

Supporting Information

Part B

Transforming 2D Azolium Salts to 3D Caged Tertiary Amines via Stereoselective Dearomative Cascade Annulation

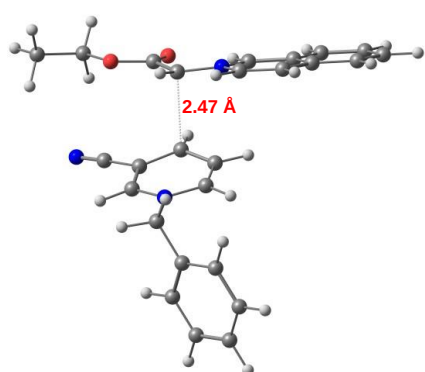
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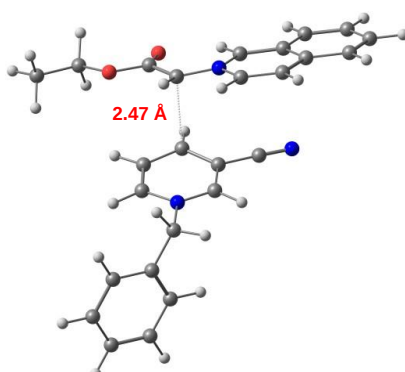
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Computational details:

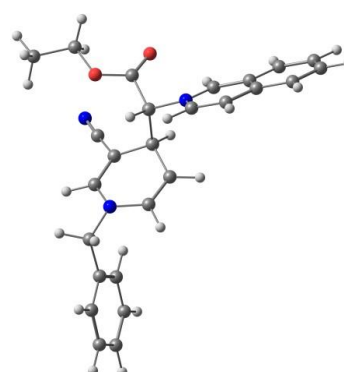
All the quantum chemical calculations were performed using Gaussian 16 program package[1], employing the density functional theory (DFT) based M062X functional in conjunction with 6-31G(d,p) basis set.[2,3] Geometries were fully relaxed in solvent (methanol) medium using polarized continuum model (PCM)[4] and characterized by frequency analysis to confirm they are true minima or saddle points on potential energy surface. Intrinsic reaction coordinate (IRC) calculations were carried out to confirm whether the transitions are connected to reactants and products.



