44708800	-2.96076600

H	-0.11838000	-2.05088100	-2.13909000
H	-0.09530600	1.59660400	-1.42512100
C	1.15136400	1.84555000	0.82959600
C	1.90276600	3.00657700	0.62516400
C	-0.08628800	2.05058500	1.44438200
C	1.48459300	4.27089900	1.05422900
C	-0.56388100	3.29190000	1.84608000
C	0.24494400	4.41318900	1.67110900
C	1.49565800	-0.79180900	1.57708600
C	1.46267700	-2.14604500	1.22832500
C	1.46315800	-0.53215500	2.94860600
C	1.33479700	-3.18045500	2.15518800
C	1.35114300	-1.53778800	3.91383200
C	1.28133800	-2.87243000	3.51459800
C	3.03182900	0.20275800	-0.33707500
C	4.17464400	0.35292300	0.45381900
C	3.26907800	-0.10278200	-1.67642600
C	5.47319400	0.21094100	-0.03038500
C	4.55336500	-0.25984000	-2.20712800
C	5.66236400	-0.10499300	-1.37777000
F	2.25455500	-0.25563600	-2.55026900
F	4.72310400	-0.55406000	-3.49681200
F	6.89154400	-0.24869500	-1.86650700
F	6.52660600	0.37231000	0.76852700
F	4.03797800	0.67951900	1.74815000
F	3.08342400	2.97064800	-0.00316400
F	2.24935300	5.34207500	0.85265300
F	-0.17950100	5.61170600	2.06438900
F	-1.79085200	3.42297100	2.36277900
F	-0.89813800	0.99668900	1.67559000
F	1.52750100	0.72137200	3.41260700
F	1.54979700	-2.52316200	-0.06324200
F	1.30964800	-1.23331000	5.20986200
F	1.26609200	-4.45189600	1.75099300
F	1.16520400	-3.84104700	4.41915300
C	-1.31119800	4.67241900	-1.33494000
C	-1.01828300	5.91856400	-0.76857500
C	-0.43027700	4.13498700	-2.28329400
C	0.14456500	6.60541100	-1.12287900
H	-1.68708800	6.34063900	-0.01524900
C	0.74161200	4.81260500	-2.62696900
H	-0.66433800	3.17796300	-2.75106200
C	1.03459100	6.04809100	-2.04359900
H	0.37174300	7.56368100	-0.65133800
H	1.43073100	4.37143200	-3.35091500
H	1.95883800	6.57064600	-2.29887800
C	-1.82366900	-2.13604900	-3.53660600
O	-2.74187500	-1.57836600	-4.09437200
O	-1.39578700	-3.36752900	-3.85381700
C	-2.05753200	-4.02156800	-4.95351900
H	-3.13887300	-4.06091000	-4.74594000
H	-1.92712100	-3.40455300	-5.85657900
C	-1.45038100	-5.39796000	-5.10818600
H	-1.60252800	-6.00247000	-4.20080000
H	-1.92015400	-5.92168800	-5.95462700
H	-0.36893400	-5.32978300	-5.29934000

P: E= -3284.73381684

H	-4.59160900	-0.84235100	-0.75821400
C	-4.16799100	-3.52965400	-0.32556500
C	-1.28743200	-4.06885400	0.23650800

H	-1.43079000	-2.05060400	0.85542000
H	-2.33878500	0.14767800	0.65497500
C	-3.03570800	1.34308000	-0.93854500
H	-3.87263700	-4.26342100	-1.09315000
H	-5.18921400	-3.18659300	-0.54563400
H	-4.18609900	-4.07166400	0.63449200
H	-1.79275700	-4.45426500	1.13497100
H	-0.20546700	-4.10159000	0.43187100
H	-1.50327200	-4.74210800	-0.60073300
H	-3.21189500	1.29588400	-2.03244100
O	-2.04286400	2.29463100	-0.63323000
H	-3.99734100	1.60147100	-0.45265000
C	-2.23547800	3.60886000	-1.12240300
H	-2.54121600	3.56499000	-2.18727100
H	-3.04487500	4.11752500	-0.56551900
C	-0.98107500	-1.92532400	-1.21664800
C	-1.16277700	-0.40825900	-1.09924400
C	-0.09786500	0.25464100	-0.32214100
O	0.76900600	-0.39345300	0.27220700
B	1.86854100	0.16825800	1.32295600
C	-3.55526300	-1.10945600	-0.52865600
C	-3.20361000	-2.38315100	-0.28551300
C	-1.72031700	-2.62977600	-0.04046400
C	-2.54099000	-0.00034700	-0.42025300
H	-1.15909800	0.04032000	-2.10737400
H	0.09126500	-2.17227700	-1.15637900
H	-0.13625500	1.34753000	-0.23386500
C	1.31238100	1.60994600	1.83480200
C	2.04957400	2.79717600	1.84323900
C	-0.01325100	1.73865500	2.26120000
C	1.50281400	4.02724200	2.21973700
C	-0.61623200	2.94678400	2.59354100
C	0.15957000	4.10604800	2.57864800
C	1.82944800	-1.02113100	2.42549700
C	1.84915400	-2.35960900	2.01858900
C	1.74137300	-0.81529500	3.80353000
C	1.72816800	-3.43192100	2.90065200
C	1.63328600	-1.86136000	4.72457700
C	1.61952000	-3.17952700	4.26896400
C	3.23621400	0.25151800	0.45662700
C	4.47079000	-0.21505300	0.91403300
C	3.26315700	0.87766800	-0.79057000
C	5.65296300	-0.08197500	0.17921300
C	4.41544400	1.04647100	-1.55298600
C	5.62594300	0.55517900	-1.06177000
F	2.12943900	1.40630900	-1.30318000
F	4.37133000	1.68544800	-2.72219300
F	6.74275000	0.69936700	-1.76627800
F	6.80437900	-0.54478100	0.65861700
F	4.58084400	-0.79920400	2.11278800
F	3.33932700	2.81512200	1.48608100
F	2.25172800	5.12732600	2.21871000
F	-0.38304500	5.27752000	2.89441500
F	-1.90629500	3.00598600	2.91726100
F	-0.79780000	0.63816900	2.31933900
F	1.75934800	0.42302900	4.31390200
F	1.99128400	-2.67439900	0.71857700
F	1.54325200	-1.61059400	6.02886500
F	1.71561100	-4.68622700	2.44784100
F	1.50902300	-4.18632700	5.12941400
C	-0.93414400	4.35638800	-0.97842500
C	-0.84444600	5.53724300	-0.23325800
C	0.22579900	3.84111500	-1.57628500

C	0.37986000	6.19862200	-0.09768100
H	-1.73427600	5.93368300	0.26211500
C	1.45315000	4.48673100	-1.42581500
H	0.17010900	2.91868500	-2.15769000
C	1.53028300	5.67331500	-0.68988300
H	0.44010900	7.10975800	0.50081300
H	2.34803000	4.05351100	-1.87743500
H	2.49064300	6.17618900	-0.56046200
C	-1.46180000	-2.35570900	-2.60013100
O	-1.65889800	-1.59637700	-3.52068600
O	-1.62004300	-3.67946300	-2.70386000
C	-2.06701500	-4.18492800	-3.97640300
H	-3.01646800	-3.69101900	-4.23617600
H	-1.33254900	-3.90053900	-4.74623300
C	-2.21446100	-5.68524800	-3.85297800
H	-2.96006300	-5.94810900	-3.08675200
H	-2.54433500	-6.10960500	-4.81350100
H	-1.25710500	-6.15352100	-3.57847000

b-endo

1: E= -619.119807369

H	-0.13203800	0.70876500	1.51026000
C	1.84050700	-1.09949800	1.88459100
C	4.54192400	0.26535100	1.08654700
H	3.11724200	1.77923900	0.36935700
H	1.22647100	1.70844000	-1.05452900
C	-0.86170800	2.22825600	-0.61053100
H	1.31914900	-1.84111400	1.25493900
H	1.22274900	-0.97036100	2.79013800
H	2.80241900	-1.53004300	2.19119100
H	4.55225500	-0.71959100	1.57326100
H	5.12918700	0.95905100	1.71427700
H	5.09437900	0.17146900	0.13426900
H	-0.71004600	3.32099800	-0.75916300
O	-1.79644100	2.00548300	0.41767700
H	-1.24256400	1.84281500	-1.57940300
C	-3.09514100	2.46157500	0.12950500
H	-3.64185800	2.42505400	1.08700600
H	-3.08151500	3.52165300	-0.19499000
C	0.69715900	0.85918600	0.81017200
C	1.98069000	0.21560400	1.15687100
C	3.16054900	0.79364800	0.84756100
C	0.44700000	1.57531500	-0.29567700
C	-3.82299300	1.62121100	-0.90282300
C	-3.57329100	0.24455800	-0.99264700
C	-4.77377400	2.19566400	-1.75532700
C	-4.26649000	-0.54169300	-1.91492900
H	-2.81918900	-0.19847000	-0.33851200
C	-5.47568100	1.40879000	-2.67267400
H	-4.96585400	3.27149300	-1.70292700
C	-5.22300200	0.03698200	-2.75516100
H	-4.05977400	-1.61301700	-1.97870900
H	-6.21559400	1.87032300	-3.33134500
H	-5.76584200	-0.57893400	-3.47620200

2: E= -2081.64724287

C	1.96287700	-0.81440000	-2.05788300
C	0.67651600	-0.41343900	-2.08925400
C	-0.31232900	-0.95208500	-1.17034300
H	-1.35753500	-0.59528900	-1.23063300

O	-0.02654600	-1.80247000	-0.31544600
H	0.35517300	0.33453600	-2.81863900
H	2.30601700	-1.56118800	-1.33690900
Cl	-0.22776900	-2.04717200	2.80286200
Cl	-3.01999800	-1.72534200	0.54999900
Cl	-0.97789100	-4.69103800	0.44365500
Al	-1.14794700	-2.65604400	0.99742500
C	2.95831900	-0.24344200	-3.01516500
O	2.69395400	0.58550000	-3.85310700
O	4.16346100	-0.77563400	-2.81148600
C	5.23136800	-0.31617700	-3.66796100
H	4.94605900	-0.51378700	-4.71355100
H	5.31884700	0.77637300	-3.55671100
C	6.49549200	-1.04121800	-3.26673100
H	7.33049800	-0.71171200	-3.90339600
H	6.75505300	-0.82977400	-2.21848400
H	6.37954500	-2.12925200	-3.38351500

RC: E= -2700.81168193

H	-0.57757200	0.61765500	2.52713900
C	1.52732700	-0.86619000	3.14423300
C	3.88332800	-0.33828400	1.34658800
H	2.53081400	1.18531700	0.50063100
H	0.70300900	2.08719100	0.14410400
C	-1.39698700	2.39671100	0.69271500
H	1.66459800	-1.88768200	2.75627500
H	0.58980300	-0.86797600	3.71442000
H	2.35615900	-0.66517400	3.84164600
H	3.80153100	-1.29120400	1.88675200
H	4.60574100	0.29505500	1.89461400
H	4.32187400	-0.54042100	0.35809700
H	-1.29956000	3.49869100	0.82275100
O	-2.31244600	1.85970000	1.60201300
H	-1.73200800	2.25378300	-0.35650300
C	-3.67910100	2.11951300	1.31545200
H	-4.22310500	1.80200700	2.21631600
H	-3.84673200	3.20479100	1.17598000
C	1.44282600	-0.78029300	-1.04435900
C	0.16504400	-0.31145200	-1.04482200
C	-0.82821500	-0.87025900	-0.17766500
H	-1.84741300	-0.45295900	-0.17996200
O	-0.56143600	-1.84752500	0.56612300
H	-0.11013800	0.53426100	-1.67590100
H	1.71212300	-1.68316400	-0.49707700
C	0.23765600	0.87457000	1.84706700
C	1.48562900	0.15532500	2.03029000
C	2.56748900	0.36110000	1.21753600
C	-0.05746900	1.75594600	0.85710800
Cl	-2.33383900	-1.44811400	3.16231200
Cl	-3.07215700	-3.74502800	0.53539000
Cl	-0.10888000	-4.21032400	2.55419100
Al	-1.55825000	-2.87386800	1.76156500
C	2.46308700	-0.11982400	-1.89254400
O	2.31544800	0.95804600	-2.42676800
O	3.58194700	-0.85335900	-1.98087500
C	4.65172000	-0.30719700	-2.77563700
H	4.28077000	-0.14897200	-3.80076700
H	4.91844300	0.68343200	-2.37349500
C	5.80944700	-1.27895300	-2.72850900
H	6.64160400	-0.89886200	-3.34043000
H	6.17236900	-1.41338300	-1.69801100
H	5.51194200	-2.26312400	-3.12069800

C	-4.16057400	1.35137900	0.10587200
C	-4.27643200	-0.04674300	0.17760700
C	-4.41593000	1.99179900	-1.11363100
C	-4.63326300	-0.78786500	-0.95037000
H	-4.07525900	-0.55531600	1.12361400
C	-4.77905400	1.25255600	-2.24462700
H	-4.33085500	3.08050300	-1.17882500
C	-4.88346800	-0.13798200	-2.16466300
H	-4.70226200	-1.87442400	-0.87503000
H	-4.97623300	1.76449500	-3.18969100
H	-5.16308200	-0.71790400	-3.04754500

TS: E= -2700.80986592

H	-0.22257800	0.74869800	1.66063000
C	1.95176400	-0.71867700	2.17046400
C	4.20555500	-0.12222200	0.37793000
H	2.84879500	1.44289800	-0.39179200
H	1.00970100	2.19488800	-0.77456400
C	-1.09271500	2.46568600	-0.23014700
H	2.12299900	-1.72386300	1.75202300
H	1.04718900	-0.77491000	2.78805400
H	2.81562700	-0.48952200	2.81697900
H	4.13986300	-1.21486100	0.49108800
H	4.66245400	0.27100700	1.30321400
H	4.89231100	0.09340800	-0.44966300
H	-0.98785600	3.57296900	-0.15739400
O	-1.97983700	1.97441800	0.72793100
H	-1.45221200	2.27316900	-1.26246900
C	-3.35217400	2.22430400	0.46349700
H	-3.87814700	1.89147000	1.36995500
H	-3.53295200	3.30982200	0.34079500
C	2.07548500	-0.49341800	-1.64707400
C	0.74999800	-0.11804900	-1.89107300
C	-0.29832400	-0.75110400	-1.20245400
H	-1.34608700	-0.49998900	-1.43072500
O	-0.04798200	-1.62389500	-0.31253200
H	0.52204600	0.64879800	-2.63123000
H	2.26300700	-1.47307000	-1.20672300
C	0.57522900	1.00557800	0.96134000
C	1.81067500	0.30523000	1.08168200
C	2.85495100	0.50474400	0.16606600
C	0.25326700	1.84403000	-0.06925300
Cl	-1.86143700	-1.40582900	2.28045100
Cl	-2.53255000	-3.56255000	-0.48401800
Cl	0.42203800	-4.07239800	1.53857500
Al	-1.03848300	-2.71375700	0.78793800
C	3.11015900	0.06592900	-2.56189300
O	3.04495300	1.16299000	-3.07090400
O	4.12701700	-0.78604200	-2.74106100
C	5.19716600	-0.34661400	-3.59967200
H	4.77980600	-0.11826900	-4.59301800
H	5.60578000	0.59474400	-3.19787100
C	6.23222900	-1.44790000	-3.65094800
H	7.06574400	-1.14838900	-4.30438900
H	6.63587300	-1.65706300	-2.64856200
H	5.79672600	-2.37718000	-4.04809200
C	-3.84814600	1.46959800	-0.74857500
C	-3.81856900	0.06540500	-0.74414600
C	-4.28157900	2.13794100	-1.90018500
C	-4.21400000	-0.65372000	-1.87318900
H	-3.48252400	-0.46251300	0.15162300
C	-4.68415800	1.41956300	-3.03129800

H	-4.30372400	3.23165700	-1.91262900
C	-4.64696900	0.02358200	-3.01950800
H	-4.17407900	-1.74410800	-1.85025400
H	-5.02169700	1.95261700	-3.92352900
H	-4.95758200	-0.54008400	-3.90260100

P: E= -2700.85825466

H	0.47493800	1.98262300	2.53470100
C	2.28635000	0.21235500	3.37733100
C	2.66554000	-1.89132400	1.32136700
H	3.36014000	0.01034700	0.68466600
H	0.83765800	2.25580100	-0.25756500
C	-1.17059400	2.15219300	0.45841700
H	1.96270200	-0.76643300	3.76873000
H	1.91250700	0.98954700	4.05872400
H	3.38939700	0.22278400	3.41044400
H	1.74704700	-2.42296400	1.60422100
H	3.35355900	-1.92718600	2.17741800
H	3.14725500	-2.43104200	0.49209600
H	-1.16270300	3.10987400	1.01310700
O	-1.94938400	1.19746400	1.14843900
H	-1.57652200	2.34514900	-0.55165900
C	-3.36288900	1.42978100	1.18635600
H	-3.71869300	0.87310900	2.06241700
H	-3.54724700	2.50634300	1.34632000
C	1.58340700	-0.41751300	-0.46346600
C	0.18385900	0.22528000	-0.41247800
C	-0.83818700	-0.69338000	0.17725900
H	-1.80440500	-0.81747300	-0.33744400
O	-0.57375300	-1.42163500	1.14672200
H	-0.13888100	0.44801100	-1.43925700
H	1.47487300	-1.46396300	-0.78942000
C	0.85034500	1.36078100	1.71622200
C	1.77023600	0.42246100	1.98019400
C	2.37525500	-0.44592500	0.89084000
C	0.23027500	1.57534100	0.36338800
Cl	-2.89862600	-1.51580700	3.31577500
Cl	-2.68750000	-3.59270900	0.42500900
Cl	-0.19737100	-3.88597700	3.04455800
Al	-1.63723300	-2.68312200	2.05372300
C	2.39872400	0.25297300	-1.56090500
O	2.05890200	1.22062400	-2.20143600
O	3.56651400	-0.37712500	-1.73947000
C	4.45924200	0.16396800	-2.73183400
H	3.94474800	0.16471300	-3.70587800
H	4.67337000	1.21446400	-2.47847400
C	5.70834800	-0.68860800	-2.74474500
H	6.41599900	-0.30570000	-3.49590100
H	6.20467300	-0.67437600	-1.76244300
H	5.46852400	-1.73305900	-2.99543600
C	-4.03575100	0.93840700	-0.07053300
C	-4.36599500	-0.42121100	-0.18422100
C	-4.26045700	1.78554000	-1.16527500
C	-4.88262600	-0.92985700	-1.37677000
H	-4.21157800	-1.08690400	0.66681700
C	-4.78737400	1.28040900	-2.35777300
H	-4.02979400	2.85138200	-1.08210200
C	-5.09177000	-0.07940000	-2.46740300
H	-5.11601900	-1.99428400	-1.44885100
H	-4.96052700	1.95040200	-3.20338500
H	-5.49850800	-0.47514600	-3.40114000

b-exo**1:** E= -619.118847308

H	0.20137100	1.93956800	-2.22713900
C	2.09774000	-0.00860000	-2.42356000
C	1.32514300	-2.18502200	-0.30485900
H	-0.49772000	-0.95262900	-0.28489200
H	-1.96739800	-0.22381800	-2.06951100
C	-2.49726900	1.89412800	-2.44713000
H	2.53726800	0.99137300	-2.26312200
H	1.96524400	-0.11954500	-3.51353100
H	2.83020100	-0.75585100	-2.09164200
H	2.29627600	-2.24564900	-0.81545500
H	0.80895900	-3.15012700	-0.45566700
H	1.51764700	-2.10647500	0.78029800
H	-2.81451100	1.85597000	-3.50668500
O	-1.98163900	3.19016000	-2.22981200
H	-3.41950000	1.73742000	-1.85001400
C	-2.20322500	3.72171400	-0.93260200
H	-1.87038600	4.76910600	-0.99107500
H	-3.28827500	3.72298200	-0.70834700
C	-0.20232100	0.93537800	-2.05671100
C	0.77371200	-0.11364200	-1.70769000
C	0.47516700	-1.04700900	-0.77975500
C	-1.52735000	0.77559100	-2.16913500
C	-1.46189000	2.99938900	0.17076700
C	-0.08657000	3.20586100	0.34811200
C	-2.10786400	2.04969900	0.97025200
C	0.63094200	2.46432400	1.28616500
H	0.42761500	3.94405600	-0.27346200
C	-1.39443900	1.30360400	1.91306500
H	-3.18133900	1.88232100	0.84511200
C	-0.02168300	1.50558400	2.06824700
H	1.70433600	2.62919700	1.40706200
H	-1.91182100	0.56085000	2.52535800
H	0.54057100	0.91896100	2.79867300

2 = b-endo 2**RC:** E= -2700.81513607

H	0.66553000	1.31357900	-1.87607200
C	2.51669100	-0.51898500	-2.20234900
C	1.39556100	-3.34627300	-1.48293200
H	-0.43411800	-2.16609600	-1.27228000
H	-1.70909600	-0.63062100	-2.07716500
C	-2.01243000	1.53967700	-2.04231500
H	2.91882900	0.20860600	-1.47741000
H	2.59227900	-0.05697600	-3.20042700
H	3.16312300	-1.40513800	-2.18808900
H	2.45806500	-3.22949400	-1.73213200
H	0.95092400	-4.06265200	-2.19616200
H	1.33223000	-3.81988000	-0.48928100
H	-2.55759800	1.54729100	-3.01100500
O	-1.24677500	2.71332200	-1.90172000
H	-2.79975100	1.46165500	-1.26996700
C	-1.90434500	3.77693700	-1.23309300
H	-1.28756400	4.66841800	-1.42276000
H	-2.90424700	3.96017600	-1.66894600
C	0.80692300	-1.08232700	1.12441300
C	0.02369200	0.02658600	1.10085300
C	-1.39407100	-0.08364900	0.96401800