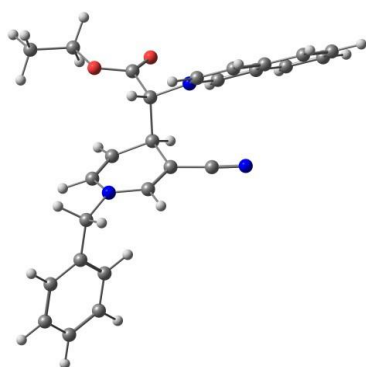
TS1_R



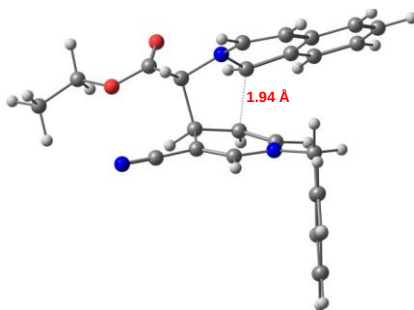
TS1_S



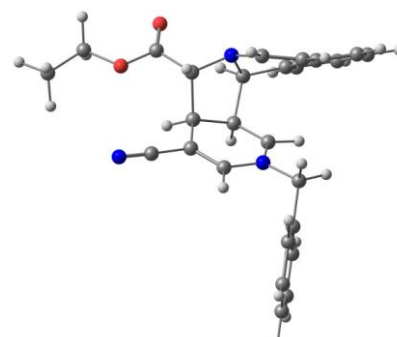
A_R



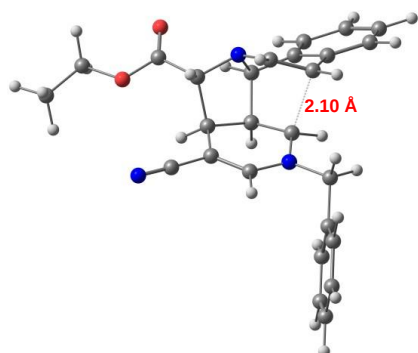
A_S



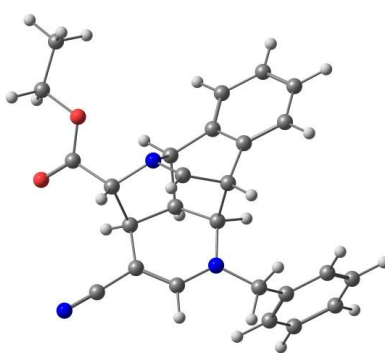
TS2_a



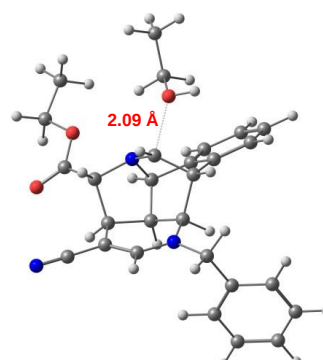
AB



TS2_b



B



TS3_F

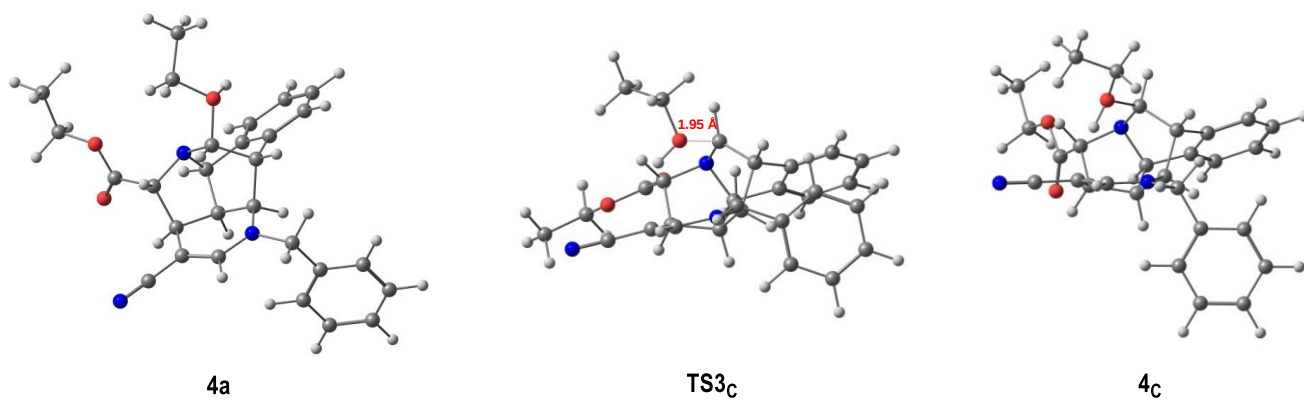


Figure S1. Optimized geometries of important intermediates and transition states for (4+2) annulation.