O	-1.96595200	-1.20509400	0.92820100
C	0.18706500	0.32959000	-1.89886300
C	1.08001600	-0.82788300	-1.86949300
C	0.62901800	-2.06460700	-1.51318700
C	-1.16200600	0.31275500	-1.97939700
H	0.46745800	1.02069500	1.08039100
H	0.36735500	-2.07731700	1.18690200
H	-2.00362600	0.82938300	0.89427600
Cl	-4.35021900	-2.97127500	2.03908100
Cl	-4.73493700	0.09893500	0.18990300
Cl	-3.28097100	-2.75290900	-1.40463300
Al	-3.67410000	-1.75037000	0.44786600
C	2.28402300	-0.96492000	1.12143100
O	2.89300000	0.08018200	1.05376300
O	2.86491200	-2.17169300	1.17637500
C	4.30153400	-2.20318400	1.11006800
H	4.70695100	-1.62812800	1.95785200
H	4.62146900	-1.68886700	0.18967100
C	4.73610700	-3.65149500	1.13771800
H	5.83411200	-3.71438900	1.09551300
H	4.39587200	-4.14620300	2.05997700
H	4.32414800	-4.20226500	0.27843800
C	-2.01963000	3.52261800	0.25389500
C	-0.85756500	3.50081300	1.04322800
C	-3.24865100	3.22093200	0.85251300
C	-0.92552900	3.18087600	2.39917400
H	0.10699600	3.72821800	0.58140600
C	-3.32107200	2.89104300	2.21028500
H	-4.15823900	3.21789900	0.24798800
C	-2.15952300	2.86733100	2.98456500
H	-0.01515500	3.16871700	3.00339000
H	-4.28457000	2.63030100	2.65245300
H	-2.21214500	2.60615600	4.04406800

TS: E= -2700.80770128

H	1.71258000	2.75673500	-1.36450000
C	3.77479800	1.06586100	-1.38878200
C	2.97591400	-1.71779400	-0.61523600
H	0.97547500	-0.83521800	-0.55750200
H	-0.39433000	0.55829100	-0.91006200
C	-0.97319800	2.65567200	-1.07363800
H	4.37438200	1.16614300	-0.46739100
H	3.83122200	2.02285600	-1.92445700
H	4.24440700	0.28663500	-2.00829400
H	4.00618600	-1.46459900	-0.33187100
H	2.99023000	-2.08593900	-1.65579400
H	2.64522800	-2.54976700	0.02188300
H	-1.56150800	2.42365800	-1.98632300
O	-0.40849300	3.93586400	-1.20291200
H	-1.70792100	2.59176900	-0.25203600
C	-0.72177500	4.84846200	-0.16281100
H	-0.36536000	5.82555800	-0.52341000
H	-1.81742600	4.92113900	-0.03100300
C	1.83353000	-0.14294600	1.50190100
C	0.83780100	0.83766100	1.71413800
C	-0.51431700	0.52255900	1.65135500
O	-0.93780500	-0.65668100	1.37074700
C	1.37608300	1.74146500	-1.14203100
C	2.35550700	0.72140100	-1.04483200
C	2.03067500	-0.54953400	-0.51087900
C	0.03251900	1.56232900	-0.93794400
H	1.12689900	1.86677700	1.91007500

H	1.54796500	-1.18049200	1.68766100
H	-1.25909200	1.31199100	1.83203400
Cl	-3.33688200	-2.78170600	1.58029200
Cl	-3.64126400	0.67020300	0.52247700
Cl	-1.74834800	-1.61501600	-1.44528800
Al	-2.48257500	-1.15272400	0.53025100
C	3.22946800	0.21899500	1.88331800
O	3.68663800	1.34082100	1.85253400
O	3.93524600	-0.86178600	2.24495900
C	5.30853700	-0.64859100	2.62067500
H	5.34120900	0.09732200	3.43016500
H	5.84714200	-0.21599300	1.76177300
C	5.88556300	-1.98132200	3.04292200
H	6.93790700	-1.85722000	3.34062800
H	5.32976600	-2.39553900	3.89759700
H	5.84241800	-2.70902900	2.21827400
C	-0.06813800	4.51599700	1.16068500
C	1.33091100	4.52736100	1.27641000
C	-0.83587400	4.18044700	2.28298500
C	1.94871000	4.22215000	2.48891900
H	1.93857800	4.77374700	0.40213700
C	-0.22114900	3.88150500	3.50429100
H	-1.92632200	4.15704200	2.20247800
C	1.17086700	3.90433400	3.60883300
H	3.03772500	4.20826400	2.55789900
H	-0.83281800	3.62301600	4.37181400
H	1.65374700	3.66100300	4.55793500

P: E= -2700.85238431

H	0.24301300	1.04207300	-3.45730300
C	2.42139100	-0.62186700	-3.43978000
C	2.07134000	-2.83109600	-1.52752800
H	0.03585400	-2.40445000	-2.00332800
H	-1.70022000	-0.76215700	-2.24843700
C	-1.94967200	1.34664300	-2.03120200
H	3.28695400	-0.50341700	-2.76644200
H	2.40613900	0.23974600	-4.12209200
H	2.60576900	-1.53002600	-4.03769900
H	3.01130900	-2.34518700	-1.22833700
H	2.25027200	-3.34285000	-2.48395100
H	1.84068100	-3.59602900	-0.77161100
H	-2.33729400	1.40913300	-3.06471000
O	-1.18258100	2.50544700	-1.76179300
H	-2.82289700	1.27195200	-1.36406100
C	-1.70305300	3.40672200	-0.79621900
H	-1.16240800	4.35169600	-0.95747300
H	-2.77736800	3.59758200	-0.97296800
C	0.48412300	-1.24021000	-0.28176900
C	-0.64560500	-0.17606500	-0.45817700
C	-1.75079100	-0.55760300	0.44515500
O	-2.89313700	-0.80003200	0.03643800
C	0.15348800	0.19050800	-2.77865800
C	1.14117700	-0.70732800	-2.66151600
C	0.91926300	-1.83407000	-1.66286200
C	-1.07808300	0.09073500	-1.91732900
H	-0.23707300	0.76918700	-0.06172900
H	0.14266800	-2.08979800	0.32956200
H	-1.54148000	-0.66872900	1.52535100
Cl	-5.17327000	-2.96650500	-0.00941800
Cl	-3.80957200	-1.45223200	2.95904300
Cl	-5.62340900	0.57175300	0.58847200
Al	-4.50685200	-1.20432800	0.95151700

C	1.67361800	-0.62861300	0.44333300
O	2.06024200	0.50694200	0.30706700
O	2.26425900	-1.52429300	1.24569400
C	3.45112500	-1.09301100	1.93847200
H	3.19784600	-0.21706400	2.55650600
H	4.19189700	-0.75951800	1.19426100
C	3.95242100	-2.25417600	2.76759000
H	4.85894800	-1.95882000	3.31755000
H	3.19273400	-2.57239200	3.49758100
H	4.20015300	-3.11572400	2.12907200
C	-1.48341400	2.91366500	0.61621800
C	-0.18007200	2.85931300	1.13501000
C	-2.53824400	2.39280000	1.37717800
C	0.06394000	2.28923400	2.38583900
H	0.65473700	3.23017200	0.53627400
C	-2.29812000	1.82390100	2.63399200
H	-3.55762500	2.41125700	0.98572500
C	-0.99518100	1.76703500	3.13720700
H	1.08649100	2.24214200	2.76663300
H	-3.12685700	1.40333500	3.20566900
H	-0.80757100	1.31461500	4.11398300

endo

1 = b-endo 1

2: E= -458.791954451

C	1.25493700	-1.38454600	-0.88867300
C	-0.01335700	-0.96472100	-0.75864500
C	-0.99527200	-1.69893600	0.08163300
H	-2.02052400	-1.25172200	0.11070700
O	-0.73970700	-2.70642800	0.70048600
H	-0.34078300	-0.06032100	-1.28103400
H	1.59713500	-2.28565700	-0.37348300
C	2.22798900	-0.64054500	-1.73301200
O	1.98187800	0.36685800	-2.35516700
O	3.42911000	-1.23844000	-1.71538000
C	4.46726400	-0.61960100	-2.49395800
H	4.13512600	-0.56053500	-3.54314100
H	4.60301300	0.41620800	-2.14281700
C	5.72401400	-1.44682600	-2.33677800
H	6.54285500	-1.00050000	-2.92158200
H	6.03557400	-1.49152000	-1.28209200
H	5.56419100	-2.47579300	-2.69331300

RC: E= -1077.93378314

H	-0.74652700	0.63108800	2.26062700
C	0.85985900	-1.45761300	2.55463100
C	3.74627400	-0.66289000	1.70085500
H	2.64487900	1.10316800	0.97768300
H	0.75911100	1.67136300	-0.20675000
C	-1.24597600	2.41439000	0.31750600
H	0.20435000	-2.06479000	1.90856000
H	0.28625100	-1.23214900	3.46970600
H	1.72643800	-2.06875000	2.83727400
H	3.60435900	-1.48193900	2.41936700
H	4.56168000	-0.02112700	2.07467600
H	4.10035800	-1.11325700	0.75784300
H	-0.94522600	3.46670400	0.12480100
O	-2.12344700	2.35283100	1.41791800
H	-1.75454100	2.07067800	-0.60787900

C	-3.47424800	2.60317100	1.11313500
H	-3.96975300	2.77544900	2.08358300
H	-3.58969900	3.53497500	0.52439900
C	1.26621500	-1.19802300	-1.20368500
C	0.03146400	-0.74133500	-1.47333100
C	-1.20095200	-1.38931000	-0.97932000
H	-2.14526100	-1.00108300	-1.42730800
O	-1.23564000	-2.26700900	-0.14137300
H	-0.08295300	0.15273900	-2.09197100
H	1.42355300	-2.11169200	-0.62815700
C	0.09905600	0.71034200	1.57017500
C	1.23717100	-0.18080700	1.84353500
C	2.49996700	0.13836500	1.47596300
C	-0.03130700	1.56782700	0.54381600
C	2.44955000	-0.45727900	-1.70205100
O	2.42310600	0.66852400	-2.15075100
O	3.57297600	-1.18759100	-1.59968900
C	4.78747600	-0.55928100	-2.04419700
H	4.66092600	-0.24779100	-3.09322600
H	4.94655400	0.35784800	-1.45406200
C	5.91617400	-1.55206600	-1.87434600
H	6.86111300	-1.10861500	-2.22383300
H	6.03863400	-1.83584600	-0.81788700
H	5.72548100	-2.46602700	-2.45709700
C	-4.15209300	1.45090200	0.39536600
C	-3.76520300	0.13070200	0.66326900
C	-5.18964200	1.68010500	-0.51795400
C	-4.40467000	-0.94029000	0.03466200
H	-2.94142500	-0.05516000	1.35374100
C	-5.83878700	0.61065000	-1.14087100
H	-5.49100600	2.70666500	-0.74683200
C	-5.44677600	-0.70324600	-0.86670700
H	-4.06426200	-1.95830600	0.23823800
H	-6.64630400	0.80439100	-1.85134500
H	-5.94728000	-1.53960000	-1.36070900

TS: E=-1077.91697551

H	0.02419100	0.94501600	1.79947600
C	2.20692600	-0.45808100	2.47183700
C	4.35078900	-0.23473900	0.44447500
H	3.04901500	1.34898100	-0.36792300
H	1.19884800	1.99001700	-0.86372800
C	-0.91955400	2.20572200	-0.39863000
H	2.18603100	-1.51641700	2.16243900
H	1.38456200	-0.31142900	3.18563800
H	3.16073500	-0.28097200	2.99455600
H	4.22147700	-1.27132600	0.79061800
H	4.96769100	0.28642700	1.19874000
H	4.91911700	-0.26269900	-0.49391000
H	-0.87442300	3.31263800	-0.28535800
O	-1.84977000	1.66444300	0.50569200
H	-1.22533300	2.02100600	-1.44719600
C	-3.18082800	2.09806100	0.30162000
H	-3.73639300	1.76233900	1.19068600
H	-3.22943700	3.20428200	0.27048100
C	2.03116800	-0.59445800	-1.39413300
C	0.66873100	-0.26006700	-1.43194800
C	-0.27841300	-1.04910700	-0.64348400
H	-1.35557500	-0.87617300	-0.87645500
O	0.05675200	-1.82202800	0.23723800
H	0.29112600	0.33206300	-2.26682500
H	2.31588400	-1.55422100	-0.96275300

C	0.81330300	1.08070900	1.05676200
C	2.04294900	0.43384500	1.26879000
C	3.03102000	0.46372400	0.27101400
C	0.44377500	1.63103200	-0.16174200
C	2.88157700	-0.03018500	-2.46198600
O	2.66681100	1.02186700	-3.03076900
O	3.96078200	-0.79493700	-2.72180100
C	4.86606100	-0.30653400	-3.72290300
H	4.31685500	-0.17976700	-4.66970500
H	5.22334100	0.69308600	-3.42593100
C	5.99789000	-1.30284200	-3.85122900
H	6.71004100	-0.96817400	-4.62120200
H	6.54161100	-1.40788200	-2.89968300
H	5.61585900	-2.29413700	-4.13911300
C	-3.79904000	1.51847300	-0.95208600
C	-3.96891800	0.12906400	-1.06008000
C	-4.16524900	2.33032700	-2.03167700
C	-4.49468200	-0.43380600	-2.22319200
H	-3.68409100	-0.51075700	-0.22101100
C	-4.69674100	1.77028000	-3.19830300
H	-4.03103300	3.41345300	-1.95972300
C	-4.85990100	0.38714100	-3.29647200
H	-4.62298200	-1.51662300	-2.29429900
H	-4.97820300	2.41633400	-4.03337100
H	-5.27187800	-0.05329300	-4.20758400

P: E= -1077.98771868

H	1.21476900	2.49285900	0.96793100
C	2.85796400	0.84602800	2.34642900
C	0.78543600	-1.69277900	1.70351000
H	2.77611900	-1.39835700	0.96683200
H	0.35091800	1.93238300	-1.25704600
C	-1.27490900	1.55999600	0.03790700
H	2.63993700	0.25045700	3.24978800
H	2.82937300	1.91057600	2.62238300
H	3.88907500	0.59066000	2.04450400
H	-0.20365600	-1.21867000	1.67159700
H	1.12748500	-1.68948000	2.75067400
H	0.68256600	-2.73746400	1.37648800
H	-1.26900000	2.58401300	0.46190700
O	-1.65193400	0.62667000	1.02423700
H	-1.99928400	1.56329100	-0.79890100
C	-2.93829100	0.81904300	1.58376100
H	-2.98132800	0.13538300	2.44550200
H	-3.03585600	1.85308300	1.96691600
C	1.48222700	-0.99206000	-0.68501900
C	0.21709400	-0.22664900	-1.08858600
C	-1.03747300	-1.06938000	-0.99059200
H	-1.97027400	-0.54035500	-1.29445200
O	-1.06972400	-2.24760500	-0.72569900
H	0.28941800	-0.06119500	-2.17889900
H	1.34509000	-2.04859200	-0.97368500
C	1.13788200	1.44875500	0.64140300
C	1.89352800	0.52097500	1.24276000
C	1.79065400	-0.93143200	0.82501900
C	0.13113100	1.20438000	-0.45727500
C	2.65356800	-0.46606000	-1.51020800
O	2.54976600	0.20140200	-2.51367400
O	3.84229500	-0.84841400	-1.01722600
C	5.00997200	-0.40256800	-1.72401400
H	4.98287700	-0.80689400	-2.74886000
H	4.97417700	0.69498200	-1.81101900

C	6.22493700	-0.87605000	-0.95639500
H	7.14448100	-0.55843800	-1.47171500
H	6.23518100	-0.45471000	0.06071600
H	6.23505300	-1.97370000	-0.87451300
C	-4.06605200	0.51787400	0.62066700
C	-4.21687100	-0.77932200	0.10343800
C	-4.95345000	1.51884400	0.20789200
C	-5.23620200	-1.06357900	-0.80595900
H	-3.52207800	-1.56786700	0.40269800
C	-5.97958000	1.23515100	-0.69927900
H	-4.83960500	2.53319700	0.60102800
C	-6.12137100	-0.05705100	-1.20878100
H	-5.34060300	-2.07611900	-1.20307100
H	-6.66542300	2.02657600	-1.01124200
H	-6.92000700	-0.28178800	-1.91987700

a-endo'

1: E= -388.203599857

H	-0.32515900	0.23887500	1.09115700
C	2.01181100	-0.74532600	2.02676900
C	4.25889200	0.05907700	0.00201700
H	2.58513500	1.24844700	-0.78559600
H	1.08381800	2.80782700	0.17685000
C	-1.10885300	2.70820700	0.31085200
H	2.98998500	-1.24294600	2.04235800
H	1.23516600	-1.52598600	1.95175100
H	1.86359800	-0.25149300	3.00265200
H	4.48612400	-0.63953600	0.81897700
H	4.96991300	0.90148600	0.07758700
H	4.48710700	-0.44977700	-0.95148600
H	-1.18483600	3.60690600	0.96526100
O	-2.09226100	1.76893800	0.64816500
H	-1.26606800	3.08555500	-0.72611100
C	-3.39794100	2.26632200	0.56737900
H	-3.56041800	3.12233400	1.25436800
H	-4.08621100	1.45628400	0.84893900
H	-3.65160400	2.60412000	-0.45857200
C	0.52663700	0.86280800	0.79884100
C	1.86517800	0.24613300	0.89793400
C	2.84541300	0.55525900	0.02293200
C	0.26446900	2.12254300	0.42230500

2: E= -2398.50446126

C	2.01869500	-2.17670700	-0.56924000
C	0.76722300	-1.95860100	-1.01082500
C	-0.26209300	-1.54233500	-0.08678800
H	-0.00106100	-1.39861300	0.97447600
O	-1.42030900	-1.34139600	-0.47165500
H	0.47652600	-2.08194500	-2.05752400
H	2.81839500	-2.49211500	-1.24363900
H	2.27821300	-2.04420400	0.48597600
B	-2.69725500	-0.83109200	0.39897200
C	-2.38427100	-1.13587700	1.96353300
C	-2.75921200	0.74680000	0.01794100
C	-3.89446700	-1.72395100	-0.23188800
C	-1.93148900	-2.39417400	2.37284600
C	-2.61936500	-0.22448500	2.99718200
C	-1.62219200	1.55181600	0.11799700
C	-3.91875000	1.40602000	-0.40005900
C	-4.83901400	-2.42701600	0.51985300

C	-4.05062500	-1.80547300	-1.62080200
F	-1.70298600	-3.34757400	1.44622600
C	-1.69559500	-2.74339000	3.70051800
F	-3.09253900	1.00019700	2.74263200
C	-2.40457800	-0.53088600	4.34470500
F	-0.46288100	1.02160800	0.57152100
C	-1.59601200	2.90774000	-0.20054700
F	-5.08563100	0.75843100	-0.48752700
C	-3.94335400	2.76457100	-0.72800300
F	-4.82520900	-2.38969900	1.86010600
C	-5.85698000	-3.19104300	-0.05838000
F	-3.23366500	-1.11379600	-2.42918400
C	-5.04769700	-2.55874800	-2.23844700
F	-1.25239800	-3.95622500	4.02323900
C	-1.93898900	-1.79710000	4.69816900
F	-2.64447100	0.37226600	5.29048600
F	-0.47491600	3.61721800	-0.08841000
C	-2.77451300	3.51983300	-0.62975100
F	-5.07288700	3.34503200	-1.12231500
F	-6.72899300	-3.84630800	0.70470500
C	-5.95981100	-3.25910300	-1.44686800
F	-5.14696600	-2.60421300	-3.56572000
F	-1.72610900	-2.10100900	5.97258200
F	-2.78355100	4.81187600	-0.93578800
F	-6.92074100	-3.98064300	-2.01332500

RC: E= -2786.74113810

H	-3.00139600	-0.63705400	0.52835500
C	-3.88632600	1.82316000	0.36510500
C	-4.83855600	2.48001500	-2.52682000
H	-4.04033500	0.46005600	-2.84963700
H	-2.48119400	-0.95632000	-2.47785500
C	-1.78841000	-2.47600400	-1.07727700
H	-2.91164300	2.03899300	0.82921500
H	-4.47947700	1.31170900	1.14134700
H	-4.38469800	2.77041700	0.12609900
H	-4.80855400	3.28656700	-1.78199000
H	-5.90029900	2.27380600	-2.75278900
H	-4.40075600	2.86931300	-3.46224500
H	-2.25506900	-3.28807100	-1.68060400
O	-1.86203200	-2.77421200	0.28907300
H	-0.73176200	-2.42222000	-1.41203400
C	-1.29156300	-4.02060900	0.60926000
H	-1.76973300	-4.84286600	0.04108100
H	-1.44866900	-4.19866900	1.68076300
H	-0.20547000	-4.03786800	0.40170500
C	-1.45414800	2.00125400	-2.80466300
C	-0.58015600	1.01348500	-2.50514000
C	0.13140400	1.05068200	-1.26420400
H	0.02956200	1.94394000	-0.63022600
O	0.86827600	0.11719300	-0.89185400
H	-0.39977500	0.16445600	-3.16731500
H	-1.99869900	2.01927300	-3.74903600
H	-1.61012500	2.84384900	-2.12677300
B	1.76527800	0.03929300	0.44680700
C	-3.05177200	-0.35907400	-0.52595800
C	-3.71742200	0.91637000	-0.82766300
C	-4.13875800	1.23263600	-2.07959100
C	-2.46908700	-1.18981900	-1.40942000
C	2.18411900	1.55727800	0.86205000
C	2.62391400	2.47695300	-0.09448200
C	2.21780800	2.01534500	2.18221900

C	3.03584400	3.77450100	0.20511700
C	2.62845600	3.30440200	2.53270300
C	3.03875400	4.19082200	1.53714800
C	3.01782800	-0.86637000	-0.05646200
C	2.78928100	-2.06128400	-0.74747800
C	4.36285100	-0.54573800	0.14333100
C	3.80353100	-2.87751300	-1.24103800
C	5.41510500	-1.33593700	-0.33222400
C	5.13362800	-2.50705300	-1.03261400
C	0.77471800	-0.68650700	1.51930200
C	1.03530600	-1.89289700	2.17418800
C	-0.45293100	-0.10501100	1.84014600
C	0.13090800	-2.48906400	3.05635700
C	-1.38844800	-0.66493900	2.70135500
C	-1.09804800	-1.88475100	3.30605300
F	1.87329300	1.21324200	3.19711800
F	2.63851700	3.68995700	3.80604100
F	3.42944700	5.42039300	1.85316000
F	3.43171700	4.60689700	-0.75596200
F	2.67167900	2.11677900	-1.39299300
F	6.67947600	-0.97851700	-0.11807900
F	6.12047200	-3.26951600	-1.49155900
F	3.51963000	-4.00637800	-1.88962200
F	1.53050300	-2.50254400	-0.92917000
F	4.72256800	0.55066700	0.82535100
F	2.18443700	-2.55397000	1.98907200
F	-0.78616200	1.08875400	1.29631300
F	0.40540300	-3.67073800	3.60841500
F	-1.99148000	-2.48342300	4.08633200
F	-2.57076000	-0.07752400	2.90419300

TS: E= -2786.73441554

H	-3.87128900	-0.60118600	0.15114700
C	-4.84485600	1.86325200	-0.07243700
C	-5.36928900	2.66658200	-2.87773500
H	-4.67687900	0.62641300	-3.30511000
H	-3.47361900	-0.95091400	-2.88457700
C	-2.62228200	-2.39282800	-1.50333800
H	-4.19479100	2.75644100	-0.10728900
H	-4.68445500	1.37701800	0.89727800
H	-5.88210500	2.23184700	-0.13083500
H	-5.03264300	3.52786900	-2.28113600
H	-6.44723700	2.53404400	-2.68401300
H	-5.25556200	2.92897000	-3.93961600
H	-2.99959500	-3.19841600	-2.17370700
O	-2.74194800	-2.75932800	-0.16139500
H	-1.55899200	-2.23829400	-1.78851900
C	-2.14140800	-4.00519900	0.12153400
H	-2.57592000	-4.80958000	-0.50370400
H	-2.33345400	-4.23701700	1.17638600
H	-1.05056500	-3.97805300	-0.04660400
C	-2.68992600	1.90747900	-3.01728500
C	-1.73826000	0.88162600	-2.83694100
C	-1.00475700	0.84322900	-1.64815500
H	-1.16823400	1.65791800	-0.93130700
O	-0.15568200	-0.05150700	-1.34450000
H	-1.53169000	0.14324800	-3.61390500
H	-2.97370900	2.16458400	-4.04059800
H	-2.62210900	2.77125400	-2.34833800
B	0.71192100	-0.05693600	-0.02924500
C	-3.94629400	-0.32005800	-0.89882600
C	-4.51865800	0.94384800	-1.21256500

C	-4.60628700	1.40708000	-2.54232700
C	-3.36251800	-1.14570400	-1.81827400
C	1.10482000	1.48830100	0.33844900
C	1.51846400	2.37784600	-0.65805400
C	1.13558300	2.00260000	1.63731200
C	1.89592600	3.69805000	-0.41236000
C	1.51079900	3.31543800	1.93321100
C	1.89258800	4.17067900	0.90011700
C	2.01519600	-0.93605500	-0.47092700
C	1.86065300	-2.12852100	-1.18502500
C	3.33923200	-0.58060500	-0.20246200
C	2.92224900	-2.90522200	-1.64164800
C	4.43827300	-1.32862600	-0.63948100
C	4.22885700	-2.49660900	-1.36878700
C	-0.23552100	-0.76717700	1.11278500
C	0.04741500	-1.97878100	1.75012300
C	-1.44620600	-0.18802100	1.50408900
C	-0.81527800	-2.58554000	2.66779600
C	-2.34408300	-0.76337200	2.39544900
C	-2.03303600	-1.98871600	2.97715500
F	0.82166700	1.23404800	2.68964400
F	1.51534400	3.75378800	3.19094100
F	2.25085500	5.42394200	1.16298200
F	2.26793600	4.50065800	-1.40925200
F	1.57679200	1.96993200	-1.93882000
F	5.67951600	-0.93405200	-0.36046300
F	5.26053600	-3.22122800	-1.79222100
F	2.70404000	-4.03555500	-2.31502100
F	0.62837000	-2.62187700	-1.42428000
F	3.63431100	0.51393500	0.51418100
F	1.17856400	-2.65312000	1.50637000
F	-1.82150300	1.01474300	1.01000100
F	-0.51569400	-3.77573300	3.18933100
F	-2.89408500	-2.59474900	3.78902400
F	-3.52184300	-0.17823000	2.64991000

P: E= -2786.79837418

H	-4.51399600	-0.77277300	-0.89616500
C	-4.72626500	1.86090600	-0.51749200
C	-1.82839500	2.85349400	-0.89516100
H	-3.07571500	2.63748000	-2.60638700
H	-2.99945200	-1.26613500	-3.10728300
C	-2.42563000	-2.42610100	-1.42536400
H	-4.32333700	2.33330800	0.39372700
H	-5.54750500	1.19591900	-0.21458200
H	-5.14664700	2.67308400	-1.13525700
H	-1.34300000	2.27838700	-0.09294200
H	-2.52076100	3.55822200	-0.41283400
H	-1.05148500	3.44528300	-1.40003100
H	-3.38314400	-2.96590300	-1.29071900
O	-1.80574800	-2.20585900	-0.17716200
H	-1.77566200	-3.04845000	-2.07089000
C	-1.28571800	-3.36684900	0.43891100
H	-2.07773400	-4.12514500	0.57701000
H	-0.90045200	-3.07143400	1.42098900
H	-0.46156500	-3.80080500	-0.15320800
C	-1.59724000	1.10543000	-2.76033100
C	-1.31966400	-0.30630900	-2.18209400
C	-0.65819800	-0.19771800	-0.85257500
H	-1.24477300	0.11019600	0.01647400
O	0.57198400	-0.32107700	-0.77181100
H	-0.61730100	-0.83256700	-2.84610400

H	-2.03552200	0.93611800	-3.75625800
H	-0.65051100	1.64047000	-2.91052200
B	1.57501700	-0.11584500	0.45860200
C	-3.68493900	-0.22838500	-1.36102600
C	-3.65533200	1.11174600	-1.26431900
C	-2.56148900	1.95201900	-1.90734600
C	-2.65343500	-1.06749400	-2.07542300
C	1.71954300	1.49839900	0.64521500
C	1.57832300	2.40594600	-0.40539700
C	2.01087500	2.07500500	1.88623700
C	1.64452500	3.79092500	-0.24410800
C	2.10577800	3.45131100	2.09147700
C	1.90845800	4.32046300	1.01669500
C	2.91551400	-0.82547700	-0.12395100
C	2.83022600	-2.03724900	-0.81787900
C	4.20228900	-0.30037200	0.00402500
C	3.92828600	-2.68290600	-1.38004700
C	5.33457900	-0.91477800	-0.54209300
C	5.19524700	-2.11141700	-1.24225600
C	0.91778000	-0.84061100	1.77305700
C	1.45525200	-1.97074700	2.40235500
C	-0.22971200	-0.32839300	2.38922000
C	0.88409700	-2.56432900	3.53374400
C	-0.84293200	-0.89068200	3.50661000
C	-0.27599400	-2.02568600	4.08758700
F	2.23065600	1.29884200	2.95607000
F	2.37898500	3.94242400	3.29779500
F	1.97720000	5.63550700	1.19440600
F	1.43418300	4.60120600	-1.28334000
F	1.34624700	1.97663500	-1.66162100
F	6.53933500	-0.36708200	-0.39657800
F	6.25912300	-2.70972000	-1.76874200
F	3.78581200	-3.83761700	-2.03045700
F	1.64379100	-2.66597900	-0.93345000
F	4.41957200	0.83617400	0.67963100
F	2.57193500	-2.55624800	1.95858700
F	-0.81428200	0.79393100	1.91297800
F	1.44114500	-3.63965800	4.08440800
F	-0.83130700	-2.58047700	5.15835500
F	-1.94091800	-0.35055900	4.02903700

a-exo'

1: E= -388.202311739

H	1.03082900	2.03566500	0.76765300
C	2.90946000	0.41760600	1.80267200
C	4.92747200	-0.28866300	-0.48396400
H	3.35977500	0.71942000	-1.65028000
H	1.02161600	0.43387600	-1.86042800
C	-0.56084200	1.90036600	-1.42390800
H	2.14449800	-0.28682400	2.17226500
H	2.79245600	1.34393600	2.39156200
H	3.89699500	-0.00303100	2.03112200
H	5.15501200	-0.57752400	0.55125700
H	5.75389100	0.34685500	-0.84867400
H	4.95198400	-1.20618500	-1.09889400
H	-0.87006300	2.52872400	-0.56184800
O	-1.57210200	0.98087000	-1.77005900
H	-0.38500700	2.59845100	-2.27459300
C	-2.76873500	1.59318500	-2.15991800
H	-3.20612100	2.21135500	-1.34841500
H	-3.48618100	0.80102900	-2.41953800

H	-2.63228800	2.24990300	-3.04460900
C	1.42733800	1.35286800	0.00331900
C	2.71037900	0.70118000	0.33354000
C	3.60977700	0.40794500	-0.62953800
C	0.70022900	1.16301800	-1.10821400

2: E= -2398.50398997

C	2.19958200	-2.09221900	0.62320200
C	1.24533500	-1.91947900	-0.31122200
C	-0.05444600	-1.37579600	0.04123400
H	-0.82000800	-1.24754900	-0.74026200
O	-0.31306300	-1.06093100	1.20955700
H	1.40619600	-2.17665100	-1.36073500
H	3.17984600	-2.50000100	0.36522100
H	2.00627000	-1.82314600	1.66652300
B	-1.66977400	-0.49290800	1.86923100
C	-2.57421000	0.14145000	0.67985900
C	-2.29030600	-1.82331800	2.56408000
C	-1.08434500	0.59992600	2.91810100
C	-2.01754700	1.03899000	-0.23630000
C	-3.94604600	-0.08354200	0.53460900
C	-2.45013500	-2.99955600	1.82734100
C	-2.71160200	-1.89115000	3.89475000
C	-1.63672300	1.86900500	3.10805400
C	0.01717400	0.29977200	3.72755700
F	-0.70378000	1.33560100	-0.15662200
C	-2.74044300	1.66484200	-1.24983800
F	-4.60427100	-0.88976600	1.37467200
C	-4.71442300	0.52549700	-0.46207000
F	-2.12088300	-3.01724300	0.51620700
C	-2.96039100	-4.18422600	2.35344000
F	-2.65125600	-0.81897000	4.69219700
C	-3.23331300	-3.05544000	4.46636000
F	-2.72496800	2.25549400	2.42777600
C	-1.11812300	2.79951700	4.01299500
F	0.58793500	-0.91871900	3.67599100
C	0.57016800	1.19874300	4.63836500
F	-2.14905700	2.50190500	-2.09873400
C	-4.10781300	1.40425800	-1.35966100
F	-6.01745200	0.27898400	-0.55795900
F	-3.08232000	-5.27412400	1.59889700
C	-3.35637900	-4.20922800	3.69179800
F	-3.62065400	-3.06995700	5.73839500
F	-1.68104000	3.99734400	4.15060100
C	-0.00493000	2.46246900	4.78172300
F	1.62528300	0.85968800	5.37717900
F	-4.82379500	1.98721200	-2.31324600
F	-3.85128200	-5.32176500	4.22122300
F	0.50225000	3.33402500	5.64638900

RC: E= -2786.74398756

H	-4.49379800	-0.40298500	-1.44248500
C	-4.20363100	-2.97311700	-1.70931200
C	-1.52723700	-3.96045200	-0.44115000
H	-1.42059800	-1.84343400	0.08585400
H	-2.13266700	0.03427600	0.47519400
C	-3.40228700	1.71224200	-0.14548000
H	-4.41181200	-2.55824800	-2.71044500
H	-5.16977300	-3.00659000	-1.17742500
H	-3.85510000	-4.00519600	-1.83507900
H	-1.57892500	-4.38046100	0.57963300

H	-0.45991700	-3.97832600	-0.70883500
H	-2.07260500	-4.63936400	-1.10996600
H	-4.34721100	1.85420100	-0.70682200
O	-2.36666000	2.49916500	-0.72150600
H	-3.57512700	2.04743000	0.89673200
C	-2.62325200	3.88414500	-0.68010200
H	-3.54810200	4.14382500	-1.23085300
H	-1.77386400	4.39457800	-1.15573800
H	-2.72007200	4.25250200	0.35743300
C	-0.81438600	-1.34714100	-2.76646700
C	-0.93764300	-0.02404900	-2.50589300
C	-0.16827400	0.58177800	-1.45972600
O	0.53309200	-0.12204300	-0.69878200
H	-1.39975600	-1.83096300	-3.55045700
B	1.56744200	0.31794300	0.39953800
C	-3.61157300	-0.68986300	-0.85630100
C	-3.22204100	-2.10180700	-0.96569500
C	-2.05163800	-2.56088700	-0.44752200
C	-2.98763800	0.27597600	-0.15672300
H	-1.63128500	0.62323600	-3.04279900
H	-0.07154500	-1.94346500	-2.23512500
H	-0.20561300	1.66995700	-1.31303800
C	1.08234200	1.79471900	0.89106900
C	1.69412100	2.99613200	0.51783400
C	-0.10758700	1.94001900	1.61087700
C	1.17156200	4.25449100	0.84056600
C	-0.66706300	3.16744000	1.94736100
C	-0.02377000	4.33880000	1.55169900
C	1.46265300	-0.89260100	1.49258000
C	1.41363400	-2.22114100	1.05559900
C	1.46540000	-0.72410600	2.87994900
C	1.29660700	-3.31233200	1.91708000
C	1.36619200	-1.78918100	3.77923200
C	1.27470200	-3.09392600	3.29420500
C	3.04859800	0.26113700	-0.27566500
C	4.15140300	0.43982000	0.56447900
C	3.34972900	0.00626900	-1.61309300
C	5.47291400	0.36810200	0.12831200
C	4.65924500	-0.08020000	-2.09523700
C	5.72767800	0.10050800	-1.21859500
F	2.37660600	-0.15941300	-2.52954000
F	4.89133700	-0.32806500	-3.38386600
F	6.97906000	0.02439900	-1.66147100
F	6.48517500	0.55109500	0.97312200
F	3.94872600	0.71759600	1.86116700
F	2.81867600	3.00537000	-0.20732600
F	1.78948100	5.36590500	0.44796500
F	-0.56670300	5.52174600	1.82323600
F	-1.84232800	3.23520800	2.57753200
F	-0.80406800	0.85234300	1.98580900
F	1.55245300	0.49560800	3.42088000
F	1.47978000	-2.51553500	-0.25814200
F	1.35709700	-1.57012700	5.09211000
F	1.21043600	-4.55439900	1.43502400
F	1.16940300	-4.11854600	4.13460000

TS: E= -2786.73962957

H	-4.67649400	-0.36453100	-1.33665000
C	-4.24758400	-2.98404100	-1.62139900
C	-1.55439200	-3.82169300	-0.70155300
H	-1.40828200	-1.72677900	-0.05189900
H	-2.05644100	0.13181700	0.21596300

C	-3.35358600	1.80712700	-0.32937500
H	-5.21819300	-2.52891500	-1.85993800
H	-4.42052100	-3.83091500	-0.93647600
H	-3.83397600	-3.41844500	-2.54800200
H	-2.07637800	-4.36348800	0.10625400
H	-0.47671500	-3.90811600	-0.51268200
H	-1.78717500	-4.34072400	-1.64419100
H	-4.26250200	1.97704800	-0.94086100
O	-2.28193300	2.60314600	-0.78778500
H	-3.60090300	2.08004100	0.71885900
C	-2.53507100	3.98810600	-0.70967600
H	-3.41586100	4.27518300	-1.31605300
H	-1.65002100	4.50729300	-1.10183200
H	-2.70373500	4.31477000	0.33227900
C	-1.03341900	-1.57327500	-2.38515800
C	-1.01856400	-0.16782300	-2.33957300
C	-0.16058000	0.48463900	-1.44587200
O	0.49076200	-0.19397300	-0.58769400
H	-1.58479300	-2.06904800	-3.18731800
B	1.56021000	0.28338200	0.41878900
C	-3.71271400	-0.62918300	-0.88773400
C	-3.29701300	-1.99139100	-1.01397000
C	-1.98162600	-2.37742200	-0.71819100
C	-2.94912800	0.36822300	-0.35934900
H	-1.65302100	0.44485000	-2.97816600
H	-0.12464700	-2.07884500	-2.05193100
H	-0.07480700	1.57902700	-1.44609900
C	1.06444000	1.75826700	0.92128600
C	1.67696500	2.97435600	0.60749000
C	-0.15072300	1.87102200	1.60140800
C	1.12968100	4.21752200	0.94979700
C	-0.73749300	3.08067200	1.95209100
C	-0.09098500	4.26948300	1.61895400
C	1.53053500	-0.89668700	1.55607700
C	1.49944100	-2.23587000	1.15357800
C	1.55623800	-0.69445100	2.93782900
C	1.42977300	-3.30882500	2.04234000
C	1.50562200	-1.73979900	3.86484500
C	1.43581300	-3.05813100	3.41428000
C	3.02840500	0.24636600	-0.29105900
C	4.15002100	0.48388400	0.50867000
C	3.29987700	-0.07117100	-1.62128000
C	5.46056700	0.41880300	0.04084500
C	4.59814300	-0.15309000	-2.13530200
C	5.68515800	0.09119300	-1.29837800
F	2.30803800	-0.31007000	-2.50029200
F	4.80168500	-0.46087200	-3.41663800
F	6.92650000	0.01917700	-1.77160400
F	6.49190600	0.66174600	0.84780800
F	3.97586200	0.81567900	1.79726200
F	2.82698000	3.01727100	-0.07521700
F	1.74885200	5.34718500	0.61296000
F	-0.65832300	5.43978300	1.90305700
F	-1.94190900	3.11805600	2.53225400
F	-0.84896100	0.76123800	1.91713900
F	1.61358400	0.54093800	3.44868700
F	1.53197100	-2.56305000	-0.15453900
F	1.51770600	-1.48884000	5.17278200
F	1.35792700	-4.56320100	1.58808600
F	1.37580600	-4.06463000	4.28206600

P: E= -2786.79217453

H	-4.75794300	-0.59485000	-1.14276100
C	-4.38444700	-3.30618300	-1.46871900
C	-1.49649100	-3.98322000	-1.45205300
H	-1.52841900	-2.27609100	-0.17332100
H	-2.18332100	-0.13221600	0.14533200
C	-3.10098700	1.52707300	-0.80669800
H	-5.40684200	-2.90333300	-1.50817500
H	-4.34514900	-4.06337600	-0.66753500
H	-4.18884900	-3.84348700	-2.41168900
H	-2.01251800	-4.67535800	-0.77070000
H	-0.41557500	-4.10876200	-1.29097100
H	-1.72759700	-4.28904400	-2.48524800
H	-3.66891600	1.77865100	-1.72615200
O	-1.94681500	2.33445600	-0.70858200
H	-3.76851000	1.69509000	0.05983400
C	-2.18410900	3.72163900	-0.62683800
H	-2.80780900	4.07382000	-1.46976200
H	-1.20960400	4.22624700	-0.66748500
H	-2.68055300	3.98599700	0.32399400
C	-1.17248300	-1.57862500	-2.16849800
C	-1.46126100	-0.07737700	-1.87818900
C	-0.26247300	0.57703300	-1.29092300
O	0.23309500	0.05633700	-0.28539900
H	-1.52167600	-1.80540500	-3.18722700
B	1.47679300	0.48912700	0.59519500
C	-3.71513300	-0.92424300	-1.09583300
C	-3.37893600	-2.21813000	-1.23739100
C	-1.89004500	-2.53137000	-1.18585300
C	-2.63414100	0.08373000	-0.83864300
H	-1.73724100	0.45092000	-2.80127000
H	-0.09193700	-1.77146500	-2.14623300
H	0.19481800	1.47300000	-1.73371200
C	1.07724700	1.98375900	1.09678800
C	1.80330600	3.15364900	0.86232300
C	-0.13527100	2.15929800	1.77392900
C	1.37722300	4.41527400	1.29597800
C	-0.60183600	3.39387800	2.21193000
C	0.16334400	4.53537900	1.96936400
C	1.47049500	-0.66995300	1.74006100
C	1.35456900	-2.00759500	1.34899800
C	1.58882500	-0.45375500	3.11384700
C	1.30770200	-3.07257300	2.24733700
C	1.56147500	-1.49185600	4.04996000
C	1.41853700	-2.80947800	3.61363500
C	2.85076500	0.34766400	-0.26748200
C	4.05114200	0.53613800	0.42753900
C	2.99607200	-0.04022000	-1.59800400
C	5.31048000	0.37052900	-0.14381500
C	4.23635200	-0.22396700	-2.21659500
C	5.40257000	-0.01863800	-1.48267400
F	1.91884600	-0.26185200	-2.38864400
F	4.30719800	-0.59267000	-3.49444700
F	6.59164500	-0.18604100	-2.05150700
F	6.41690300	0.57300700	0.56583300
F	4.00744500	0.91334800	1.71230000
F	2.95957200	3.13198500	0.18860200
F	2.10946000	5.49927300	1.04843500
F	-0.27739100	5.72847700	2.35585800
F	-1.79358900	3.50687000	2.80223800
F	-0.92280300	1.09927600	2.01797500
F	1.72466800	0.78413100	3.60268800
F	1.27706500	-2.32652400	0.04152000
F	1.66945200	-1.23503500	5.35168700