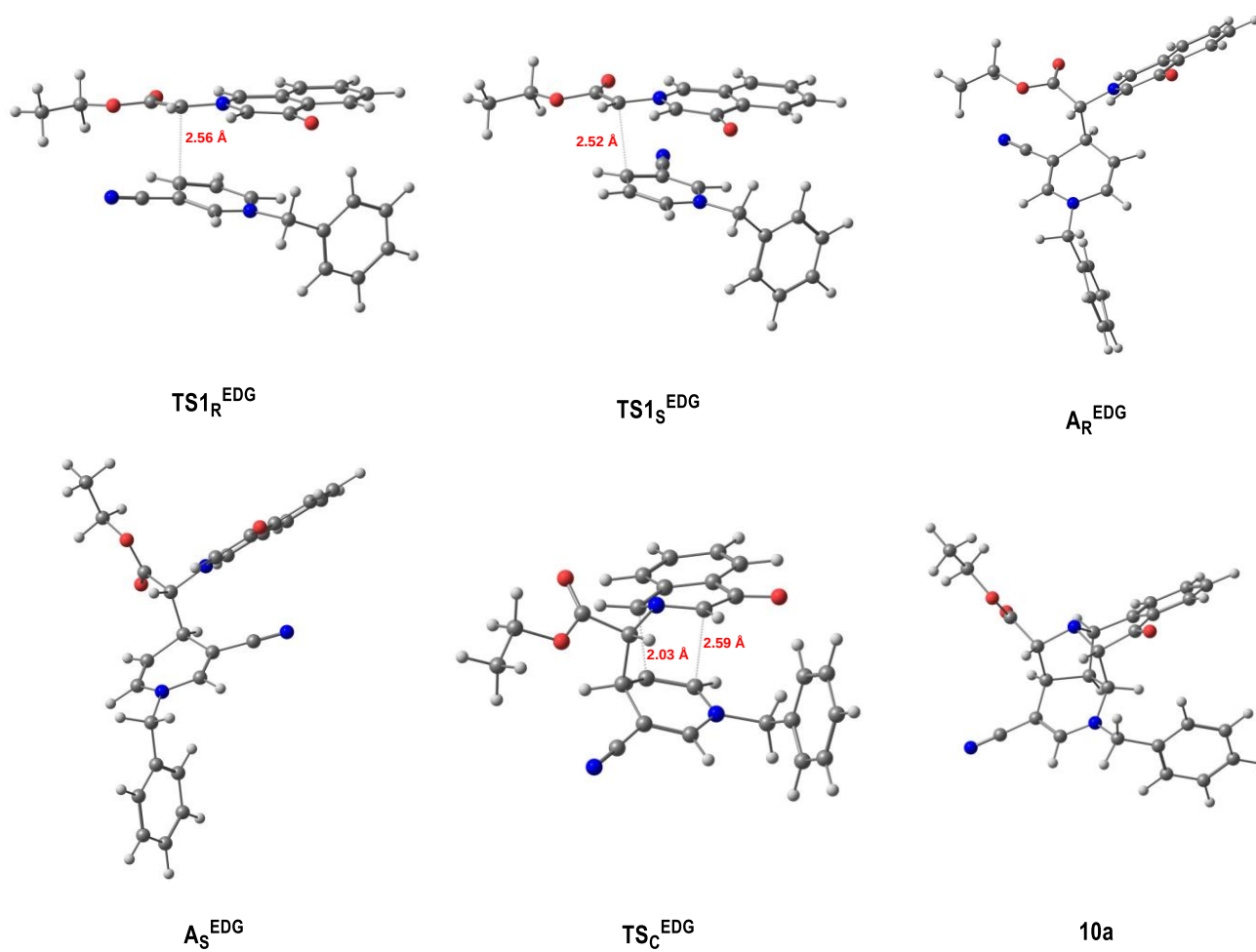


Figure S2. Optimized geometries of important intermediates and transition states for (3+2) annulation.

References:

1. Gaussian 16, Revision C.01, Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A. V., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., Izmaylov, A. F., Sonnenberg, J. L., Williams-Young, D., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V. G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery, J. A., Jr., Peralta, J. E., Ogliaro, F., Bearpark, M. J., Heyd, J. J., Brothers, E. N., Kudin, K. N., Staroverov, V. N., Keith, T. A., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A. P., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Millam, J. M., Klene, M., Adamo, C., Cammi, R., Ochterski, J. W., Martin, R. L., Morokuma, K., Farkas, O., Foresman, J. B., and Fox, D. J., Gaussian, Inc., Wallingford CT (2019).
2. Zhao Y. & Truhlar, D.G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: Two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor Chem Acc.* **120**, 215–241 (2008).
3. Ditchfield, R., Hehre, W. J. and Pople, J. A. Self-Consistent Molecular Orbital Methods. 9. Extended Gaussian-type basis for molecular-orbital studies of organic molecules. *J. Chem. Phys.* **54**, 724 (1971).
4. Cossi, M., Rega, N., Scalmani, G., Barone, V. Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. *J. Comput. Chem.* **24**, 669-681 (2003).

Coordinates:

TS1_R

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H	-4.963309000	-4.434991000	2.209518000
C	-4.077863000	-2.703812000	1.338157000
H	-4.527750000	-2.006954000	2.037862000
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H	6.522247000	-0.385693000	2.326509000
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TS1s

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C	3.239074000	0.530001000	-0.081354000
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C	-4.577634000	-1.416497000	-0.782770000
H	-3.552525000	-1.452231000	-1.141362000
C	-5.613691000	-1.825388000	-1.621479000
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H	-1.377299000	2.097124000	-1.381500000

TS2a

C	-0.211600000	3.130970000	0.871735000
C	0.435524000	4.374616000	0.923749000
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C	0.278660000	5.282603000	-0.111201000
H	0.781912000	6.242479000	-0.065077000
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C	-0.588513000	0.152500000	-1.260372000
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C	1.194785000	-1.386638000	0.294569000
H	1.974121000	-1.925926000	0.818847000
C	0.750430000	0.517164000	-1.024230000
H	1.162233000	1.407686000	-1.492017000
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H	0.538703000	2.325386000	2.776713000
C	-0.874255000	1.033809000	1.901485000
C	-2.143984000	-0.574803000	0.592059000
H	-2.035956000	-1.184518000	1.491717000
C	-3.589842000	-0.701802000	0.124959000
O	-3.896716000	-1.987196000	0.012397000
C	-5.235809000	-2.287831000	-0.447464000
H	-5.375680000	-1.816114000	-1.423103000
H	-5.944465000	-1.843916000	0.255710000
C	-5.355289000	-3.792222000	-0.512194000
H	-6.355750000	-4.063101000	-0.855246000
H	-4.624336000	-4.207312000	-1.209168000
H	-5.193884000	-4.234073000	0.473128000
C	-0.354335000	-3.201848000	0.534678000
C	2.855150000	0.434205000	0.224859000
H	2.759838000	0.683614000	1.286650000
H	2.982675000	1.366193000	-0.330163000
C	4.000387000	-0.516870000	-0.016929000
C	4.288373000	-0.943485000	-1.316616000
H	3.683248000	-0.589341000	-2.147381000
C	5.344633000	-1.817537000	-1.545688000

H	5.565076000	-2.145537000	-2.555924000
C	6.121558000	-2.268865000	-0.477865000
H	6.946601000	-2.949887000	-0.658315000
C	5.837182000	-1.847069000	0.817349000
H	6.437155000	-2.198234000	1.650020000
C	4.774410000	-0.974578000	1.048390000
H	4.547479000	-0.647360000	2.059142000
N	-1.765827000	0.784344000	0.860877000
N	-0.662938000	-4.257284000	0.897176000
N	1.561621000	-0.139194000	-0.207266000
O	-4.331481000	0.218399000	-0.116959000
H	-0.872665000	0.296519000	2.695440000

AB

C	-0.821049000	3.270679000	0.756582000
C	-0.490454000	4.629101000	0.803480000
H	0.000901000	5.028853000	1.685307000
C	-0.798561000	5.457837000	-0.269833000
H	-0.541508000	6.510948000	-0.227049000
C	-1.439260000	4.944078000	-1.398241000
H	-1.680433000	5.595256000	-2.231151000
C	-1.767214000	3.591668000	-1.456175000
H	-2.261221000	3.181908000	-2.332637000
C	-1.458239000	2.758876000	-0.385271000
C	-1.710684000	1.283734000	-0.435872000
H	-2.539276000	1.054193000	-1.110310000
C	-0.488576000	0.383681000	-0.927523000
H	-0.404206000	0.496838000	-2.014164000
C	-0.931870000	-1.023003000	-0.480480000
H	-1.400101000	-1.549844000	-1.314058000
C	0.198589000	-1.856582000	0.041039000
C	1.385511000	-1.341082000	0.384874000
H	2.205078000	-1.918072000	0.792871000
C	0.795564000	0.833704000	-0.352337000
H	1.099701000	1.869674000	-0.477683000
C	-0.557938000	2.344734000	1.851800000
H	0.035154000	2.665384000	2.700191000
C	-1.160778000	1.134849000	1.883989000
C	-2.024233000	-0.742811000	0.644609000
H	-1.793845000	-1.282190000	1.566383000
C	-3.387201000	-1.213551000	0.153148000
O	-3.368819000	-2.536535000	0.026399000
C	-4.570730000	-3.151765000	-0.489392000
H	-4.793302000	-2.706329000	-1.462288000
H	-5.393467000	-2.920657000	0.191668000
C	-4.300992000	-4.635393000	-0.584156000
H	-5.183264000	-5.143291000	-0.978679000
H	-3.458412000	-4.830490000	-1.251160000
H	-4.072019000	-5.048504000	0.400375000
C	-0.039987000	-3.259939000	0.225891000

C	2.922283000	0.545989000	0.795430000
H	2.850162000	0.421466000	1.878719000
H	2.960370000	1.612465000	0.568788000
C	4.107023000	-0.194080000	0.229859000
C	4.423902000	-0.071642000	-1.125980000
H	3.819600000	0.563004000	-1.769054000
C	5.513220000	-0.757679000	-1.650349000
H	5.757421000	-0.659812000	-2.702617000
C	6.292978000	-1.566654000	-0.822946000
H	7.143718000	-2.099975000	-1.233709000
C	5.981305000	-1.689067000	0.527907000
H	6.586224000	-2.316555000	1.173422000
C	4.886760000	-1.005238000	1.054200000
H	4.640382000	-1.098507000	2.108301000
N	-1.992289000	0.687448000	0.862281000
N	-0.275445000	-4.384285000	0.364339000
N	1.645861000	0.035643000	0.222091000
O	-4.321499000	-0.499166000	-0.111381000
H	-1.058211000	0.465530000	2.731917000

B

C	0.220119000	2.166547000	0.938081000
C	0.827537000	3.348257000	1.340151000
H	1.496564000	3.364315000	2.194243000
C	0.558082000	4.509492000	0.616060000
H	1.024506000	5.443152000	0.911112000
C	-0.304104000	4.484057000	-0.481007000
H	-0.504199000	5.397949000	-1.029215000
C	-0.914538000	3.294723000	-0.875926000
H	-1.591754000	3.270009000	-1.723616000
C	-0.636980000	2.137311000	-0.159053000
C	-1.199646000	0.782821000	-0.437703000
H	-1.995024000	0.798051000	-1.182303000
C	-0.166088000	-0.352146000	-0.701573000
H	0.230933000	-0.327517000	-1.715276000
C	-1.024681000	-1.639919000	-0.451868000
H	-1.405870000	-2.022225000	-1.402088000
C	-0.246066000	-2.699377000	0.258807000
C	0.992521000	-2.486103000	0.787978000
H	1.533120000	-3.305564000	1.250607000
C	0.979115000	-0.118072000	0.316257000
H	1.731417000	0.529221000	-0.142233000
C	0.408563000	0.809005000	1.556287000
H	1.074706000	0.786951000	2.415980000
C	-0.890798000	0.163231000	1.809718000
C	-2.264117000	-1.147417000	0.407392000
H	-2.433527000	-1.779761000	1.280741000
C	-3.560404000	-1.075407000	-0.384704000
O	-4.203034000	0.068408000	-0.214009000
C	-5.456850000	0.204250000	-0.929651000