F	1.16848800	-4.32572600	1.81370100
F	1.38511800	-3.80664100	4.49214800

b-endo'

1 = a-exo' 1

2: E= -1814.63504545

C	1.49211500	-0.96084900	-1.91017800
C	0.43159800	-0.13707000	-2.00438400
C	-0.86621800	-0.50990100	-1.46486600
H	-1.71483900	0.19334700	-1.56181300
O	-1.06219200	-1.59340500	-0.89567100
H	0.50071600	0.84072400	-2.48752100
H	2.46817200	-0.68268400	-2.31501400
H	1.39516400	-1.93479500	-1.42121500
Cl	-4.01682000	-0.68187400	-0.50230900
Cl	-2.98213700	-4.04641300	-1.26455300
Cl	-2.09688700	-2.54446200	1.90920500
Al	-2.67087500	-2.29825800	-0.11292300

RC: E= -2202.87495296

H	-0.56076300	-0.22313500	1.81093200
C	1.53093800	-1.73190100	1.95551100
C	3.95845300	-0.51804200	0.45068400
H	2.47568900	1.05340000	0.06285800
H	0.59670100	1.90199800	-0.09975000
C	-1.48840500	1.99460300	0.56489900
H	2.48874600	-2.25975800	1.87604600
H	0.72413600	-2.39366500	1.60466400
H	1.33088800	-1.55387100	3.02556300
H	3.98642900	-1.59220100	0.67763900
H	4.63309300	-0.01081600	1.16473800
H	4.40048900	-0.36711300	-0.54736500
H	-2.21883700	1.31738500	1.04680900
O	-1.88067600	2.30346200	-0.75829100
H	-1.45328400	2.92868700	1.16846000
C	-3.14138600	2.92883500	-0.83384700
H	-3.93969000	2.28137500	-0.42860900
H	-3.35002000	3.12742000	-1.89457800
H	-3.14853900	3.89042700	-0.28341400
C	1.51358200	-0.92490700	-1.84354400
C	0.41699500	-0.15400400	-2.03915500
C	-0.86849000	-0.52686300	-1.52067400
H	-1.70319900	0.18321900	-1.62842300
O	-1.07592600	-1.63867500	-0.96724800
H	0.47204400	0.81454300	-2.54018900
H	2.48957400	-0.64210000	-2.24022200
H	1.42525200	-1.89362800	-1.34858700
C	0.21909200	0.26719800	1.21876700
C	1.50750000	-0.42599200	1.20319300
C	2.58192100	0.06773400	0.52556100
C	-0.13027000	1.36961200	0.52076600
Cl	-4.00541900	-0.65341300	-0.38282900
Cl	-3.11457900	-4.04043700	-1.24148600
Cl	-2.04444400	-2.59279300	1.87828800
Al	-2.62759300	-2.28658200	-0.15717300

TS: E= -2202.87299303

H	-0.06686700	0.52590000	1.71721000
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C	2.08363400	-1.00521300	1.79627500
C	4.35122200	0.05788500	0.21615100
H	2.96665400	1.74150800	-0.14380300
H	1.11158100	2.62488800	-0.22561500
C	-0.99459400	2.68958800	0.36798800
H	2.28377600	-1.83785900	1.10026100
H	1.16202100	-1.25014300	2.33653100
H	2.92780700	-0.97704300	2.50550400
H	4.28611300	-1.03716000	0.12895800
H	4.88256900	0.27379900	1.16011700
H	4.97882900	0.43093900	-0.60585700
H	-1.74006500	1.97599000	0.76696300
O	-1.31226700	3.07485900	-0.95008700
H	-0.99985900	3.58081900	1.03624700
C	-2.60288900	3.62978900	-1.07091700
H	-3.38244500	2.90453300	-0.77581900
H	-2.74829400	3.90012200	-2.12618800
H	-2.71134600	4.54223900	-0.45169400
C	2.17106700	-0.02221700	-1.72097300
C	1.00819200	0.66705900	-2.02558800
C	-0.25560300	0.20593200	-1.60166000
H	-1.14583300	0.80576100	-1.83997100
O	-0.40680000	-0.88694300	-0.96375000
H	1.02940500	1.61758100	-2.56105600
H	3.10930500	0.25975700	-2.20054700
H	2.09233200	-1.05107000	-1.36596800
C	0.71416400	0.99831000	1.11517900
C	1.96165100	0.29347100	1.04746000
C	2.99685900	0.71115000	0.21666800
C	0.37147300	2.08156900	0.36557900
Cl	-3.41967200	-0.05908100	-0.60334600
Cl	-2.28541700	-3.43276200	-1.20716800
Cl	-1.52523300	-1.75642900	1.87829900
Al	-1.94616600	-1.58516800	-0.22114500

P: E=-2202.91582330

H	-0.62863400	0.39640700	1.99581900
C	1.48509300	-1.24817400	2.49225900
C	3.49161500	-1.11211600	0.33469000
H	2.68632000	0.87039700	0.27869400
H	0.69724600	2.12667700	-0.02519300
C	-1.44371700	1.93725200	0.02944300
H	1.53602400	-2.28406400	2.11800600
H	0.65502300	-1.19853300	3.20959400
H	2.42930500	-1.05447700	3.02770000
H	3.17286500	-2.16563600	0.29892400
H	4.05805100	-0.96227600	1.26520300
H	4.18282300	-0.94556400	-0.50617900
H	-2.20447700	1.17616900	0.29885100
O	-1.71697400	2.47351900	-1.24088900
H	-1.49069800	2.71947700	0.81369300
C	-3.02440200	2.98676600	-1.36248800
H	-3.78348100	2.20087000	-1.18732700
H	-3.13701900	3.37323700	-2.38503700
H	-3.20474800	3.81297600	-0.64777500
C	1.59375900	-0.32408600	-1.13389800
C	0.26483200	0.44229500	-1.27386900
C	-0.92767200	-0.41145400	-1.39441700
H	-1.83769700	0.01558500	-1.85143900
O	-0.98635800	-1.53459000	-0.87610000
H	0.25803800	1.15459000	-2.10965200
H	2.28320600	0.00281700	-1.92684900

H	1.40910600	-1.39716100	-1.29212300
C	0.16937400	0.46561800	1.25122000
C	1.27616500	-0.28714800	1.36123100
C	2.29572000	-0.16454900	0.23958300
C	-0.04889800	1.31478000	0.03630300
Cl	-4.06047000	-1.07837200	-0.71704300
Cl	-2.52467600	-4.28800400	-1.34830400
Cl	-2.05718400	-2.60685900	1.83062300
Al	-2.50746000	-2.48637000	-0.24325500

b-exo'

1 = a-endo' 1

2 = b-endo' 2

RC: E= -2202.87259782

H	1.15878900	1.54075200	0.18035700
C	3.25879100	-0.00922900	-0.44945400
C	2.16382700	-2.81928400	-1.29994600
H	0.28085300	-1.69926100	-1.18343900
H	-0.57637000	0.24021500	-1.99643900
C	-1.24518300	2.06080200	-0.96801600
H	3.62914600	0.73854300	-1.17119200
H	3.92246200	-0.88187900	-0.49611400
H	3.36312600	0.44581600	0.55091800
H	3.24092600	-2.68898700	-1.12753700
H	2.02841500	-3.16414600	-2.34047200
H	1.81056900	-3.64771100	-0.66113800
H	-1.11742200	2.84103700	-1.75170700
O	-1.05463400	2.61856000	0.31325000
H	-2.27912600	1.68102800	-1.07710000
C	-1.94751600	3.67023300	0.59735200
H	-1.82642800	4.51044400	-0.11415800
H	-1.72398900	4.03288700	1.61083500
H	-2.99863300	3.32845900	0.56150200
C	0.97782900	-1.54619600	2.06655500
C	0.24446900	-0.41662200	2.14926700
C	-1.04688600	-0.32706900	1.51518700
O	-1.58308400	-1.32429100	0.97672400
H	1.98013700	-1.61193000	2.49528600
C	0.87639400	0.77268400	-0.54849600
C	1.81430400	-0.34653300	-0.72218800
C	1.36265700	-1.57945800	-1.05758700
C	-0.28241000	0.94411900	-1.21279400
H	0.62419800	0.49121800	2.62197200
H	0.57082700	-2.43136300	1.57444000
H	-1.57624400	0.63897900	1.51248700
Cl	-4.12235500	-3.19374300	0.93085300
Cl	-4.16655600	0.37486200	0.44163600
Cl	-2.56208200	-1.73945500	-1.97383400
Al	-3.19880400	-1.50348300	0.05298800

TS: E= -2202.86640726

H	1.96500000	2.39641400	-0.06256900
C	3.90254700	0.58836800	-0.43537000
C	2.83435400	-2.16535000	-0.85451200
H	0.88885600	-1.13772900	-0.75929900
H	-0.31549800	0.50465300	-0.90663000
C	-0.71306500	2.57046700	-0.31620200
H	4.38977200	0.27074600	-1.37255700

H	4.39148800	0.02253400	0.37593800
H	4.11483900	1.65521400	-0.28501200
H	3.78026000	-2.14500300	-0.29216400
H	3.09290800	-2.18134700	-1.92832000
H	2.32063100	-3.11212600	-0.63389400
H	-1.09391500	2.87086400	-1.32015200
O	-0.03908100	3.62399800	0.31202500
H	-1.62013600	2.26181100	0.24341300
C	-0.82556400	4.77650600	0.47334800
H	-1.15988100	5.18694900	-0.50026100
H	-0.21139600	5.53247500	0.98263500
H	-1.72665100	4.57712400	1.08635300
C	1.55806400	-1.22866900	1.60982700
C	0.61997200	-0.29473000	2.03772100
C	-0.72458400	-0.41258500	1.66568600
O	-1.15409900	-1.38730600	0.96215300
H	2.59215200	-1.16403500	1.95318500
C	1.52889900	1.43621300	-0.35117900
C	2.42228400	0.31829300	-0.48351300
C	1.95218000	-0.98763700	-0.55432100
C	0.17819100	1.39209700	-0.50265200
H	0.91796800	0.61168700	2.56636800
H	1.20260000	-2.21757900	1.31764800
H	-1.44753100	0.36216400	1.96884600
Cl	-3.63004900	-3.30496400	0.29666900
Cl	-3.67560800	0.31567400	0.23704800
Cl	-1.63886400	-1.46622400	-2.08424400
Al	-2.60168300	-1.51027300	-0.15799400

P: E= -2202.91178016

H	1.58981500	1.92593800	-0.94615700
C	3.69759700	0.15518500	-0.92242800
C	2.79134200	-2.56956500	-0.24069500
H	1.15842100	-1.78493300	-1.37590100
H	-0.50283900	-0.14205300	-1.31551900
C	-1.08240100	1.74774200	-0.53792000
H	4.08376000	-0.41471800	-1.78465300
H	4.29218100	-0.16192600	-0.04963200
H	3.89611000	1.22138500	-1.10266700
H	3.39847500	-2.34805000	0.65175200
H	3.47110500	-2.65176500	-1.10106500
H	2.32766600	-3.55661700	-0.08901200
H	-0.83096900	2.41437400	-1.38750000
O	-0.97862300	2.43024300	0.68854600
H	-2.12276100	1.40501600	-0.70694300
C	-1.94517400	3.44385000	0.84751700
H	-1.86022800	4.21624900	0.05889600
H	-1.77530400	3.91652200	1.82499600
H	-2.97059100	3.02735900	0.82178100
C	0.68080900	-1.54282700	0.69789100
C	-0.16709200	-0.26583300	0.82464100
C	-1.59929200	-0.45946100	1.10720400
O	-2.26281100	-1.36454600	0.58157800
H	1.21396600	-1.69881600	1.64889900
C	1.31169200	0.88188500	-0.77403100
C	2.23296100	-0.09460700	-0.71265200
C	1.71560100	-1.50567300	-0.46137700
C	-0.13323200	0.55304700	-0.53926800
H	0.23197700	0.42403300	1.57781700
H	0.02528500	-2.41362300	0.54936600
H	-2.12915200	0.30439100	1.70466800
Cl	-4.82939500	-3.27289500	0.63260500

Cl	-4.79423900	0.25013100	1.48304000
Cl	-4.00067800	-0.73983600	-1.84834700
Al	-4.13398300	-1.32960800	0.19456900

d-endo'

1 = a-exo' 1

2: E= -516.118358545

C	2.12193800	-1.84325300	-0.12003600
C	0.87876600	-2.13464700	-0.54000600
C	-0.30229500	-1.62652300	0.15261000
H	-1.30405100	-1.89336600	-0.23020300
O	-0.22697000	-0.90849300	1.15192200
H	0.70048100	-2.76332800	-1.41631000
H	3.00414500	-2.22458400	-0.63981100
H	2.27450700	-1.21162900	0.76007800
B	-1.64719900	-0.31760800	1.95747500
F	-1.48315600	1.01593800	1.84511900
F	-2.65311000	-0.84990100	1.20608700
F	-1.49816100	-0.85012000	3.18715100

RC: E= -904.352247494

H	-0.61627800	-0.20098000	1.76711000
C	1.39139600	-1.79098200	1.89223600
C	3.92482900	-0.59504300	0.52680800
H	2.50419500	1.03561900	0.15161500
H	0.60186800	1.93043300	-0.09363100
C	-1.49791100	2.01801400	0.56619200
H	2.28772800	-2.40331800	1.73361400
H	0.50706200	-2.35052100	1.55223100
H	1.27130400	-1.64857100	2.98025900
H	3.92382400	-1.65722700	0.80549300
H	4.62428200	-0.07400300	1.20597000
H	4.35861100	-0.50618900	-0.48317200
H	-2.20191400	1.34084900	1.08322300
O	-1.93040900	2.27001500	-0.75966600
H	-1.47264700	2.97527900	1.13217700
C	-3.27564100	2.68188100	-0.82977500
H	-3.95598800	1.89468100	-0.45491000
H	-3.50832400	2.88278400	-1.88541000
H	-3.44939100	3.60831200	-0.24726400
C	1.51355900	-0.94481800	-1.93750600
C	0.41501700	-0.17842200	-2.10594800
C	-0.84952500	-0.52687000	-1.50455500
H	-1.67147600	0.20031400	-1.54916500
O	-1.03180000	-1.62520200	-0.93240600
H	0.45169900	0.77903100	-2.62997600
H	2.47895500	-0.66266200	-2.36162100
H	1.44789900	-1.89515200	-1.40467100
B	-2.36699100	-1.91811000	-0.08222600
F	-3.11118000	-0.75343400	-0.13378300
F	-2.95712400	-2.97805000	-0.69140000
F	-1.88001000	-2.17598800	1.17783800
C	0.18660600	0.28327500	1.20257300
C	1.45462600	-0.45201300	1.19923500
C	2.56751000	0.03406200	0.58928700
C	-0.13436100	1.40300600	0.52122800

TS: E= -904.347754700

H	-0.13597200	0.51955700	1.67950500
C	1.95527200	-1.07395000	1.73296700
C	4.28435900	-0.01554300	0.22466500
H	2.95137300	1.71269500	-0.09249600
H	1.11234300	2.63388000	-0.20480600
C	-1.01446400	2.68822500	0.34035700
H	2.21599600	-1.87513200	1.02147000
H	0.99032800	-1.33930700	2.17936700
H	2.73946900	-1.07240100	2.50960800
H	4.20336800	-1.10759600	0.11814200
H	4.79515000	0.17874100	1.18400700
H	4.93649600	0.35847300	-0.57770200
H	-1.75274100	1.95844500	0.71916200
O	-1.31740700	3.07053500	-0.98414400
H	-1.04378700	3.57904900	1.00845800
C	-2.65137800	3.49250000	-1.14277800
H	-3.36218100	2.68249300	-0.89172300
H	-2.78787500	3.77484600	-2.19631800
H	-2.88190300	4.37095700	-0.50770300
C	2.18485900	0.03769800	-1.70901800
C	0.98691600	0.68330400	-2.01074400
C	-0.24443400	0.17958300	-1.54668300
H	-1.16657800	0.73627400	-1.75028100
O	-0.31515200	-0.89946700	-0.87706300
H	0.96369800	1.62934200	-2.55320500
H	3.09993400	0.35774700	-2.21115500
H	2.14065500	-1.01311900	-1.41679100
B	-1.63219500	-1.29938600	-0.11433800
F	-2.48863300	-0.20543700	-0.20177700
F	-2.12090800	-2.41567200	-0.72376900
F	-1.21689600	-1.51150300	1.18926900
C	0.66720200	0.99104000	1.10845400
C	1.88733900	0.25225000	1.02980400
C	2.93846200	0.66020100	0.20049000
C	0.35504000	2.08765600	0.36091500

P: E= -904.393931817

H	-0.30063100	0.42919000	2.26712200
C	1.95556300	-1.08383000	2.58636400
C	3.57100400	-1.13764100	0.12309000
H	2.71801700	0.82475400	0.04471700
H	0.67355500	2.03806400	0.01375200
C	-1.42786100	1.81072600	0.31762000
H	2.06481600	-2.14854900	2.32218500
H	1.23401900	-1.01096600	3.41251000
H	2.93943600	-0.75092600	2.95794800
H	3.27529800	-2.19586100	0.19971900
H	4.26254600	-0.91814300	0.94951900
H	4.12956000	-1.01819900	-0.81821400
H	-2.15613800	1.03410200	0.63569800
O	-1.81561000	2.37924400	-0.90710500
H	-1.41172400	2.57213700	1.12356800
C	-3.10345800	2.94666000	-0.88644300
H	-3.87786800	2.19119400	-0.64923200
H	-3.30380900	3.35831500	-1.88540000
H	-3.17695900	3.76360700	-0.14234500
C	1.45088500	-0.49673100	-1.08804300
C	0.13313700	0.30099300	-1.11177400
C	-1.08788000	-0.53821300	-1.22044700
H	-2.02504500	-0.04495100	-1.52850800
O	-1.11758200	-1.73522800	-0.94045600
H	0.08240900	0.99951900	-1.96167400

H	2.02078200	-0.28867700	-2.00640900
H	1.21881300	-1.57185300	-1.09191700
B	-2.58760000	-2.60920900	-0.95737300
F	-3.51782300	-1.64607500	-1.23873600
F	-2.37844800	-3.50842300	-1.94354700
F	-2.63262100	-3.09142500	0.30419600
C	0.36455700	0.42836500	1.39778200
C	1.51045900	-0.27167000	1.40628200
C	2.35097800	-0.21611300	0.13897100
C	-0.03477600	1.20580800	0.17658100

d-exo'

1 = a-endo' 1

2 = d-endo' 2

RC: E= -904.350551571

H	0.97089800	1.60197000	0.20208400
C	3.17074100	0.16763400	-0.24612400
C	2.32369000	-2.70072500	-1.16803600
H	0.37088900	-1.70467100	-1.20667500
H	-0.62845300	0.14358200	-1.97802400
C	-1.41930900	1.95393500	-1.01345500
H	3.89322300	-0.65819100	-0.25943000
H	3.17557600	0.60759800	0.76630800
H	3.54047300	0.95207200	-0.92855500
H	3.37421500	-2.50228400	-0.91474700
H	2.29124700	-3.06217600	-2.21135100
H	1.97355900	-3.54473500	-0.54790800
H	-1.31600500	2.73008100	-1.80435700
O	-1.28741300	2.54040700	0.26462800
H	-2.42611100	1.51040000	-1.13431700
C	-2.17800200	3.60487900	0.48455400
H	-2.00705900	4.43610800	-0.22781000
H	-2.01133800	3.97708200	1.50562700
H	-3.23375800	3.28376300	0.38976300
C	0.88040900	-1.36559400	2.34535800
C	-0.00715300	-0.36355700	2.20785500
C	-1.15630500	-0.49178800	1.33367400
O	-1.42032600	-1.56795900	0.76106200
H	1.76841500	-1.26094700	2.97289000
B	-2.62762800	-1.70402100	-0.31084300
F	-1.97118500	-1.87128100	-1.50532200
F	-3.33379300	-2.78242700	0.10873800
F	-3.31776100	-0.51122900	-0.24078500
C	0.76022400	0.80202400	-0.51655300
C	1.77404800	-0.25927700	-0.62619800
C	1.42861100	-1.51339600	-1.00077800
C	-0.38935000	0.88770300	-1.21349100
H	0.12577600	0.60430800	2.69560400
H	0.72714200	-2.31279600	1.82397000
H	-1.81819000	0.37350600	1.19264500

TS: E= -904.340707433

H	1.80827500	2.29526100	-0.11704800
C	3.90593700	0.62893900	-0.28763700
C	3.08114800	-2.19961500	-0.70005900
H	1.06189100	-1.32082400	-0.78444800
H	-0.24225400	0.17631200	-1.04073800
C	-0.87139800	2.19010500	-0.51777700

H	4.36085200	0.14596100	0.59457300
H	4.03538500	1.71499200	-0.18971000
H	4.48839600	0.28905100	-1.16052000
H	3.96726700	-2.11799800	-0.05209100
H	3.43506600	-2.17164500	-1.74535400
H	2.62738500	-3.18733700	-0.53536700
H	-1.17275500	2.46792700	-1.55530400
O	-0.37456300	3.29442900	0.18364600
H	-1.79376700	1.77795300	-0.06001100
C	-1.28392700	4.36157800	0.26755400
H	-1.54909600	4.75716600	-0.73324800
H	-0.80704000	5.16330300	0.84882400
H	-2.22223500	4.06272200	0.77516700
C	1.54492500	-1.37033000	1.53289800
C	0.49651300	-0.51217300	1.90132700
C	-0.79026000	-0.69270400	1.39006800
O	-1.08083200	-1.66434900	0.61295900
H	2.52068600	-1.24833100	2.00980000
B	-2.25574700	-1.55822100	-0.40800700
F	-1.60260300	-1.36174800	-1.62407800
F	-2.95769100	-2.72123100	-0.34884700
F	-2.99958700	-0.43491100	-0.06079600
C	1.47837900	1.29108400	-0.39728300
C	2.45765300	0.25284800	-0.43055200
C	2.08233800	-1.09876400	-0.45651700
C	0.14437100	1.10853900	-0.62269900
H	0.68255600	0.39158100	2.48325700
H	1.27598200	-2.39628900	1.27222600
H	-1.58448500	0.02876800	1.62760200