H	-6.135963000	-0.572285000	-0.570126000
H	-5.262049000	0.030878000	-1.990527000
C	-5.973258000	1.596946000	-0.657339000
H	-6.918816000	1.741983000	-1.183430000
H	-6.143564000	1.743889000	0.410984000
H	-5.261142000	2.346681000	-1.008814000
C	-0.826553000	-3.996307000	0.364766000
C	3.004832000	-1.161553000	1.276975000
H	3.309877000	-2.140583000	1.653003000
H	3.009243000	-0.468383000	2.125218000
C	3.954596000	-0.676178000	0.205142000
C	4.166466000	-1.448026000	-0.941143000
H	3.651410000	-2.399112000	-1.051491000
C	5.031477000	-1.003666000	-1.934537000
H	5.194876000	-1.609274000	-2.819829000
C	5.690962000	0.218253000	-1.791767000
H	6.366282000	0.563849000	-2.567473000
C	5.479604000	0.993003000	-0.655505000
H	5.986317000	1.945644000	-0.542393000
C	4.609950000	0.547015000	0.339656000
H	4.439359000	1.152746000	1.226036000
N	-1.732038000	0.159720000	0.813722000
N	-1.338611000	-5.035098000	0.441130000
N	1.635899000	-1.302994000	0.767046000
O	-3.925201000	-2.000822000	-1.066485000
H	-1.086023000	-0.487145000	2.658586000

TS3_F

C	0.044780000	2.120839000	0.138058000
C	0.295703000	3.474824000	0.317627000
H	0.844217000	3.825630000	1.186176000
C	-0.174932000	4.371900000	-0.642440000
H	0.011804000	5.433315000	-0.520161000
C	-0.883373000	3.918197000	-1.755893000
H	-1.244959000	4.629602000	-2.490136000
C	-1.137165000	2.557754000	-1.927879000
H	-1.700132000	2.200410000	-2.784397000
C	-0.662971000	1.666077000	-0.973641000
C	-0.893052000	0.189752000	-0.965384000
H	-1.574114000	-0.131252000	-1.755286000
C	0.374344000	-0.703042000	-0.884140000
H	0.900956000	-0.791678000	-1.833819000
C	-0.234011000	-2.074130000	-0.449117000
H	-0.448231000	-2.672031000	-1.339058000
C	0.678599000	-2.828001000	0.468495000
C	1.738002000	-2.239007000	1.086382000
H	2.387753000	-2.825223000	1.728767000
C	1.295175000	-0.021739000	0.168349000
H	1.998433000	0.623192000	-0.367123000
C	0.432278000	1.001528000	1.062368000

H	0.978788000	1.321222000	1.948937000
C	-0.789314000	0.208799000	1.395404000
H	-0.870145000	-0.343475000	2.325778000
C	-1.604512000	-1.697876000	0.236528000
H	-1.705784000	-2.153105000	1.224290000
C	-2.819592000	-2.107411000	-0.583041000
O	-3.733729000	-1.149522000	-0.646811000
C	-4.940694000	-1.466331000	-1.379740000
H	-5.410319000	-2.331059000	-0.904873000
H	-4.658897000	-1.742135000	-2.398808000
C	-5.816508000	-0.236179000	-1.335884000
H	-6.743071000	-0.427384000	-1.880761000
H	-6.066366000	0.021518000	-0.304206000
H	-5.309366000	0.613156000	-1.799283000
C	0.406376000	-4.202495000	0.714777000
C	3.327279000	-0.428443000	1.518017000
H	3.721135000	-1.195742000	2.190076000
H	3.118795000	0.454780000	2.131551000
C	4.347756000	-0.079338000	0.452402000
C	4.525180000	-0.901296000	-0.663478000
H	3.906961000	-1.787294000	-0.785704000
C	5.485505000	-0.586647000	-1.620577000
H	5.616032000	-1.229895000	-2.484639000
C	6.277555000	0.551016000	-1.470264000
H	7.025214000	0.795512000	-2.217544000
C	6.101166000	1.375561000	-0.362190000
H	6.708382000	2.266953000	-0.243613000
C	5.134927000	1.063588000	0.592006000
H	4.991156000	1.712741000	1.451616000
C	-3.062544000	2.145309000	1.336894000
H	-3.308988000	1.301317000	0.684265000
H	-2.649024000	2.948711000	0.716851000
C	-4.281169000	2.601292000	2.116066000
H	-5.061991000	2.923225000	1.422578000
H	-4.670763000	1.783069000	2.725305000
H	-4.036836000	3.441799000	2.770523000
N	-1.457787000	-0.244122000	0.350863000
N	0.148699000	-5.320104000	0.897057000
N	2.078213000	-0.939134000	0.958807000
O	-2.911626000	-3.202188000	-1.081999000
O	-2.048829000	1.653051000	2.228882000
H	-1.569760000	2.399907000	2.616818000

4a

C	0.275420000	2.338398000	-0.079895000
C	0.692750000	3.655518000	0.081439000
H	1.197693000	3.965171000	0.991244000
C	0.458298000	4.563406000	-0.952007000
H	0.781049000	5.593327000	-0.844986000
C	-0.186190000	4.157137000	-2.120440000

H	-0.361498000	4.874595000	-2.914732000
C	-0.615008000	2.838592000	-2.274143000
H	-1.125075000	2.522540000	-3.178764000
C	-0.379384000	1.932844000	-1.247173000
C	-0.774080000	0.488088000	-1.232491000
H	-1.364197000	0.212578000	-2.109842000
C	0.400361000	-0.501602000	-1.018168000
H	1.017548000	-0.640328000	-1.906005000
C	-0.360542000	-1.804389000	-0.664601000
H	-0.574516000	-2.343116000	-1.591850000
C	0.410480000	-2.683367000	0.277187000
C	1.416786000	-2.190698000	1.043610000
H	1.962444000	-2.842500000	1.719444000
C	1.263325000	0.089155000	0.134022000
H	2.110275000	0.610217000	-0.324384000
C	0.454264000	1.201934000	0.891018000
H	0.950390000	1.498702000	1.816626000
C	-0.929438000	0.622610000	1.169659000
H	-0.932380000	-0.115413000	1.973241000
C	-1.709602000	-1.296665000	-0.069476000
H	-1.909095000	-1.696934000	0.927630000
C	-2.923131000	-1.616399000	-0.940041000
O	-4.043698000	-1.262538000	-0.317191000
C	-5.271087000	-1.464086000	-1.051780000
H	-5.365235000	-2.529208000	-1.278021000
H	-5.200983000	-0.918228000	-1.996045000
C	-6.398839000	-0.960970000	-0.180995000
H	-7.350189000	-1.098004000	-0.698990000
H	-6.433899000	-1.512281000	0.760941000
H	-6.272860000	0.102210000	0.036704000
C	0.052078000	-4.053550000	0.400767000
C	3.076513000	-0.532579000	1.693266000
H	3.271907000	-1.272455000	2.474959000
H	2.950641000	0.431089000	2.197698000
C	4.250472000	-0.453766000	0.733160000
C	4.344027000	-1.313378000	-0.363910000
H	3.554105000	-2.033825000	-0.560336000
C	5.444827000	-1.250621000	-1.214726000
H	5.506088000	-1.921861000	-2.065111000
C	6.463038000	-0.329902000	-0.976489000
H	7.319904000	-0.281473000	-1.640285000
C	6.372818000	0.532685000	0.113659000
H	7.157756000	1.258105000	0.301091000
C	5.268219000	0.474129000	0.959981000
H	5.195291000	1.154696000	1.804245000
C	-3.157383000	1.361159000	2.142598000
H	-3.025381000	0.663534000	2.969161000
H	-3.572618000	0.853751000	1.270389000
C	-3.903908000	2.607622000	2.541214000
H	-4.905882000	2.309321000	2.856595000
H	-3.413849000	3.112480000	3.374705000
H	-4.010524000	3.298173000	1.701538000

N	-1.579444000	0.169303000	-0.009234000
N	-0.267286000	-5.167866000	0.479878000
N	1.822504000	-0.899231000	1.043478000
O	-2.876958000	-2.098174000	-2.047222000
O	-1.760786000	1.741702000	1.787194000
H	-1.746293000	2.513938000	1.180563000