P: E= -904.392415890

H	1.53869000	2.13265300	-0.62705400
C	3.70221400	0.44810700	-0.46420300
C	2.84585000	-2.36359300	-0.19353100
H	1.34698400	-1.53084400	-1.46990100
H	-0.37616900	0.11086200	-1.55384300
C	-1.11813500	1.86751700	-0.60532900
H	4.18142800	0.06120400	0.45034700
H	3.87007000	1.53399100	-0.50497100
H	4.23628000	-0.01229600	-1.31286300
H	3.31003800	-2.21241200	0.79428900
H	3.64309600	-2.33444300	-0.95044400
H	2.41413600	-3.37631300	-0.20417500
H	-0.77870600	2.61352400	-1.35246200
O	-1.13309200	2.42252700	0.68554000
H	-2.14124800	1.56135400	-0.90798800
C	-1.94439800	3.56437300	0.80558900
H	-1.59857700	4.38252600	0.14376900
H	-1.89026700	3.90601200	1.84870900
H	-3.00127400	3.34424800	0.55683200
C	0.58964600	-1.49694100	0.53585700
C	-0.39672800	-0.31641600	0.57620700
C	-1.83085700	-0.69490400	0.60743200
O	-2.25281600	-1.79663000	0.26005600
H	1.00922100	-1.63480800	1.54484800
B	-3.93635100	-2.13653700	0.21569500
F	-4.12118200	-2.40938700	-1.09474100
F	-4.03867600	-3.17343700	1.07323100
F	-4.49642300	-0.96660300	0.64609500
C	1.28701100	1.06836400	-0.59482600
C	2.23688700	0.12481400	-0.49893700
C	1.76010300	-1.32143900	-0.46401600

C	-0.16590600	0.67575600	-0.62574300
H	-0.24018400	0.31368700	1.46523700
H	0.05143100	-2.42273400	0.28680900
H	-2.56209800	0.06822100	0.92848300

e-endo'

1 = a-exo' 1

2: E= -1506.16128055

C	-2.59297800	2.15398100	-3.27366900
C	-2.01086000	1.05024700	-2.77466600
C	-1.01973200	1.16020400	-1.72631900
H	-0.75298400	2.15724700	-1.34004800
O	-0.48168300	0.15265400	-1.25690000
H	-2.24233200	0.04344300	-3.13230900
H	-3.33954100	2.10021200	-4.06958100
H	-2.33518000	3.14851500	-2.89581800
B	0.56938900	0.08280200	-0.03639100
C	1.18571400	1.57161400	0.20632200
C	1.76292100	2.28626900	-0.85096500
C	1.32700100	2.19986700	1.45089900
C	2.40456300	3.51540800	-0.73465400
C	1.96342500	3.42672400	1.63831500
C	2.50347400	4.08721900	0.53506500
C	1.77047500	-0.88754600	-0.52392800
C	1.94494000	-1.47729000	-1.77846200
C	2.82862400	-1.11449400	0.36476400
C	3.05969000	-2.23893200	-2.13316100
C	3.96311500	-1.86260400	0.07471700
C	4.07379700	-2.43112900	-1.19655200
C	-0.42119900	-0.48666800	1.11919800
C	-0.32785400	-1.72644100	1.76402700
C	-1.52791000	0.27153200	1.52165200
C	-1.22100400	-2.16377500	2.74384500
C	-2.45619100	-0.10543000	2.48331100
C	-2.28928600	-1.34488300	3.10498700
F	0.83901000	1.60301800	2.54901900
F	1.67402100	1.75395400	-2.09659300
F	1.00059700	-1.31714400	-2.73072000
F	2.73353200	-0.57496600	1.59799300
F	0.66253200	-2.57353500	1.44248500
F	-1.71879100	1.47889500	0.92494800
H	-3.27933200	0.56605600	2.73046700
H	-2.99620300	-1.67317600	3.86990800
H	-1.06128400	-3.14139400	3.20054700
H	4.73069900	-1.98898300	0.83921100
H	3.11011400	-2.66335800	-3.13686400
H	4.95287900	-3.02491600	-1.45612700
H	2.81824100	3.99207200	-1.62426300
H	3.00658100	5.04776100	0.66488800
H	2.02894000	3.83700400	2.64689500

RC: E= -1894.38856134

H	-2.50982800	-0.80658600	0.79689700
C	-3.91690900	1.37503100	0.84439800
C	-5.36581900	1.86339300	-1.87175400
H	-4.21233500	0.06791000	-2.38490300
H	-2.46164900	-1.12175700	-2.26717200
C	-1.17759900	-2.34762900	-1.00129700
H	-2.95129500	1.81287500	1.14915600

H	-4.24697100	0.74881500	1.68992300
H	-4.64275600	2.18788100	0.72165500
H	-5.43450100	2.62406100	-1.08254100
H	-6.37649700	1.44181600	-2.01911400
H	-5.11197900	2.37792600	-2.81442700
H	-0.18017700	-1.86101500	-1.03049800
O	-1.26593500	-3.31447700	-2.01918500
H	-1.27192700	-2.80487700	0.00352900
C	-0.14950900	-4.17010600	-2.04962400
H	0.78266000	-3.61232900	-2.25800700
H	-0.31575900	-4.90831500	-2.84749200
H	-0.01564100	-4.70825800	-1.08988100
C	-1.94866500	2.11573800	-2.47168300
C	-0.93157100	1.23760000	-2.33268500
C	-0.24801100	1.13835800	-1.07561500
H	-0.53407900	1.82153000	-0.25977100
O	0.67573800	0.32460600	-0.89378900
H	-0.60598700	0.57064500	-3.13422800
H	-2.49345800	2.22121600	-3.41126300
H	-2.23225600	2.78372700	-1.65549400
B	1.54675000	0.17374600	0.43761800
C	-2.80023500	-0.58171400	-0.23436000
C	-3.74766900	0.52879400	-0.39307200
C	-4.37892500	0.77801100	-1.56827300
C	-2.21882000	-1.30106300	-1.21583500
C	2.19538100	1.64289200	0.73441200
C	2.73461300	2.40563200	-0.31082600
C	2.39328600	2.21046200	2.00070800
C	3.37729800	3.63146500	-0.15619900
C	3.03072700	3.43007600	2.22290400
C	3.52264100	4.14642500	1.13214300
C	2.75372900	-0.84744000	0.05919000
C	2.97379500	-1.52551600	-1.14414500
C	3.74565400	-1.08106900	1.02052100
C	4.07829900	-2.33986600	-1.39604200
C	4.86774000	-1.88115300	0.83559700
C	5.03445300	-2.51448400	-0.39711900
C	0.48528200	-0.39263100	1.54768700
C	0.37741100	-1.74382100	1.90722100
C	-0.43985500	0.42283100	2.21263300
C	-0.51829300	-2.24332300	2.85392400
C	-1.34999800	-0.00446700	3.17294600
C	-1.38265700	-1.36112200	3.49854700
F	1.95572700	1.55896600	3.09155500
F	2.63322100	1.92859800	-1.57311100
F	2.07017100	-1.43487300	-2.14905100
F	3.59379000	-0.50259200	2.23048900
F	1.15279300	-2.65801100	1.29667500
F	-0.49668100	1.74395400	1.89184800
H	-2.01298600	0.72255600	3.64269300
H	-2.08670200	-1.72984500	4.24725800
H	-0.51847700	-3.31352700	3.06429100
H	5.58119800	-1.99649400	1.65254100
H	4.16511000	-2.82244900	-2.37063000
H	5.90564500	-3.14824200	-0.57603800
H	3.75894700	4.14803600	-1.03787900
H	4.02649700	5.10296200	1.28677200
H	3.13385800	3.79051900	3.24727500

TS: E= -1894.38139002

H	-3.45004100	-0.84112200	0.27657300
C	-5.00141500	1.30022900	0.28508100

C	-5.93386700	2.08930500	-2.42942900
H	-4.86305800	0.26306200	-3.02682900
H	-3.45582800	-1.14391800	-2.80511900
C	-2.06542000	-2.29107300	-1.60528700
H	-4.38839700	2.21831300	0.36124300
H	-4.82578900	0.72310900	1.20233200
H	-6.05470900	1.61711600	0.25654700
H	-5.72239200	2.97967600	-1.81780500
H	-6.94452400	1.73724000	-2.16024400
H	-5.96643100	2.40585700	-3.48206500
H	-1.09449700	-1.74999300	-1.53975900
O	-2.07195800	-3.16470100	-2.70166500
H	-2.17552800	-2.82835600	-0.64132300
C	-0.90690200	-3.95750900	-2.77743700
H	-0.00690800	-3.33568300	-2.92693500
H	-1.02694600	-4.63785700	-3.63239900
H	-0.76262400	-4.56046700	-1.85969800
C	-3.15084600	1.90724000	-2.80058100
C	-2.03787500	1.04782800	-2.78643600
C	-1.24454000	0.97567100	-1.63189800
H	-1.51963500	1.61555200	-0.78031100
O	-0.23238800	0.22437700	-1.51241900
H	-1.75495500	0.44908400	-3.65469800
H	-3.56362200	2.19598100	-3.76988000
H	-3.18896900	2.69761700	-2.04490800
B	0.62334900	0.15499600	-0.19633400
C	-3.73684800	-0.59270100	-0.74871000
C	-4.60556800	0.51457800	-0.93330700
C	-4.91119900	0.99922100	-2.22007300
C	-3.12879800	-1.27380300	-1.77213400
C	1.27315900	1.63446800	0.06010800
C	1.79903700	2.36935200	-1.01243400
C	1.48865500	2.23679700	1.30739900
C	2.44061600	3.60081600	-0.89761800
C	2.12642300	3.46325900	1.48933500
C	2.60184700	4.15167000	0.37371900
C	1.85741000	-0.86537300	-0.49996100
C	2.16754800	-1.50822100	-1.70285800
C	2.78619500	-1.11474200	0.51877600
C	3.29148100	-2.31264500	-1.89784800
C	3.92295500	-1.90569300	0.39255300
C	4.17721000	-2.50964000	-0.84012900
C	-0.43287500	-0.37816400	0.95112600
C	-0.57303400	-1.72938500	1.29959300
C	-1.33362900	0.45080000	1.63460500
C	-1.46920300	-2.22158700	2.24992900
C	-2.24181200	0.03121000	2.60307200
C	-2.30405100	-1.32686500	2.91694200
F	1.06687100	1.61698900	2.42448400
F	1.69340300	1.85792000	-2.25810600
F	1.34103900	-1.38983900	-2.76864000
F	2.55596900	-0.55712600	1.72610300
F	0.16936400	-2.65743600	0.66465900
F	-1.37580500	1.77332200	1.33141200
H	-2.87619000	0.77158000	3.09200200
H	-3.00466800	-1.68639100	3.67340500
H	-1.48944600	-3.29380000	2.44940500
H	4.58110900	-2.03469500	1.25282000
H	3.44962400	-2.76727500	-2.87700900
H	5.06269300	-3.13473600	-0.97413700
H	2.81042800	4.09324000	-1.79807300
H	3.10546800	5.11314300	0.49573200
H	2.24161900	3.85073500	2.50257200

P: E= -1894.44599434

H	-3.63650600	-1.25005500	0.32364000
C	-4.42536500	1.24991700	0.79885300
C	-2.53839000	2.98794400	-0.82980700
H	-4.18891200	2.12207700	-1.85694500
H	-3.04649200	-1.53004600	-2.35722200
C	-1.64425900	-2.36497800	-0.99702000
H	-3.79978300	1.88513200	1.44787100
H	-4.81510200	0.42517700	1.41276700
H	-5.27681100	1.86837600	0.46643400
H	-1.65989400	2.72250100	-0.22516000
H	-3.21989300	3.54621900	-0.17157600
H	-2.21791200	3.67480500	-1.62850800
H	-1.13319000	-2.11262600	-0.05204200
O	-0.72774800	-2.78924500	-1.96706000
H	-2.37573400	-3.16676200	-0.75814300
C	0.22281400	-3.70580900	-1.48291300
H	0.77138000	-3.30332000	-0.61158200
H	0.94248900	-3.89680500	-2.28994600
H	-0.24872000	-4.66359800	-1.18406800
C	-2.45590700	1.10776200	-2.60206200
C	-1.54235500	-0.04426900	-2.16623600
C	-0.43313600	0.43868800	-1.29510900
H	-0.26340500	1.52002300	-1.17477900
O	0.31876200	-0.34333300	-0.71870500
H	-1.02363400	-0.49104900	-3.03550000
H	-3.16899300	0.69767300	-3.33303200
H	-1.87838300	1.88010100	-3.13502900
B	1.39667200	-0.06054900	0.43937300
C	-3.28602700	-0.56184400	-0.45340900
C	-3.62706800	0.73398200	-0.36774100
C	-3.23795500	1.75131900	-1.43035100
C	-2.41475500	-1.15676000	-1.52940800
C	1.72627600	1.52904700	0.50849000
C	2.11591700	2.23293700	-0.63743900
C	1.78847000	2.28993100	1.68368700
C	2.50299300	3.56936400	-0.66509100
C	2.17431300	3.62906400	1.72717900
C	2.53044600	4.27122200	0.54108700
C	2.74536300	-0.84348500	0.01698300
C	3.05216200	-1.40197200	-1.22629100
C	3.79215400	-0.90151300	0.94412400
C	4.27663200	-1.99815500	-1.53118700
C	5.03314900	-1.47890700	0.70414300
C	5.27108400	-2.03616300	-0.55486500
C	0.51593000	-0.68816300	1.65776200
C	0.72234400	-1.92935700	2.27083800
C	-0.66761800	-0.05723700	2.06200500
C	-0.12915200	-2.48001600	3.22988500
C	-1.56396900	-0.55143500	3.00086200
C	-1.27807700	-1.78145500	3.59745400
F	1.46858700	1.71671700	2.85465100
F	2.10009500	1.57217600	-1.82250600
F	2.13173400	-1.37851400	-2.21493800
F	3.57375100	-0.36146900	2.16108000
F	1.78103900	-2.67954100	1.91526200
F	-0.99338300	1.11947000	1.46702900
H	-2.45864100	0.02183500	3.24548200
H	-1.95694300	-2.19890700	4.34403800
H	0.12101200	-3.45035600	3.66072100
H	5.78400100	-1.48390300	1.49521600

H	4.42813100	-2.41314200	-2.52864700
H	6.23611900	-2.49750500	-0.77528500
H	2.78175300	4.02802200	-1.61460500
H	2.83534700	5.31971800	0.55711700
H	2.19318700	4.14104800	2.69017400

e-exo'

1 = a-exo' 1

2: E= -1506.16063697

C	-0.82409100	-1.84028500	-2.37828400
C	-0.92938100	-0.50049100	-2.31791000
C	-0.14694800	0.26691000	-1.35836400
O	0.62407200	-0.30224400	-0.58134000
H	-1.40636400	-2.42528400	-3.09419700
B	1.64447700	0.31548900	0.52632200
H	-1.59622000	0.06111900	-2.97664300
H	-0.14485400	-2.36813600	-1.70109000
H	-0.24118900	1.36402200	-1.33130600
C	1.12877000	1.81331400	0.87174800
C	1.95605700	2.93954500	0.96150300
C	-0.21082500	2.07631300	1.18153200
C	1.50693400	4.21569500	1.30043700
C	-0.72601900	3.32236100	1.52133700
C	0.15393000	4.40495500	1.57903600
C	1.47970100	-0.75435900	1.73415800
C	1.45893500	-2.13645300	1.50297800
C	1.37303100	-0.40817200	3.08586000
C	1.30561800	-3.10341600	2.49150100
C	1.22084000	-1.32737500	4.12334200
C	1.18092200	-2.68682300	3.81793100
C	3.05916000	0.23656800	-0.26490100
C	4.23011900	-0.33514700	0.24774800
C	3.20989200	0.76387300	-1.55190400
C	5.43433500	-0.40906300	-0.45155600
C	4.37671900	0.71981300	-2.30587300
C	5.50276700	0.11887900	-1.74045100
F	2.14116400	1.38910000	-2.11796500
F	4.22766000	-0.83267200	1.49637800
F	3.27391000	2.80716100	0.73207900
F	-1.08574400	1.03859900	1.14108600
F	1.43717100	0.89023900	3.43953400
F	1.62088200	-2.58843700	0.23577200
H	-0.21567200	5.39657700	1.84856400
H	-1.78918000	3.42189100	1.74382500
H	2.22745100	5.03323800	1.34780600
H	4.38952000	1.16034600	-3.30358700
H	6.29628600	-0.87193200	0.03073300
H	6.43781900	0.07101900	-2.30253500
H	1.30054100	-4.15742400	2.21037600
H	1.14412000	-0.95992500	5.14748400
H	1.06310600	-3.42424100	4.61483300

RC: E= -1894.39330221

H	-4.46900600	-0.48327000	-1.50811400
C	-4.27402800	-3.09945300	-1.59347300
C	-1.49620100	-4.01800900	-0.48481800
H	-1.37476600	-1.88048000	-0.05801700
H	-2.22453400	-0.08175900	0.55768000
C	-3.39709700	1.61828200	-0.17892400

H	-4.54398800	-2.72358600	-2.59569900
H	-5.20652200	-3.11335800	-1.00340300
H	-3.93106200	-4.13570600	-1.70286200
H	-1.37222500	-4.36374300	0.55707100
H	-0.48557000	-4.03675300	-0.92403600
H	-2.12613900	-4.74705200	-1.01202700
H	-4.31844000	1.77969100	-0.77432600
O	-2.30854400	2.32832900	-0.75492300
H	-3.58430200	2.01164000	0.84122000
C	-2.46652200	3.72496900	-0.74264500
H	-3.32191000	4.04511700	-1.37024600
H	-1.54284100	4.16985000	-1.13946900
H	-2.61947400	4.10884500	0.28277100
C	-0.83385400	-1.21503500	-2.86488000
C	-0.96002000	0.09578700	-2.57335300
C	-0.16098900	0.68100300	-1.52399700
O	0.40118900	-0.04438000	-0.68501300
H	-1.41371700	-1.68010800	-3.66459600
B	1.48535500	0.38313000	0.39827800
C	-3.63062800	-0.78216200	-0.86487700
C	-3.24825300	-2.20098300	-0.94766800
C	-2.04267700	-2.62710500	-0.49681000
C	-3.04132900	0.16895700	-0.12146400
H	-1.63049300	0.76363700	-3.11510100
H	-0.10447700	-1.82612700	-2.33096100
H	-0.02747700	1.77040900	-1.47057600
C	1.03897200	1.86903200	0.89354600
C	1.69822900	3.06351000	0.57586200
C	-0.11370900	2.06115600	1.66716600
C	1.29461500	4.32775400	1.01217500
C	-0.56517300	3.28645500	2.14215700
C	0.15765600	4.43390400	1.81026600
C	1.39049600	-0.82442000	1.49127000
C	1.36035000	-2.16211700	1.07406000
C	1.42421700	-0.67478600	2.88348500
C	1.31395300	-3.26316800	1.92583500
C	1.38343900	-1.73363000	3.78971500
C	1.32167000	-3.03877600	3.30302500
C	2.94885600	0.28905100	-0.30993100
C	4.07993600	0.46801600	0.49699700
C	3.25201100	-0.01303600	-1.63843400
C	5.39491000	0.35266300	0.06092700
C	4.54553000	-0.14613900	-2.14212000
C	5.62539400	0.03702600	-1.27991900
F	2.24421200	-0.18324200	-2.53343900
F	3.88006400	0.79177100	1.79063300
F	2.78776300	3.03123600	-0.21322900
F	-0.85957400	0.97932100	1.98556300
F	1.50476600	0.55934700	3.41022600
F	1.38863900	-2.43489200	-0.25543300
H	-0.17008000	5.41174500	2.16989500
H	-1.46342500	3.32210000	2.75981200
H	1.88307600	5.19856800	0.72034000
H	4.67989400	-0.38682500	-3.19762500
H	6.20821400	0.51267500	0.76996300
H	6.64713500	-0.06181400	-1.65254600
H	1.29156200	-4.26736500	1.50082300
H	1.40659000	-1.51365400	4.85787200
H	1.29035800	-3.88204300	3.99631800