TS3c

C	1.635662000	1.841497000	0.633870000
C	2.825457000	2.441644000	1.024824000
H	3.497575000	1.941820000	1.715335000
C	3.136592000	3.696469000	0.500577000
H	4.061369000	4.183576000	0.790448000
C	2.271234000	4.330439000	-0.391823000
H	2.528031000	5.307345000	-0.786750000
C	1.076499000	3.722190000	-0.777291000
H	0.398642000	4.214948000	-1.467000000
C	0.769414000	2.470991000	-0.258452000
C	-0.455975000	1.664934000	-0.554604000
H	-1.204078000	2.232866000	-1.109140000
C	-0.196010000	0.282393000	-1.173821000
H	0.052186000	0.314798000	-2.234336000
C	-1.561379000	-0.419604000	-0.955848000
H	-2.184006000	-0.250915000	-1.839047000
C	-1.392082000	-1.900226000	-0.773032000
C	-0.164953000	-2.451644000	-0.514287000
H	-0.063161000	-3.530559000	-0.441077000
C	0.992758000	-0.304062000	-0.371706000
H	1.908105000	-0.042292000	-0.907965000
C	1.142671000	0.468445000	1.020613000
H	1.800795000	-0.042489000	1.722501000
C	-0.231973000	0.650024000	1.597011000
C	-2.224178000	0.375879000	0.258703000
H	-2.577586000	-0.284051000	1.049792000
C	-3.414022000	1.207041000	-0.198138000
O	-4.368240000	0.388564000	-0.624076000
C	-5.570539000	1.011712000	-1.132180000
H	-5.289090000	1.683559000	-1.946733000
H	-6.011972000	1.608063000	-0.329949000
C	-6.482861000	-0.100852000	-1.592817000
H	-7.404672000	0.325085000	-1.993822000
H	-6.002176000	-0.691845000	-2.375346000
H	-6.737023000	-0.760119000	-0.760352000
C	-2.508102000	-2.751822000	-1.020492000
C	2.135151000	-2.425772000	0.278556000
H	2.044547000	-3.487784000	0.036733000
H	2.105239000	-2.332409000	1.371469000
C	3.432157000	-1.871569000	-0.259683000
C	3.733059000	-1.994818000	-1.619663000
H	3.034584000	-2.505693000	-2.277658000

C	4.911889000	-1.460643000	-2.127657000
H	5.139660000	-1.560704000	-3.183711000
C	5.801915000	-0.798779000	-1.280214000
H	6.721341000	-0.382168000	-1.677939000
C	5.508471000	-0.674063000	0.074099000
H	6.196718000	-0.160713000	0.737367000
C	4.323983000	-1.207867000	0.581727000
H	4.097774000	-1.114347000	1.641278000
N	-1.114543000	1.221138000	0.719292000
N	-3.446200000	-3.407361000	-1.214222000
N	0.962004000	-1.750504000	-0.296693000
O	-3.475028000	2.411328000	-0.189157000
O	-0.554601000	-1.227229000	1.992967000
C	-0.930908000	-1.509338000	3.361626000
H	-1.056585000	-1.783195000	1.363036000
H	-0.281560000	-0.881649000	3.976262000
H	-0.663684000	-2.550874000	3.551239000
C	-2.398186000	-1.243014000	3.622626000
H	-2.630742000	-1.490083000	4.660674000
H	-2.652842000	-0.191217000	3.463596000
H	-3.029495000	-1.865118000	2.981010000
H	-0.418234000	0.774430000	2.658440000

4c

C	0.505581000	2.238004000	1.073954000
C	1.161391000	3.245015000	1.768787000
H	1.716108000	3.020494000	2.674453000
C	1.097264000	4.547945000	1.272801000
H	1.603857000	5.348668000	1.800885000
C	0.390331000	4.828485000	0.103706000
H	0.350486000	5.846100000	-0.269722000
C	-0.270400000	3.812121000	-0.587358000
H	-0.827775000	4.029016000	-1.493435000
C	-0.205919000	2.515581000	-0.093618000
C	-0.874328000	1.307799000	-0.678791000
H	-1.491688000	1.570738000	-1.539153000
C	0.077131000	0.127551000	-1.026943000
H	0.597256000	0.249864000	-1.977088000
C	-0.901949000	-1.078262000	-1.080047000
H	-1.128793000	-1.311068000	-2.123482000
C	-0.337997000	-2.322209000	-0.415028000
C	0.931748000	-2.352104000	0.126448000
H	1.384183000	-3.297763000	0.413687000
C	1.110295000	0.073440000	0.127048000
H	1.970201000	0.683326000	-0.162098000
C	0.496710000	0.765384000	1.391776000
H	1.060804000	0.537496000	2.300234000
C	-0.981069000	0.384477000	1.560032000
C	-2.191862000	-0.547865000	-0.382738000
H	-2.658578000	-1.267472000	0.291924000
C	-3.276256000	-0.146139000	-1.382322000