TS: E= -1894.38597099

H	-4.69679700	-0.49058000	-1.30653500
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C	-4.20100100	-3.07866000	-1.73650100
C	-1.44472200	-3.86190700	-0.96583500
H	-1.35961500	-1.81891800	-0.16975900
H	-2.04626200	0.01742700	0.19820000
C	-3.39292600	1.67412500	-0.28346300
H	-5.20034400	-2.65160400	-1.89696600
H	-4.30615500	-3.98144000	-1.11215100
H	-3.81517400	-3.42226500	-2.71239600
H	-1.88889500	-4.46595200	-0.15557600
H	-0.35385500	-3.90406000	-0.85245300
H	-1.71990300	-4.33870300	-1.91934500
H	-4.33317800	1.82950900	-0.85118200
O	-2.36770000	2.51033400	-0.76731000
H	-3.60569200	1.91948500	0.78020500
C	-2.64374200	3.88250800	-0.63488400
H	-3.52180300	4.18230900	-1.24091100
H	-1.75874300	4.43200000	-0.98298500
H	-2.83193600	4.16061900	0.41871300
C	-1.03701800	-1.49595500	-2.46861900
C	-1.08584300	-0.09485000	-2.34716500
C	-0.23219900	0.54752000	-1.43249400
O	0.41374500	-0.14177700	-0.58950000
H	-1.56474100	-1.96672600	-3.30181100
B	1.49593000	0.34217500	0.41924800
C	-3.71374000	-0.75078600	-0.89772900
C	-3.26604900	-2.08814100	-1.10027400
C	-1.92386000	-2.43666000	-0.87449600
C	-2.95079800	0.24766900	-0.36233800
H	-1.73492000	0.52542500	-2.96327200
H	-0.09240500	-1.96402500	-2.18224600
H	-0.14904000	1.64182800	-1.41054100
C	1.05486400	1.84742900	0.87801000
C	1.73790800	3.03425400	0.58679100
C	-0.12422800	2.05444400	1.60428900
C	1.32969800	4.30287500	1.00740200
C	-0.58251100	3.28219000	2.06467000
C	0.16436100	4.42243600	1.76147300
C	1.43926600	-0.79955100	1.59397200
C	1.41308000	-2.16041700	1.26087000
C	1.48077100	-0.56758500	2.97428900
C	1.38163300	-3.20920400	2.17703900
C	1.45667400	-1.57016400	3.94380700
C	1.40089500	-2.90291000	3.53836300
C	2.95670800	0.22089000	-0.29541800
C	4.10223500	0.44818200	0.47755600
C	3.23496000	-0.17203500	-1.60613500
C	5.40959000	0.30412000	0.02733600
C	4.52072200	-0.33799300	-2.12250300
C	5.61593900	-0.09842400	-1.29432200
F	2.21443300	-0.40786600	-2.46891800
F	3.92571600	0.85140400	1.75300800
F	2.85865400	2.99199600	-0.15566300
F	-0.89784300	0.97618300	1.89002600
F	1.54823300	0.69667800	3.42859600
F	1.42840400	-2.51557400	-0.05084200
H	-0.16569100	5.40378200	2.10944900
H	-1.50241900	3.32655000	2.64921600
H	1.93831900	5.16737500	0.73877600
H	4.63666000	-0.64909300	-3.16178200
H	6.23553400	0.50922200	0.70974200
H	6.63093700	-0.22168400	-1.67828300
H	1.36266300	-4.23775400	1.81350500
H	1.48689100	-1.28524300	4.99643500

H 1.38285700 -3.70298000 4.28164300

P: E= -1894.44567444

H	-4.78608500	-0.51729500	-1.28386000
C	-4.49520500	-3.23388600	-1.60933800
C	-1.63994800	-4.01410600	-1.50836600
H	-1.66043800	-2.33142400	-0.19353200
H	-2.26161600	-0.12619400	0.11130800
C	-3.06596500	1.55285600	-0.90412400
H	-5.50049500	-2.79369600	-1.68109300
H	-4.51149300	-3.99584200	-0.81163100
H	-4.28843100	-3.77406700	-2.54836500
H	-2.18930000	-4.70037600	-0.84701300
H	-0.56500400	-4.17728800	-1.33925300
H	-1.86552000	-4.29452400	-2.55015700
H	-3.53310800	1.82536100	-1.87380200
O	-1.89189100	2.30220900	-0.69155900
H	-3.80737600	1.75241200	-0.10603400
C	-2.03912500	3.70112900	-0.72076100
H	-2.43036900	4.04507900	-1.69790300
H	-1.04833900	4.13958300	-0.54485700
H	-2.72105500	4.04926700	0.07661100
C	-1.18066100	-1.61756700	-2.15340600
C	-1.44136700	-0.11064200	-1.87429800
C	-0.24757100	0.51822000	-1.24058300
O	0.18501900	0.01314100	-0.20226700
H	-1.46823300	-1.83189200	-3.19425800
B	1.45126600	0.47523900	0.65429500
C	-3.75617600	-0.87965900	-1.20174100
C	-3.45928600	-2.18347700	-1.33750400
C	-1.98648700	-2.55312600	-1.22604700
C	-2.65449700	0.09213900	-0.89782400
H	-1.66025600	0.41920600	-2.81224800
H	-0.11079600	-1.84236500	-2.05802200
H	0.26076600	1.38388600	-1.68778900
C	1.02403400	1.96578500	1.14404200
C	1.67933600	3.16541400	0.84916400
C	-0.13516100	2.13319900	1.91482000
C	1.27001600	4.41886300	1.31218200
C	-0.59414200	3.34791000	2.41024000
C	0.12882600	4.50393100	2.10765900
C	1.51495600	-0.66714800	1.81042500
C	1.41991300	-2.02245200	1.47039900
C	1.71724700	-0.43956000	3.17593100
C	1.48721700	-3.07659200	2.37685200
C	1.79980400	-1.44982700	4.13394400
C	1.67974100	-2.77830000	3.72697300
C	2.80393400	0.34856000	-0.24476500
C	4.02272600	0.62954700	0.39114200
C	2.96078400	-0.11858600	-1.55040100
C	5.27731000	0.48257500	-0.18766700
C	4.18536100	-0.29135400	-2.19417100
C	5.35496300	0.01372700	-1.50120100
F	1.85878900	-0.43531100	-2.29312000
F	3.97339500	1.08000300	1.65903100
F	2.77204500	3.15194500	0.06263900
F	-0.87026300	1.03827300	2.20364100
F	1.84123500	0.82383600	3.61967600
F	1.25676500	-2.35375300	0.16412600
H	-0.20324500	5.47304100	2.48655800
H	-1.49954700	3.36932800	3.01810600
H	1.85746400	5.29772200	1.04304500

H	4.19687000	-0.66207200	-3.21996700
H	6.16489600	0.73381200	0.39433900
H	6.32673800	-0.11375800	-1.98262700
H	1.39940200	-4.10171700	2.01426700
H	1.95655000	-1.17560600	5.17807400
H	1.74108500	-3.58373600	4.46206700

f-endo'

1 = a-endo' 1

2: E= -2931.95840784

C	-3.14590200	1.33155200	-2.94454600
C	-1.85730600	0.97375000	-2.79299700
C	-1.28469400	0.88940200	-1.46940700
H	-1.92235600	1.12155400	-0.59691100
O	-0.10480100	0.56108500	-1.28817500
H	-1.20573300	0.73897700	-3.63909400
H	-3.60796900	1.40574900	-3.93190400
H	-3.77669800	1.56071300	-2.07950400
B	0.69594800	0.52100900	0.15653800
C	1.52421800	1.90837400	0.13135000
C	0.89977900	3.13094300	-0.15929600
C	2.88987100	1.94638800	0.44901900
C	1.60068000	4.33898400	-0.13999700
C	3.59593400	3.15376700	0.48712500
C	2.95814500	4.35823000	0.18796700
C	1.62342200	-0.78589700	0.02067300
C	2.25423200	-1.10846900	-1.19279200
C	1.90141300	-1.60043100	1.12722900
C	3.11177100	-2.20530700	-1.29982400
C	2.77046800	-2.69391200	1.02916700
C	3.37954600	-3.00554600	-0.18560200
C	-0.43228600	0.42708500	1.30703800
C	-1.26908000	-0.70274400	1.37592700
C	-0.63432300	1.43075200	2.26557200
C	-2.27678600	-0.81208600	2.33642700
C	-1.62656400	1.31615700	3.24734800
C	-2.45914500	0.19812200	3.28493900
H	-1.12810800	-1.52305500	0.66738800
H	-0.00885700	2.32471600	2.25302300
H	-3.23777600	0.11214300	4.04236400
H	2.08111600	-0.48738400	-2.07332600
H	1.44324100	-1.37832200	2.09302200
H	4.06192100	-3.85155300	-0.26176900
H	3.41910500	1.01819000	0.66990300
H	-0.16599400	3.16452900	-0.39880900
H	3.51001700	5.29778500	0.20849300
C	0.90104900	5.61452000	-0.53194900
C	5.04655200	3.15446700	0.90162100
C	3.00231800	-3.55913100	2.24186300
C	3.71412900	-2.55432700	-2.63656100
C	-3.20669500	-1.99822300	2.30491500
C	-1.76111800	2.39717100	4.29127100
F	-1.57984100	3.61858400	3.75856000
F	-2.97192600	2.38369400	4.87384100
F	-0.84729800	2.25352500	5.26665000
F	-4.19482900	-1.81022500	1.40285200
F	-3.79285500	-2.21421100	3.49164600
F	-2.56682500	-3.12374000	1.95001600
F	4.10302600	-4.31866100	2.11857400
F	3.14020600	-2.81971200	3.35666000

F	1.96546800	-4.39266400	2.45301900
F	4.86928000	-3.22694900	-2.50891300
F	2.88317600	-3.33158400	-3.36051600
F	3.96041900	-1.45742300	-3.37496800
F	5.70529200	4.22035400	0.41550100
F	5.17187500	3.18901500	2.24130000
F	5.68436700	2.05172400	0.47518500
F	-0.40222300	5.59018600	-0.19182200
F	0.94919000	5.81196400	-1.86464300
F	1.45289200	6.69154000	0.04650900

RC: E= -3320.20434499

H	-2.57568700	-1.81708800	-0.17314900
C	-4.41137500	0.04410800	0.10923200
C	-5.87276900	0.54137900	-2.59707900
H	-4.31204200	-0.85082500	-3.27132400
H	-2.18390600	-1.37628300	-3.18618500
C	-0.84223600	-2.68366600	-2.04785800
H	-5.37145400	0.57301200	0.07539100
H	-3.65012700	0.75068800	0.48647800
H	-4.48029600	-0.75071100	0.86786900
H	-6.11456300	1.17854000	-1.73586500
H	-6.75625300	-0.08774700	-2.80760200
H	-5.74930600	1.19437900	-3.47754100
H	-1.04768500	-3.57910200	-2.67656900
O	-0.62525500	-3.04904300	-0.71501800
H	0.06961700	-2.22100100	-2.48311600
C	0.25607800	-4.13867700	-0.54904100
H	-0.20395600	-5.08176400	-0.90142100
H	0.47897600	-4.22634200	0.52243800
H	1.19993600	-3.98141500	-1.09676100
C	-2.67101600	1.78414800	-2.81812100
C	-1.43213300	1.24823300	-2.73812900
C	-0.86570500	0.98563800	-1.44810800
H	-1.49002200	1.16928600	-0.55959100
O	0.31741200	0.61897200	-1.28815300
H	-0.83558000	1.00562300	-3.62087800
H	-3.13844600	2.00823800	-3.77874700
H	-3.22097200	2.07095300	-1.92077600
B	1.06539000	0.48691900	0.12906300
C	-2.82384400	-1.41564300	-1.15651600
C	-4.00564700	-0.54917800	-1.21824900
C	-4.65782900	-0.30861700	-2.38474300
C	-2.00263500	-1.74942100	-2.17369200
C	1.91797200	1.85844200	0.26556800
C	1.51342000	3.06908100	-0.31191200
C	3.07866500	1.88605000	1.05740900
C	2.22614400	4.25717300	-0.10976400
C	3.78883400	3.06869000	1.27311800
C	3.36924200	4.26660800	0.68731400
C	2.01404200	-0.80405900	-0.05035300
C	2.49273800	-1.18640600	-1.31245900
C	2.43875100	-1.56564200	1.04909700
C	3.34110300	-2.28556400	-1.47311800
C	3.29163200	-2.66334800	0.89556800
C	3.75265600	-3.03294300	-0.36853700
C	-0.07591300	0.34791700	1.27489900
C	-0.61836800	-0.90611100	1.60440900
C	-0.62165800	1.46779000	1.92281300
C	-1.63503100	-1.03978900	2.55295000
C	-1.67090700	1.34397500	2.84170600
C	-2.17397400	0.08666300	3.17784900

H	-0.26096000	-1.79524100	1.08927400
H	-0.22906400	2.46391700	1.70879600
H	-2.97191500	-0.01200500	3.91392700
H	2.19582500	-0.61685000	-2.19429700
H	2.09420800	-1.30991500	2.05288400
H	4.41255100	-3.89115200	-0.49101500
H	3.44450400	0.96501700	1.51416600
H	0.62031100	3.11456400	-0.93815800
H	3.92693300	5.18900400	0.84758600
C	1.77240300	5.51303100	-0.80633000
C	4.98869600	3.07057900	2.18640200
C	3.62139000	-3.51242500	2.09450400
C	3.71644900	-2.71890200	-2.86395000
C	-2.20189900	-2.40351400	2.84913900
C	-2.32653000	2.58180100	3.39313400
F	-3.29304300	3.01934200	2.55086700
F	-2.91471400	2.36257200	4.57936300
F	-1.45826800	3.59283900	3.54466000
F	-3.21875700	-2.70550600	2.00074300
F	-2.70516100	-2.48323400	4.09053100
F	-1.28684700	-3.37399100	2.71246900
F	4.74711400	-4.22303300	1.92142500
F	3.76804200	-2.77630900	3.20785200
F	2.63029400	-4.39943700	2.34122700
F	4.78636300	-3.52687500	-2.88118200
F	2.69682600	-3.40354600	-3.44128400
F	3.97671200	-1.67524300	-3.66847000
F	5.89310000	3.99595100	1.81990000
F	4.63739000	3.34756600	3.45686100
F	5.60930700	1.87913700	2.20096600
F	0.42711600	5.60410700	-0.83236200
F	2.18428100	5.54394400	-2.08907000
F	2.24132200	6.62169700	-0.21335300

TS: E= -3320.19952703

H	-3.37852800	-2.05558700	-0.55300000
C	-5.60246700	-0.59147300	-0.63280200
C	-6.09200200	0.66411400	-3.26559800
H	-4.26305300	-0.42126200	-3.83058600
H	-2.50256100	-1.35050200	-3.42646600
C	-1.20967200	-2.51287700	-2.11508000
H	-6.62525800	-0.87818700	-0.92881300
H	-5.65527500	0.47272300	-0.34019400
H	-5.31132300	-1.17063100	0.25147000
H	-6.39680900	1.34546400	-2.45680200
H	-6.91207400	-0.06043200	-3.40770100
H	-6.00887700	1.25280400	-4.19047800
H	-1.15250700	-3.34313200	-2.85481100
O	-1.20904400	-2.99394300	-0.80547600
H	-0.31696000	-1.88112400	-2.31476100
C	-0.23854100	-3.99089800	-0.54680200
H	-0.51733100	-4.94686200	-1.02894200
H	-0.19374100	-4.13177600	0.54030500
H	0.75623800	-3.68814400	-0.90784000
C	-3.46985200	1.50253900	-2.62458500
C	-2.12317400	1.10369400	-2.60813000
C	-1.46387500	0.86353200	-1.39597600
H	-2.03965500	0.95581800	-0.46120400
O	-0.22662900	0.58978800	-1.30690900
H	-1.54872100	1.02048000	-3.53428900
H	-3.83253500	2.02440600	-3.51267500
H	-3.91415600	1.85272200	-1.68860400

B	0.60270700	0.54493500	0.03312300
C	-3.48028800	-1.58446100	-1.53150600
C	-4.63428100	-0.78177600	-1.76577100
C	-4.80078900	-0.05076600	-2.95424000
C	-2.43852100	-1.72854600	-2.40472500
C	1.46620000	1.91494300	0.06579700
C	1.17439700	3.02445500	-0.73702500
C	2.53760200	2.04090500	0.96718000
C	1.91540500	4.21033500	-0.64825700
C	3.27163900	3.22356000	1.07129100
C	2.96754700	4.32054800	0.25880000
C	1.57223900	-0.74178300	-0.13327900
C	2.09263800	-1.08165300	-1.39180800
C	1.95623700	-1.54284800	0.95203000
C	2.93604300	-2.18263800	-1.56468200
C	2.81259100	-2.63742700	0.78874100
C	3.31046500	-2.96820400	-0.47235500
C	-0.41540300	0.41836300	1.29385900
C	-1.14305900	-0.76870500	1.49095800
C	-0.62871800	1.45578900	2.21390000
C	-2.03460500	-0.91527700	2.55722400
C	-1.52016600	1.31501400	3.28550700
C	-2.22891100	0.12675600	3.46739700
H	-1.02198100	-1.59468400	0.78852000
H	-0.09166100	2.39905300	2.09743500
H	-2.91758300	0.01496000	4.30407600
H	1.82646800	-0.47644600	-2.26063000
H	1.57229100	-1.32285000	1.94988500
H	3.96793400	-3.82699000	-0.60364800
H	2.81169300	1.19565300	1.60201000
H	0.35313600	2.97930700	-1.45402100
H	3.54429900	5.24213300	0.33178900
C	1.59387900	5.34778100	-1.58091300
C	4.36297200	3.34431600	2.10347900
C	3.09700900	-3.53226400	1.96539000
C	3.33460400	-2.58132700	-2.95882900
C	-2.79283300	-2.20686300	2.69849300
C	-1.67296700	2.44435700	4.27225400
F	-1.68259100	3.64016400	3.65575500
F	-2.81462600	2.34537100	4.97771800
F	-0.66123100	2.46837800	5.15790200
F	-3.77767600	-2.31195200	1.76123100
F	-3.39144500	-2.32716600	3.89133000
F	-2.00146500	-3.27811500	2.52710300
F	4.22709200	-4.24001700	1.80685600
F	3.20275800	-2.84228200	3.11172200
F	2.09599700	-4.42704100	2.14022200
F	4.38189400	-3.41888400	-2.97824300
F	2.30944600	-3.21857700	-3.57988200
F	3.64223300	-1.52149100	-3.72397900
F	5.33433300	4.18742500	1.70952100
F	3.88479600	3.81715700	3.27125200
F	4.93798700	2.15847900	2.36741800
F	0.26358900	5.49186800	-1.74766500
F	2.11411000	5.14553500	-2.80801200
F	2.07332000	6.52184800	-1.13847600

P: E= -3320.25202648

H	-3.42496000	-2.40587000	-0.84345400
C	-5.25986700	-0.41911400	-0.41778400
C	-4.86660800	1.82244500	-2.30237400
H	-4.29246900	0.13242700	-3.48269200

H	-2.71462200	-1.65847900	-3.61317700
C	-1.31449700	-2.75958600	-2.44188900
H	-6.26799700	-0.36430500	-0.86245500
H	-5.13516900	0.49601000	0.18440100
H	-5.22567700	-1.27859500	0.26499300
H	-4.63633100	2.31553500	-1.34464500
H	-5.94008800	1.58519500	-2.31044900
H	-4.68146100	2.55387200	-3.10422600
H	-1.86888100	-3.71741800	-2.47556400
O	-0.65740700	-2.61722000	-1.20136300
H	-0.57584400	-2.77138200	-3.26782700
C	0.28436300	-3.63910500	-0.92655700
H	-0.21330500	-4.62512200	-0.88833800
H	0.73558300	-3.43094400	0.05141100
H	1.08077600	-3.66410100	-1.68896800
C	-2.51524800	0.96771500	-2.62695300
C	-1.52011600	-0.23414300	-2.53496400
C	-0.84546100	-0.11948600	-1.22032600
H	-1.45385800	-0.33075700	-0.32996400
O	0.30582900	0.30996200	-1.08582700
H	-0.76200100	-0.16831000	-3.32869100
H	-2.34507200	1.49041400	-3.57969600
H	-2.29090100	1.70817500	-1.83981300
B	1.12823800	0.41766500	0.33693700
C	-3.37084400	-1.58377700	-1.56117200
C	-4.19630200	-0.52759300	-1.47134300
C	-4.00898400	0.57322400	-2.50780700
C	-2.27822400	-1.59430000	-2.59918200
C	1.83878100	1.85747200	0.25886400
C	1.23389500	2.95267700	-0.37512800
C	3.07409500	2.07989800	0.88614700
C	1.83562800	4.21476800	-0.39124400
C	3.67370200	3.34302200	0.88936800
C	3.06030500	4.42010000	0.24602800
C	2.15661800	-0.81931900	0.22087800
C	2.74014500	-1.15145500	-1.01313100
C	2.50398900	-1.60779400	1.32659500
C	3.59973700	-2.24374400	-1.14430800
C	3.37177800	-2.69946000	1.20231700
C	3.92322100	-3.02961100	-0.03531800
C	0.03486700	0.28339600	1.52169700
C	-0.62576000	-0.93765800	1.75051500
C	-0.37355300	1.37924600	2.29724700
C	-1.67392400	-1.04979500	2.66605900
C	-1.39652000	1.26502300	3.24684200
C	-2.06409400	0.05283500	3.42928900
H	-0.34800000	-1.81971600	1.17442000
H	0.10495200	2.34946100	2.15398300
H	-2.87669200	-0.03001500	4.15077900
H	2.50656900	-0.55457000	-1.89645000
H	2.08109500	-1.38313000	2.30754700
H	4.59308600	-3.88325800	-0.13461600
H	3.58680300	1.25126400	1.37888200
H	0.26945200	2.83006800	-0.87140700
H	3.53070600	5.40304100	0.24009600
C	1.17963300	5.33996800	-1.14775700
C	4.96699900	3.55359400	1.63498700
C	3.61522600	-3.58372500	2.39700600
C	4.09585200	-2.63129400	-2.51160100
C	-2.43674600	-2.34476900	2.74900400
C	-1.75699700	2.45630100	4.09899800
F	-1.65203500	3.60633600	3.41093700
F	-3.01673300	2.37559100	4.56361600

F	-0.94700100	2.56051000	5.16730400
F	-3.38646500	-2.41016000	1.77996900
F	-3.07045500	-2.49245400	3.92063400
F	-1.64025700	-3.41079400	2.57166200
F	4.73507500	-4.31328500	2.27089600
F	3.71255300	-2.87629000	3.53403600
F	2.59368500	-4.45221400	2.56252800
F	5.20920100	-3.37663400	-2.46098100
F	3.16313000	-3.36535900	-3.17074100
F	4.35065200	-1.56130000	-3.28053000
F	5.67255000	4.58342300	1.13602200
F	4.74524500	3.82199700	2.93614700
F	5.75179900	2.46320000	1.58882200
F	-0.16423400	5.26584300	-1.08205500
F	1.50382000	5.31096400	-2.45589600
F	1.54202300	6.54477700	-0.67919500

f-exo'

1 = a-exo' 1

2: E= -2931.95593041

C	-0.79053900	-1.79320800	-3.69890700
C	-1.51014100	-0.95009100	-2.93497200
C	-0.97801000	-0.38196400	-1.70798200
O	0.16195100	-0.64154800	-1.29844400
H	-1.20019300	-2.21580400	-4.61939900
B	0.85558300	-0.14704400	0.11937200
H	-2.52731100	-0.65678500	-3.20596200
H	0.22741000	-2.07486200	-3.41476000
H	-1.61049100	0.30802000	-1.12228900
C	0.04241600	1.16155200	0.59753000
C	0.06302400	2.32694300	-0.19145400
C	-0.69741000	1.21017400	1.78834600
C	-0.63634000	3.47757500	0.17946200
C	-1.39031300	2.36449900	2.17284200
C	-1.36664900	3.50496300	1.37039100
C	0.67008100	-1.44592700	1.06263300
C	-0.58138400	-2.05914400	1.22493900
C	1.74344600	-1.97857500	1.79209600
C	-0.76187900	-3.15093800	2.07744500
C	1.57237000	-3.07315600	2.64643000
C	0.31845100	-3.66720500	2.79595400
C	2.38156400	0.12463500	-0.31334500
C	3.11913500	1.19595200	0.20963300
C	3.05116700	-0.75458300	-1.18092900
C	4.46573100	1.38714700	-0.12319500
C	4.38989600	-0.56201000	-1.52780800
C	5.10960800	0.51201700	-0.99728100
H	-0.72860700	0.33750300	2.44262000
H	0.65117300	2.34532500	-1.11265500
H	-1.89840200	4.40666700	1.67284500
H	2.64452700	1.89552400	0.90027900
H	2.52227900	-1.61868900	-1.58735600
H	6.15906300	0.65614000	-1.25219200
H	-1.45309600	-1.68778000	0.68010800
H	2.73428900	-1.53121900	1.69973800
H	0.18445400	-4.52002800	3.46100600
C	-2.20998000	2.34643700	3.43935000
C	-0.63601900	4.67228400	-0.74030300
C	5.04155200	-1.49337100	-2.51695300
C	5.19902100	2.58063400	0.43495600

C	-2.14165700	-3.72725600	2.26302900
C	2.76754000	-3.65159400	3.36255300
F	6.53205900	2.43520700	0.35940400
F	4.88462600	2.79459600	1.72460700
F	4.88306000	3.70516500	-0.23553000
F	4.59745600	-2.75619400	-2.37902900
F	4.77150300	-1.12554200	-3.78663700
F	6.37715600	-1.51481000	-2.38882200
F	-2.85091300	-3.68686900	1.11676400
F	-2.10526900	-5.00485700	2.67169300
F	-2.84489000	-3.03552500	3.17840600
F	2.41174700	-4.31326000	4.47662600
F	3.64337000	-2.69674100	3.71683700
F	3.43080400	-4.52338200	2.57952000
F	-3.40488200	1.75835200	3.23403500
F	-2.45169200	3.58420800	3.90005000
F	-1.59716700	1.65786800	4.41572100
F	-1.52599200	4.50880000	-1.74237100
F	-0.96463800	5.80430400	-0.10063500
F	0.56415200	4.85698600	-1.31402000

RC: E= -3320.20046755

H	-4.76939500	-0.30501500	-2.09601000
C	-4.93813000	-2.88699200	-1.80902500
C	-2.44262900	-3.99739800	-0.29695700
H	-2.03705800	-1.85585600	-0.14203400
H	-2.73823400	0.17732100	0.15782600
C	-3.68686900	1.84707500	-0.92778600
H	-5.05272200	-2.63385800	-2.87704800
H	-5.91237500	-2.68458800	-1.33270800
H	-4.74558600	-3.96394700	-1.73653400
H	-2.35165100	-4.18534200	0.78583500
H	-1.46023300	-4.26456900	-0.72004800
H	-3.18795600	-4.69464300	-0.70078900
H	-4.46906100	1.96099500	-1.70514200
O	-2.48630300	2.47976600	-1.34033000
H	-4.06340700	2.33881900	-0.00927600
C	-2.62011600	3.87339700	-1.50806500
H	-3.33196000	4.11763300	-2.32071800
H	-1.63130100	4.27786500	-1.75853300
H	-2.97388500	4.35514900	-0.57836900
C	-1.27556900	-1.80907300	-3.08113600
C	-1.28833100	-0.47269700	-2.88916200
C	-0.57973600	0.13863000	-1.79446700
O	0.12375300	-0.54220700	-1.01327400
H	-1.84812800	-2.27579600	-3.88515400
B	1.05775200	0.00611900	0.16792400
C	-4.04123500	-0.59783600	-1.32823500
C	-3.85411400	-2.04639300	-1.17981700
C	-2.76760800	-2.56188500	-0.55011000
C	-3.42883700	0.39760500	-0.65941600
H	-1.88798600	0.19801200	-3.50598300
H	-0.66823300	-2.45822900	-2.44857800
H	-0.68673500	1.22130100	-1.63100300
C	0.47399500	1.44867700	0.61654800
C	1.03676100	2.65814100	0.18582900
C	-0.68815900	1.53003200	1.40377300
C	0.46281500	3.89196300	0.51669600
C	-1.27089900	2.75461000	1.72966000
C	-0.69301800	3.94927100	1.29255400
C	0.96650600	-1.14069200	1.30054700
C	0.84991100	-2.49866600	0.94957800

C	1.09130400	-0.84247400	2.66288600
C	0.84112200	-3.50447600	1.91539100
C	1.08793700	-1.84914900	3.63899100
C	0.96003000	-3.18581000	3.27384300
C	2.53649300	0.09242000	-0.48905700
C	3.67732900	-0.12711400	0.30058200
C	2.74738200	0.45789300	-1.82525800
C	4.96555300	0.01807500	-0.22016500
C	4.03419200	0.61103600	-2.35334100
C	5.15481400	0.39142500	-1.55329700
H	-1.15484700	0.61383900	1.76860700
H	1.94362500	2.64773300	-0.42124600
H	-1.14181900	4.91028600	1.54479300
H	3.56306000	-0.41388100	1.34729100
H	1.90079200	0.62943100	-2.49375800
H	6.15875700	0.50820700	-1.96056400
H	1.19901000	0.19644700	2.98221900
H	0.77593100	-2.77583300	-0.10191800
H	0.96195500	-3.96808000	4.03303100
C	-2.52702700	2.80804300	2.55757800
C	1.04971500	5.15901100	-0.04829700
C	6.16274700	-0.28950300	0.64355700
C	4.19325100	1.07634000	-3.77696400
C	0.69588900	-4.95291900	1.53109200
C	1.19634400	-1.45189200	5.08892100
F	0.73560700	-5.13653200	0.19691000
F	-0.48010300	-5.46156300	1.96194300
F	1.66203300	-5.71291100	2.07006500
F	2.23927100	-0.62823500	5.29516700
F	1.35015800	-2.51235200	5.89809000
F	0.09419900	-0.79314900	5.49654900
F	-3.18112500	1.63086000	2.55456400
F	-2.28363500	3.12736800	3.83704300
F	-3.38792000	3.73709200	2.08057000
F	2.38490800	5.09615200	-0.14802400
F	0.74127300	6.23528800	0.69245500
F	0.57664000	5.39548600	-1.29619200
F	5.40561700	0.78758300	-4.27483000
F	3.27594400	0.51168000	-4.58733900
F	4.02829900	2.40984500	-3.87902400
F	7.24170200	0.42252000	0.27360100
F	5.92538200	-0.02489000	1.93913100
F	6.50417400	-1.58999300	0.56334000

TS: E= -3320.19552924

H	-4.56197200	-0.18770500	-1.52644500
C	-4.35832300	-2.79859000	-1.94047300
C	-1.76182000	-3.92069600	-1.05405800
H	-1.45390200	-1.89551900	-0.25139100
H	-1.95780900	0.06625700	0.11002600
C	-3.15301900	1.83224500	-0.43317100
H	-5.28627300	-2.24810200	-2.14478800
H	-4.60487300	-3.67580600	-1.31997700
H	-3.97721200	-3.19433900	-2.89786600
H	-2.23357000	-4.45497500	-0.21272800
H	-0.68376600	-4.11403500	-0.97829600
H	-2.12835200	-4.37142300	-1.98823300
H	-4.01001200	2.05440400	-1.10070900
O	-2.02150300	2.58720700	-0.79742800
H	-3.46764200	2.09005200	0.60006400
C	-2.24997600	3.97936000	-0.76839800
H	-3.01452900	4.27799200	-1.51204000

H	-1.30099100	4.47646600	-1.00407100
H	-2.58509800	4.31037000	0.23103200
C	-0.98764900	-1.61668600	-2.57628100
C	-0.88632000	-0.22380400	-2.45529200
C	-0.04303800	0.35582600	-1.49473800
O	0.58867600	-0.36705200	-0.65588500
H	-1.54529200	-2.03782600	-3.41551300
B	1.56861300	0.14843900	0.45592800
C	-3.63519600	-0.54904100	-1.06700800
C	-3.33382300	-1.93283700	-1.26089100
C	-2.06652700	-2.45047400	-0.96797900
C	-2.82272700	0.37412100	-0.47911100
H	-1.47478600	0.45221700	-3.07427800
H	-0.14058900	-2.21329700	-2.23323600
H	0.03750700	1.44797100	-1.42454900
C	1.01847500	1.58582000	0.97607700
C	1.56592500	2.80758000	0.55873000
C	-0.10636200	1.64453700	1.81514200
C	1.01938800	4.03102100	0.96367300
C	-0.65966700	2.86047500	2.22076700
C	-0.09213000	4.06647900	1.80506300
C	1.50737800	-0.99325000	1.60429300
C	1.13769500	-2.31334100	1.30852800
C	1.85432000	-0.71316600	2.93557300
C	1.09012900	-3.30290100	2.29577200
C	1.83357100	-1.70229400	3.92385400
C	1.44249800	-3.00627100	3.61353200
C	3.04439100	0.21913900	-0.20549200
C	4.13363500	0.66230100	0.56676100
C	3.31340500	-0.15802400	-1.52642300
C	5.42373600	0.73363600	0.04140000
C	4.60636600	-0.08500200	-2.06319600
C	5.67112300	0.36194600	-1.28490500
H	-0.56659000	0.71637100	2.16011400
H	2.43985300	2.81238400	-0.09519800
H	-0.51841900	5.01949800	2.11840000
H	3.97479600	0.96778900	1.60270900
H	2.50882300	-0.52780100	-2.16413300
H	6.67656100	0.42282000	-1.70062400
H	2.13069700	0.30410900	3.22084100
H	0.88196700	-2.57674000	0.28204100
H	1.40962900	-3.77418400	4.38571300
C	-1.86599000	2.87666700	3.11983700
C	1.56933500	5.31932400	0.41152600
C	6.57552400	1.16170600	0.91427300
C	4.81688400	-0.44736900	-3.50944300
C	0.58694700	-4.67532600	1.94283800
C	2.27264400	-1.36170800	5.32509400
F	0.96882000	-5.05095200	0.70414900
F	-0.76826600	-4.71893300	1.94894300
F	1.00836800	-5.61667600	2.79794600
F	3.61158200	-1.41983700	5.44992400
F	1.75495700	-2.20690600	6.23415600
F	1.90119500	-0.11648100	5.67241600
F	-2.63853500	1.78250300	2.93242300
F	-1.54088300	2.90710100	4.42002100
F	-2.64900400	3.95116400	2.88330200
F	2.87567900	5.23436400	0.12571900
F	1.39799400	6.34771400	1.25799200
F	0.93856200	5.65734100	-0.74099000
F	6.10857700	-0.67297000	-3.79788500
F	4.12681100	-1.55424900	-3.84879000
F	4.39290800	0.53478500	-4.33098400

F	7.50579500	1.83731100	0.21538200
F	6.17390200	1.95275000	1.92399600
F	7.19602400	0.10164100	1.46652800

P: E= -3320.24831418

H	-5.16541400	-0.40052100	-1.13637200
C	-4.98705400	-3.11354800	-1.28614900
C	-2.21903500	-3.99530000	-1.76760000
H	-1.95118700	-2.33134700	-0.45391300
H	-2.61981900	0.19838100	-0.11877700
C	-3.54258700	1.66677600	-1.33673400
H	-5.97527400	-2.64015800	-1.19666900
H	-4.86140800	-3.80826900	-0.43864800
H	-4.98199900	-3.73233900	-2.19830900
H	-2.66199800	-4.65558500	-1.01027000
H	-1.14357800	-4.22416600	-1.80095400
H	-2.64904000	-4.25249700	-2.74894700
H	-4.03642700	1.76118400	-2.32676900
O	-2.46861800	2.56980700	-1.23111700
H	-4.30454800	1.87642800	-0.56179600
C	-2.83865100	3.92937700	-1.27025600
H	-3.38886800	4.17313200	-2.19913300
H	-1.91643900	4.52364500	-1.23360700
H	-3.47164100	4.19697900	-0.40382600
C	-1.76434900	-1.61308600	-2.47959200
C	-1.84608600	-0.11583300	-2.14750100
C	-0.65348700	0.41090600	-1.44807100
O	0.12889500	-0.33869000	-0.85073900
H	-2.26361300	-1.78712300	-3.44468000
B	1.20912700	0.11943400	0.29648800
C	-4.13901700	-0.77166200	-1.22324700
C	-3.89158100	-2.08809200	-1.30592300
C	-2.43731400	-2.52060200	-1.42977500
C	-3.03084700	0.24515800	-1.14419500
H	-2.00366000	0.49266000	-3.05204200
H	-0.71135300	-1.90679200	-2.60622800
H	-0.54377300	1.50241600	-1.36850400
C	0.64664300	1.54195700	0.82104200
C	1.19197100	2.77439100	0.42681200
C	-0.55977700	1.57293000	1.53816200
C	0.55134400	3.98048600	0.72702200
C	-1.22145700	2.77278200	1.81094900
C	-0.66218000	3.98748400	1.41932000
C	1.07265300	-1.08013400	1.36588300
C	0.68455300	-2.37161500	0.98029100
C	1.35383900	-0.87289300	2.72508100
C	0.54421600	-3.40240300	1.91348700
C	1.25099700	-1.90983700	3.65818900
C	0.83246400	-3.18174200	3.26124900
C	2.64640800	0.16377200	-0.41786900
C	3.76519600	0.55543600	0.33962700
C	2.86785800	-0.17848500	-1.75693500
C	5.04196900	0.61082600	-0.21918600
C	4.14721600	-0.11997000	-2.32582800
C	5.24295000	0.27576900	-1.56265700
H	-1.01720800	0.63318900	1.85686800
H	2.12387800	2.79735000	-0.14038900
H	-1.17441000	4.92613300	1.63005500
H	3.64042600	0.82969200	1.38917800
H	2.03814700	-0.50928400	-2.38397400
H	6.23811200	0.32496300	-2.00392400
H	1.64117900	0.12109100	3.07483500

H	0.47225400	-2.58033800	-0.06835100
H	0.72671600	-3.98357800	3.99130800
C	-2.56087500	2.73219200	2.49747000
C	1.09630700	5.28779400	0.21357300
C	6.22738000	0.98218800	0.63572600
C	4.31101200	-0.43774200	-3.78938800
C	0.00129500	-4.72990600	1.45662400
C	1.62522400	-1.65571800	5.09649200
F	0.48587000	-5.08370400	0.25104400
F	-1.34661700	-4.68387000	1.32707300
F	0.27745000	-5.72220300	2.31411900
F	2.95091800	-1.78509400	5.28962100
F	1.01856600	-2.51534200	5.93298600
F	1.29302900	-0.41085200	5.48247200
F	-3.35161000	1.77271000	1.95981300
F	-2.45746100	2.45673100	3.80517600
F	-3.22479300	3.89650700	2.37987500
F	2.39079700	5.20681200	-0.11980300
F	0.96174200	6.27479500	1.11384500
F	0.42552900	5.68292100	-0.89622100
F	5.58569500	-0.70190200	-4.11435000
F	3.56943300	-1.50252500	-4.15018500
F	3.90815400	0.59114100	-4.56256000
F	7.16183400	1.64258200	-0.07054600
F	5.87267200	1.76328000	1.67035500
F	6.82313700	-0.10943600	1.15039800

g-endo'

1 = a-exo' 1

2: E= -1524.25053021

C	-2.96845700	0.56312700	-3.37647400
C	-1.72899300	0.97596900	-3.05373500
C	-1.15965900	0.61992700	-1.77360400
H	-1.75831700	0.00855600	-1.07404500
O	-0.02505200	0.98539900	-1.44087300
H	-1.11487000	1.58139100	-3.72598400
H	-3.42547300	0.81568000	-4.33630800
H	-3.56306400	-0.04193100	-2.68428200
B	0.76734400	0.56939700	-0.05538900
C	1.54397400	1.92054600	0.34710200
C	2.08085400	2.78286700	-0.62886400
C	1.78245700	2.23868200	1.69724100
C	2.81034000	3.91890200	-0.28453200
C	2.51922400	3.36364100	2.06923300
C	3.01960000	4.19328600	1.06729400
C	1.75222300	-0.61391400	-0.55366100
C	1.29137000	-1.67779300	-1.35287600
C	3.10052600	-0.64508100	-0.15280200
C	2.12078200	-2.72781000	-1.74049400
C	3.95273900	-1.68725000	-0.51922700
C	3.44855700	-2.71536900	-1.31349600
C	-0.36857700	0.10835300	0.99853700
C	-0.48087000	-1.20906100	1.47808800
C	-1.30857500	1.05110600	1.47013600
C	-1.48260200	-1.58374800	2.37701300
C	-2.32404200	0.70288100	2.35764800
C	-2.39568500	-0.61991600	2.79760300
H	-3.05251800	1.42625400	2.72243300
H	-1.57047200	-2.60204300	2.75437200
H	4.99656200	-1.71648000	-0.20858900

H	1.76798300	-3.55183000	-2.35948000
H	3.22392100	4.59267400	-1.03407500
H	2.70900400	3.61310400	3.11256500
H	0.24925100	-1.70431600	-1.68555500
H	3.49588400	0.16569700	0.46209000
H	1.38273100	1.59163800	2.48138200
H	1.92532300	2.55995200	-1.68669300
H	-1.23594600	2.09099400	1.13915700
H	0.23458900	-1.96423300	1.14703300
N	4.33993900	-3.81973100	-1.71644200
O	5.49452100	-3.78638100	-1.32314600
O	3.86643400	-4.69932400	-2.41909400
N	-3.47011200	-1.00636600	3.73448000
O	-4.26357500	-0.14122500	4.06910000
O	-3.50024200	-2.16649000	4.11102000
N	3.79085300	5.39227100	1.44517400
O	3.96582400	5.60061200	2.63531900
O	4.20662400	6.10424100	0.54431200

RC: E= -1912.48190876

H	-2.58988200	-0.98519900	0.64567500
C	-4.24914600	1.03302300	0.76668700
C	-5.64599200	1.51800600	-1.95267300
H	-4.30879200	-0.12595500	-2.53119100
H	-2.48738100	-1.13225500	-2.43148100
C	-1.14892600	-2.36212600	-1.23805300
H	-3.43705500	1.74502500	0.99961900
H	-4.30807600	0.35519100	1.63214800
H	-5.18766400	1.59771600	0.71373900
H	-5.73487900	2.28639400	-1.17309700
H	-6.62379800	1.00957400	-2.03516000
H	-5.48713600	2.02842800	-2.91672600
H	-0.19252300	-1.85326900	-0.99067800
O	-1.02245500	-3.06587600	-2.44615200
H	-1.35972200	-3.04216700	-0.38643400
C	-0.02564100	-4.05721800	-2.40756900
H	0.96847000	-3.63332300	-2.16851500
H	0.01634400	-4.52823700	-3.39958400
H	-0.25329200	-4.83822300	-1.65463800
C	-2.31403900	2.08292600	-2.44535700
C	-1.21222900	1.29486600	-2.41257100
C	-0.54273300	1.07236900	-1.16830200
H	-0.97384900	1.52972500	-0.26411700
O	0.52683400	0.42858600	-1.07207000
H	-0.81497300	0.80181500	-3.30318100
H	-2.84607800	2.28536700	-3.37622700
H	-2.65976400	2.60791800	-1.55349900
B	1.38391500	0.28318000	0.29156800
C	-2.88733700	-0.73580000	-0.37678700
C	-3.94088500	0.27248900	-0.49975100
C	-4.55761700	0.52402900	-1.68673600
C	-2.23355600	-1.34686300	-1.39010800
C	2.08574400	1.72021400	0.52929800
C	2.36047700	2.60840400	-0.52855300
C	2.51954800	2.09593900	1.81632000
C	3.01704200	3.82098600	-0.32248000
C	3.18366000	3.29861900	2.04949800
C	3.41856300	4.15156700	0.97104800
C	2.48612800	-0.84320500	-0.04435900
C	2.67887300	-1.37209100	-1.33384700
C	3.32898000	-1.31576800	0.98151300
C	3.65217900	-2.33727100	-1.59539900

C	4.30809200	-2.27788700	0.74827400
C	4.45376700	-2.78144100	-0.54559200
C	0.32229000	-0.14404400	1.44642600
C	0.09253200	-1.49403000	1.77542000
C	-0.48199700	0.81728700	2.09343500
C	-0.91779000	-1.88136600	2.65569500
C	-1.51593200	0.46007200	2.95786900
C	-1.73123700	-0.89362900	3.21065800
H	-2.15870500	1.20129000	3.43113200
H	-1.10341400	-2.92649400	2.90225700
H	4.95808400	-2.64813700	1.54020800
H	3.80167700	-2.75347700	-2.59114900
H	3.22904700	4.51153900	-1.13801000
H	3.51671300	3.59340600	3.04400700
H	2.04865600	-1.02660000	-2.15479500
H	3.21473800	-0.92371100	1.99536100
H	2.32555300	1.43462100	2.66415400
H	2.06482500	2.34561900	-1.54693100
H	-0.29543200	1.87972300	1.91733300
H	0.71558000	-2.26658900	1.32150700
N	5.47626500	-3.80873900	-0.80744600
O	6.16780400	-4.17215700	0.13117000
O	5.56916600	-4.23800600	-1.94758700
N	-2.86733700	-1.29057700	4.05915400
O	-3.72269700	-0.44443300	4.28347700
O	-2.89594000	-2.43769100	4.47018400
N	4.10615800	5.43385100	1.20426400
O	4.45194500	5.69116600	2.34675900
O	4.28625300	6.16293000	0.24095800

TS: E= -1912.47911825

H	-3.34566300	-1.01332900	0.25969600
C	-5.12817300	0.95288100	0.30377800
C	-6.01735500	1.79194000	-2.39844000
H	-4.73187200	0.12244100	-3.04640500
H	-3.22604900	-1.16467800	-2.82814100
C	-1.83241600	-2.32286700	-1.64619900
H	-4.73428200	1.98208600	0.39495900
H	-4.85487300	0.41405500	1.22029200
H	-6.22503700	1.04336800	0.26547600
H	-5.90493800	2.66945600	-1.74352600
H	-7.00028500	1.34261200	-2.17368900
H	-6.05014900	2.14675800	-3.43851100
H	-0.89743100	-1.77465200	-1.39546900
O	-1.68617200	-3.02122500	-2.85190300
H	-2.02303200	-3.00191100	-0.78831700
C	-0.63859600	-3.96251900	-2.82485800
H	0.33373300	-3.48864200	-2.59429600
H	-0.58445300	-4.42787900	-3.81862000
H	-0.82149800	-4.75493500	-2.07217300
C	-3.16414100	1.92871600	-2.65806800
C	-1.99847900	1.15737900	-2.71618500
C	-1.22233100	1.00053300	-1.55922800
H	-1.58714600	1.48861500	-0.64309300
O	-0.13222200	0.35279500	-1.49428400
H	-1.67459500	0.67260000	-3.64004900
H	-3.61836300	2.26398900	-3.59196600
H	-3.29928900	2.60866900	-1.81327100
B	0.72968900	0.26155100	-0.15736300
C	-3.61661900	-0.74668100	-0.76459400
C	-4.58539900	0.28815000	-0.93084700
C	-4.91576000	0.78474900	-2.19759500

C	-2.93586800	-1.33942900	-1.79053600
C	1.41954500	1.70813300	0.06574800
C	1.63509300	2.60499700	-0.99824400
C	1.89224400	2.09081100	1.33706200
C	2.27328500	3.83078100	-0.81281700
C	2.53781800	3.30691900	1.55013700
C	2.71498100	4.16747500	0.46612700
C	1.85222900	-0.85587900	-0.46531700
C	2.08265800	-1.36075600	-1.75863700
C	2.67322900	-1.33923000	0.57297100
C	3.07014100	-2.31325600	-2.01234200
C	3.66641700	-2.28912600	0.34811900
C	3.84873100	-2.76966600	-0.94995700
C	-0.31578000	-0.15965100	1.02341900
C	-0.55932400	-1.50742500	1.35253700
C	-1.11450600	0.80730100	1.66988500
C	-1.58049100	-1.88732100	2.22414100
C	-2.16204700	0.45913600	2.52095200
C	-2.39417800	-0.89347700	2.76876900
H	-2.80088900	1.20724400	2.98923800
H	-1.77579000	-2.93104900	2.46986200
H	4.29938500	-2.66794900	1.14975700
H	3.24915700	-2.71037100	-3.01106600
H	2.43952800	4.52798300	-1.63331700
H	2.90059500	3.60674000	2.53266800
H	1.46934500	-1.00213200	-2.58695800
H	2.52948200	-0.96649100	1.59040300
H	1.74391500	1.42315700	2.18943900
H	1.30329000	2.33750600	-2.00404400
H	-0.91520200	1.86786300	1.49738000
H	0.06138400	-2.28522600	0.90353200
N	4.88478800	-3.78471800	-1.20280800
O	5.55697800	-4.15809600	-0.25377700
O	5.00849400	-4.19625100	-2.34682600
N	-3.54660300	-1.28065200	3.59648800
O	-4.41126200	-0.43382100	3.78638300
O	-3.58348800	-2.42100800	4.02519200
N	3.38174800	5.46344200	0.67816100
O	3.76209100	5.72717900	1.80853600
O	3.51221600	6.19889200	-0.28867800

P: E= -1912.52921756

H	-2.90566700	-1.35240900	0.43165200
C	-4.45463300	0.85345800	0.90944800
C	-4.55276800	2.63416100	-1.43957100
H	-4.55731100	0.66747400	-2.27630000
H	-3.01702200	-1.21968500	-2.52946100
C	-1.41275400	-2.25420800	-1.59276700
H	-4.12355400	1.84959400	1.24733000
H	-4.27929300	0.14481400	1.72968600
H	-5.54353600	0.92826300	0.74969900
H	-3.95877900	3.27872600	-0.77157200
H	-5.56444000	2.55257100	-1.01775200
H	-4.63813500	3.15074400	-2.40825700
H	-0.72691400	-2.17094000	-0.72817100
O	-0.69602400	-2.42755500	-2.78676400
H	-2.06800600	-3.12684700	-1.39126400
C	0.03196300	-3.63149400	-2.83758400
H	0.76849800	-3.70045300	-2.01476300
H	0.56949200	-3.65692800	-3.79576200
H	-0.63654100	-4.51267500	-2.78006600
C	-2.55042300	1.41797900	-2.39664100

C	-1.54233100	0.27753400	-2.17238900
C	-0.58220000	0.61799200	-1.09238500
H	-0.84297000	1.40783100	-0.36599300
O	0.47495700	0.00236700	-0.94269000
H	-0.96847500	0.02394100	-3.07648900
H	-2.77139000	1.49797300	-3.47094400
H	-2.08480900	2.37805800	-2.11638100
B	1.41712500	0.12098300	0.41162100
C	-3.01934600	-0.68878300	-0.43060000
C	-3.74723500	0.43872000	-0.34751400
C	-3.89473900	1.26547700	-1.62225300
C	-2.29760200	-1.02220900	-1.71248100
C	1.95302700	1.63728100	0.47197900
C	2.16265200	2.40784100	-0.68872500
C	2.31611900	2.21524500	1.70469300
C	2.68501200	3.69911100	-0.63313900
C	2.84956800	3.50045000	1.78793600
C	3.01937800	4.23011300	0.61185500
C	2.59456600	-0.93830300	0.14475900
C	2.70975900	-1.68001500	-1.04542100
C	3.56453000	-1.15256200	1.14353800
C	3.74000800	-2.60172600	-1.23665800
C	4.60189400	-2.06647100	0.97706000
C	4.67350800	-2.78405900	-0.21835200
C	0.36362100	-0.31383800	1.56614100
C	0.15970200	-1.67331900	1.87165300
C	-0.50511500	0.62039600	2.16421400
C	-0.88617800	-2.09585800	2.69205600
C	-1.56845000	0.22604300	2.97475500
C	-1.75393100	-1.13501900	3.21108000
H	-2.25842600	0.94476200	3.41477900
H	-1.05573000	-3.14761300	2.92098200
H	5.35359200	-2.23757000	1.74674300
H	3.83353700	-3.18209900	-2.15397800
H	2.84632100	4.29895500	-1.52815400
H	3.12914200	3.95127700	2.73949500
H	1.97353200	-1.54115200	-1.83824700
H	3.50828600	-0.59046200	2.07941600
H	2.17296300	1.64848100	2.62770600
H	1.92739000	1.98774300	-1.67000200
H	-0.35805700	1.68790700	1.98335800
H	0.82898300	-2.42187400	1.44195800
N	5.76040100	-3.76070600	-0.40729700
O	6.56673400	-3.89345800	0.49997100
O	5.78811900	-4.38050600	-1.45974100
N	-2.91264900	-1.57088700	4.00920100
O	-3.78037800	-0.74010100	4.24255400
O	-2.94515000	-2.73327400	4.37545700
N	3.56658600	5.59734300	0.68579200
O	3.86034700	6.02955000	1.78898200
O	3.68964000	6.21390200	-0.36102200

g-exo'

1 = a-exo' 1

2: E= -1524.24787346

C	-0.76457200	-1.82025400	-2.74296800
C	-0.87039200	-0.50232300	-2.49150100
C	-0.12769400	0.13833800	-1.41802000
O	0.62975400	-0.49329800	-0.66916800
H	-1.32557200	-2.29121500	-3.55366200

B	1.60074400	0.12936900	0.51269900
H	-1.51940700	0.14430400	-3.08731700
H	-0.11011100	-2.45312100	-2.13689500
H	-0.24558400	1.22493600	-1.26263100
C	0.98052100	1.56827100	0.90473000
C	1.67008400	2.77758600	0.70461500
C	-0.30878000	1.64549800	1.47616900
C	1.11031300	4.01098400	1.04666200
C	-0.89558300	2.86203600	1.81653800
C	-0.17060200	4.03356500	1.59270600
C	1.51533100	-0.98394100	1.67356200
C	1.51868700	-2.35900700	1.36525400
C	1.51458200	-0.62487900	3.03389200
C	1.50317200	-3.33655200	2.35721600
C	1.51077800	-1.58355200	4.04832900
C	1.49845200	-2.93063100	3.69231600
C	3.04486600	0.18685300	-0.21479200
C	4.20351400	-0.25580600	0.44958400
C	3.20671100	0.72798300	-1.50467800
C	5.46742500	-0.16029300	-0.13357700
C	4.45482600	0.82885800	-2.11533200
C	5.57360600	0.37918700	-1.41414900
H	-1.89048800	2.92646600	2.25583400
H	1.64281200	4.94969400	0.89743900
H	4.58365200	1.24576900	-3.11344700
H	6.36740100	-0.49883400	0.37863300
H	1.50086500	-4.40096600	2.12525100
H	1.51254800	-1.31064300	5.10300400
H	-0.86541300	0.72407500	1.66971200
H	2.67360400	2.75917500	0.27527400
H	4.11699300	-0.68594700	1.44926100
H	2.33800100	1.09422800	-2.06012100
H	1.51770100	0.43126100	3.31204400
H	1.54030600	-2.67407100	0.31938700
N	1.48235300	-3.95524900	4.75325600
O	1.48991600	-3.57035500	5.91162800
O	1.46106100	-5.12631500	4.40748600
N	6.90227100	0.47690700	-2.04816200
O	7.86385300	0.08259100	-1.40881700
O	6.95690100	0.94627400	-3.17427200
N	-0.78013300	5.33188200	1.94548400
O	-1.90934400	5.31640500	2.40873000
O	-0.11867000	6.33788800	1.74826500

RC: E= -1912.48578218

H	-4.64807200	-0.31985500	-1.47743500
C	-4.57711900	-2.90465300	-1.58770400
C	-1.89667300	-4.02311900	-0.44593700
H	-1.59663900	-1.89729700	-0.04944100
H	-2.23010600	0.08403400	0.37319600
C	-3.46909900	1.77831000	-0.31885400
H	-4.81046100	-2.53336100	-2.60025300
H	-5.50901400	-2.82618600	-1.00251500
H	-4.32099100	-3.96767500	-1.66839000
H	-1.77661000	-4.34883500	0.60216900
H	-0.90623200	-4.15760100	-0.91335100
H	-2.60148000	-4.70693900	-0.93599700
H	-4.44173100	1.89512100	-0.83731800
O	-2.46355300	2.51780500	-0.99086700
H	-3.59380200	2.18169200	0.70701100
C	-2.73090700	3.90251400	-1.02870600
H	-3.62843800	4.12483900	-1.63807400

H	-1.86041100	4.39749700	-1.48058500
H	-2.88895600	4.31279300	-0.01525100
C	-1.09065100	-1.46124100	-3.03166400
C	-1.15520500	-0.15046400	-2.71573000
C	-0.37843600	0.40609600	-1.63547200
O	0.43198600	-0.29330400	-0.98896500
H	-1.71262700	-1.89032600	-3.81978000
B	1.36927500	0.16681400	0.23296700
C	-3.76962400	-0.63601400	-0.90043800
C	-3.48490500	-2.07545200	-0.95738400
C	-2.31844700	-2.59036000	-0.49204400
C	-3.08721900	0.33181100	-0.25828000
H	-1.84782900	0.53512400	-3.20570800
H	-0.39125800	-2.12446100	-2.52017500
H	-0.53188200	1.46052700	-1.36331300
C	0.81835000	1.60617800	0.73210300
C	1.36347900	2.80710200	0.23825300
C	-0.29627700	1.70968900	1.58800700
C	0.82015800	4.05175500	0.55725200
C	-0.86780700	2.93727800	1.91456300
C	-0.30130300	4.09529000	1.38378800
C	1.23376800	-1.04590500	1.29424700
C	1.06071400	-2.37335800	0.85473400
C	1.36611500	-0.83931800	2.68065800
C	0.98332900	-3.44240700	1.74344400
C	1.30270500	-1.89272300	3.59324100
C	1.09798400	-3.18406500	3.10960700
C	2.86695500	0.21473100	-0.37004000
C	3.93354600	0.52704100	0.49722900
C	3.18143000	-0.04003900	-1.71649000
C	5.25009700	0.59409400	0.05141900
C	4.49349700	0.01718300	-2.18977300
C	5.51282500	0.33667600	-1.29588900
H	-1.73968000	3.01733300	2.56286300
H	1.23797600	4.98225600	0.17406700
H	4.74259000	-0.17873900	-3.23211600
H	6.07655000	0.83815600	0.71792100
H	0.84163000	-4.46864800	1.40708100
H	1.39936600	-1.73511900	4.66690800
H	-0.73482300	0.80201500	2.00850300
H	2.23502200	2.76767300	-0.41894000
H	3.72735500	0.72349300	1.55248200
H	2.38807900	-0.29437900	-2.42247500
H	1.51605100	0.17274100	3.06332800
H	0.98869700	-2.57471900	-0.21550200
N	0.99746400	-4.30404400	4.06084100
O	1.15202500	-4.05722600	5.24641000
O	0.75914000	-5.41279900	3.60533500
N	6.90086800	0.40436000	-1.78422600
O	7.77180400	0.69087800	-0.97757500
O	7.09767700	0.17075800	-2.96720100
N	-0.92239800	5.39661700	1.67873100
O	-2.02671400	5.38856200	2.20752200
O	-0.31112900	6.40379700	1.36397800

TS: E= -1912.47934835

H	-4.60661700	-0.17174200	-1.27845400
C	-4.39757000	-2.81108400	-1.51890100
C	-1.73305300	-3.83878500	-0.73565000
H	-1.39483700	-1.76289800	-0.10412500
H	-1.90101800	0.19821900	0.16050000
C	-3.13340200	1.92388800	-0.42216800

H	-5.34407600	-2.28652900	-1.70542100
H	-4.59278900	-3.63798100	-0.81604600
H	-4.07314500	-3.27996000	-2.46408200
H	-2.20655700	-4.32326900	0.13556800
H	-0.65139300	-4.01213600	-0.65301600
H	-2.09709600	-4.35405500	-1.63730100
H	-4.05511500	2.09785900	-1.01352300
O	-2.05134700	2.65403700	-0.94616000
H	-3.34605300	2.25983200	0.61669200
C	-2.29448900	4.04407800	-0.97699900
H	-3.10071600	4.29728800	-1.69276300
H	-1.36542200	4.53551300	-1.29418100
H	-2.58117800	4.42564200	0.01909400
C	-1.10394600	-1.64235000	-2.45309900
C	-0.97123800	-0.24436600	-2.40045300
C	-0.06785700	0.34957000	-1.50389400
O	0.59513700	-0.36619200	-0.68527500
H	-1.72344300	-2.08522900	-3.23637000
B	1.57603700	0.14183400	0.43662700
C	-3.64711800	-0.49693800	-0.86125500
C	-3.34305700	-1.88652600	-0.97842800
C	-2.04544800	-2.36597900	-0.74477400
C	-2.80027700	0.46561000	-0.39440700
H	-1.58110000	0.41938600	-3.01154200
H	-0.23402600	-2.23397300	-2.16127700
H	0.02405700	1.44258600	-1.45931000
C	1.00349200	1.57481800	0.94732000
C	1.54002800	2.79814400	0.50523900
C	-0.13578500	1.63364800	1.77572900
C	0.96650000	4.02334500	0.84715900
C	-0.74068900	2.83965400	2.11949400
C	-0.17918700	4.02358600	1.64045200
C	1.52241300	-1.02883700	1.55614000
C	1.29320200	-2.36927800	1.18729500
C	1.75580100	-0.76941700	2.92002700
C	1.26631500	-3.40129100	2.12213200
C	1.74479700	-1.78355400	3.87757500
C	1.48909600	-3.09092500	3.46438400
C	3.05672800	0.22283400	-0.20961700
C	4.13918500	0.63706700	0.59353800
C	3.33851900	-0.11575400	-1.54498200
C	5.43627600	0.72449200	0.09705800
C	4.62991800	-0.03970900	-2.06931800
C	5.66473800	0.38365500	-1.23814800
H	-1.63037900	2.88640000	2.74681100
H	1.37850700	4.97194200	0.50392800
H	4.85192500	-0.30005100	-3.10367400
H	6.27352200	1.04777600	0.71460500
H	1.08260400	-4.43779700	1.84073000
H	1.92002600	-1.58435100	4.93427200
H	-0.56141000	0.70438900	2.16325300
H	2.42941100	2.79381300	-0.12872600
H	3.96096300	0.90021700	1.63931100
H	2.53372800	-0.45422900	-2.20112500
H	1.93891300	0.25652000	3.24871200
H	1.13781100	-2.60793900	0.13348600
N	1.44928000	-4.16916200	4.46548300
O	1.67239400	-3.87301900	5.62911500
O	1.19065300	-5.29775000	4.07312300
N	7.03047200	0.47315800	-1.78031800
O	7.91562700	0.85217900	-1.02865100
O	7.19818800	0.16413100	-2.95075400
N	-0.83422300	5.30260700	1.94932000

O	-1.96075700	5.25979100	2.42926200
O	-0.23096400	6.33076300	1.69040500

P: E= -1912.53296615

H	-4.91342900	-0.24870700	-1.01551300
C	-4.75423300	-2.96289300	-1.08743400
C	-1.98725300	-3.87875000	-1.52249700
H	-1.70761900	-2.17638400	-0.25916500
H	-2.38875300	0.38783500	0.01119200
C	-3.27258300	1.80197500	-1.29659600
H	-5.73899700	-2.47873500	-1.02137100
H	-4.64556700	-3.63599500	-0.22023000
H	-4.74625600	-3.60579700	-1.98280000
H	-2.44688100	-4.51871000	-0.75585800
H	-0.91167000	-4.11241000	-1.54576800
H	-2.40972800	-4.16224100	-2.49982300
H	-3.72457400	1.85796500	-2.30959500
O	-2.20264700	2.70613100	-1.17745200
H	-4.07198700	2.04531100	-0.56855800
C	-2.58331700	4.06352500	-1.22875200
H	-3.10184200	4.30508100	-2.17605200
H	-1.67060500	4.66947600	-1.15856100
H	-3.24705800	4.32636900	-0.38424900
C	-1.51680100	-1.51882700	-2.29938900
C	-1.56741800	-0.02028100	-1.97787200
C	-0.38478100	0.47305900	-1.23553300
O	0.37850100	-0.29821500	-0.64327500
H	-2.02850300	-1.69513900	-3.25760200
B	1.47775200	0.14372700	0.50394000
C	-3.88817400	-0.62723100	-1.08271500
C	-3.64961600	-1.94728600	-1.12418000
C	-2.19736800	-2.39377300	-1.22774800
C	-2.77610100	0.38721000	-1.02612700
H	-1.66515100	0.58684600	-2.89217100
H	-0.46968200	-1.83147600	-2.42970400
H	-0.26650100	1.56225500	-1.13018800
C	0.91308000	1.56714400	1.02475000
C	1.42013500	2.79160300	0.55287200
C	-0.26689800	1.60667800	1.79667500
C	0.75639000	3.99823800	0.78105700
C	-0.95590800	2.79420000	2.02870300
C	-0.43993100	3.97527500	1.49577400
C	1.38254700	-1.07190700	1.55708100
C	1.09927800	-2.38934600	1.14638200
C	1.64882200	-0.86060200	2.92296900
C	1.06295200	-3.44915600	2.05002900
C	1.62988700	-1.90535700	3.84662500
C	1.32900600	-3.18969300	3.39479400
C	2.90699000	0.18933100	-0.22885600
C	4.03305100	0.58581100	0.52137600
C	3.11695300	-0.16148200	-1.57414600
C	5.30658900	0.64445900	-0.03714000
C	4.38348600	-0.11392200	-2.15863000
C	5.46376700	0.29320300	-1.37932900
H	-1.88884000	2.82474100	2.59024000
H	1.12975100	4.94598500	0.39452200
H	4.55143300	-0.38435400	-3.20050700
H	6.17862400	0.95353500	0.53804100
H	0.83813000	-4.46894700	1.73963500
H	1.83384800	-1.74718300	4.90502000
H	-0.67423700	0.67468700	2.19679100
H	2.33987500	2.79945600	-0.03622500

H	3.90934000	0.85636700	1.57315800
H	2.27703700	-0.48875600	-2.19085300
H	1.86770000	0.14924200	3.27893900
H	0.90209100	-2.59244200	0.09191500
N	1.28709400	-4.30099700	4.36168300
O	1.53832200	-4.04615000	5.52910900
O	1.00095400	-5.41010100	3.93702900
N	6.80477300	0.35407800	-1.98695300
O	7.73084500	0.71712900	-1.27884800
O	6.90853400	0.03919300	-3.16262200
N	-1.21199200	5.22072300	1.63870800
O	-2.28757000	5.15837500	2.21603000
O	-0.74705800	6.23702700	1.14585500