O	-4.411281000	0.136961000	-0.757598000
C	-5.509978000	0.550692000	-1.599933000
H	-5.708589000	-0.245505000	-2.321817000
H	-5.203386000	1.443516000	-2.150916000
C	-6.691785000	0.812799000	-0.695737000
H	-7.547266000	1.129141000	-1.295948000
H	-6.966755000	-0.091608000	-0.149078000
H	-6.460227000	1.602225000	0.022277000
C	-1.005379000	-3.563954000	-0.648006000
C	3.016945000	-1.331525000	0.896112000
H	3.202274000	-2.368288000	1.188776000
H	3.098324000	-0.715282000	1.797619000
C	4.018052000	-0.868282000	-0.140829000
C	4.005468000	-1.417528000	-1.426015000
H	3.268420000	-2.173787000	-1.684873000
C	4.931138000	-0.998844000	-2.375711000
H	4.916206000	-1.430579000	-3.370965000
C	5.877107000	-0.026765000	-2.048920000
H	6.598438000	0.299451000	-2.790823000
C	5.890433000	0.526628000	-0.772051000
H	6.619376000	1.287894000	-0.514851000
C	4.959147000	0.109633000	0.178136000
H	4.963845000	0.546817000	1.172939000
N	-1.763458000	0.662363000	0.342224000
N	-1.588677000	-4.549426000	-0.833619000
N	1.640572000	-1.256993000	0.394245000
O	-3.118223000	-0.090039000	-2.580191000
O	-1.114079000	-1.055650000	1.926159000
C	-0.658585000	-1.479874000	3.273757000
H	-0.792976000	-1.709606000	1.193631000
H	-0.927869000	-0.654474000	3.931725000
H	0.426451000	-1.588202000	3.228818000
C	-1.374857000	-2.761294000	3.617341000
H	-1.061933000	-3.066648000	4.617907000
H	-2.454830000	-2.610380000	3.617308000
H	-1.117004000	-3.564388000	2.923539000
H	-1.429209000	0.873052000	2.426509000

TS1_R^{EDG}

C	-1.544190000	-1.955525000	0.918010000
C	-2.880425000	-2.392405000	0.994642000
H	-3.511457000	-1.964774000	1.767428000
C	-3.358059000	-3.341664000	0.117289000
H	-4.388261000	-3.676739000	0.179370000
C	-2.502236000	-3.885889000	-0.866426000
H	-2.883879000	-4.630475000	-1.557621000
C	-1.188983000	-3.487043000	-0.948495000
H	-0.526722000	-3.912435000	-1.696822000
C	-0.677320000	-2.515517000	-0.048324000
C	0.676547000	-2.111460000	-0.119490000

H	1.374574000	-2.510119000	-0.839157000
C	0.650715000	0.660493000	-1.375610000
H	0.650717000	-0.089054000	-2.155435000
C	1.850633000	1.189684000	-0.879337000
H	2.799636000	0.977732000	-1.354992000
C	1.753753000	2.242572000	0.060955000
C	0.524951000	2.631339000	0.547362000
H	0.412180000	3.412199000	1.289681000
C	-0.545872000	1.053031000	-0.818074000
H	-1.494452000	0.622470000	-1.114535000
C	-1.033911000	-0.930871000	1.832254000
C	0.340946000	-0.639709000	1.703563000
C	2.471123000	-0.736505000	0.698590000
H	2.776300000	-0.127789000	1.534694000
C	3.442795000	-1.149753000	-0.246006000
O	4.620596000	-0.499520000	-0.003356000
C	5.669076000	-0.741430000	-0.944874000
H	5.315580000	-0.504316000	-1.953261000
H	5.935064000	-1.803236000	-0.929908000
C	6.836458000	0.133864000	-0.541874000
H	7.666375000	-0.004051000	-1.238411000
H	6.544313000	1.186807000	-0.551105000
H	7.180062000	-0.121661000	0.463128000
C	2.945359000	2.870476000	0.557745000
C	-1.880176000	2.367842000	0.825844000
H	-1.843326000	3.441642000	1.018371000
H	-1.847022000	1.812854000	1.769093000
C	-3.101141000	1.990008000	0.036369000
C	-3.511256000	2.749014000	-1.063621000
H	-2.956277000	3.640975000	-1.342767000
C	-4.626268000	2.358736000	-1.797972000
H	-4.946483000	2.949419000	-2.649762000
C	-5.332502000	1.209581000	-1.438489000
H	-6.200344000	0.906931000	-2.015413000
C	-4.925384000	0.453451000	-0.342353000
H	-5.470111000	-0.443217000	-0.063539000
C	-3.810814000	0.844051000	0.397711000
H	-3.468311000	0.270920000	1.256831000
N	1.163304000	-1.223152000	0.763892000
N	3.921924000	3.351565000	0.948946000
N	-0.603203000	2.033799000	0.114528000
O	3.316910000	-1.890998000	-1.222813000
H	0.809881000	0.083048000	2.357836000
O	-1.783147000	-0.340838000	2.660971000

TS1s^{EDG}

C	-0.872572000	-2.216889000	0.769751000
C	-2.172781000	-2.754771000	0.714418000

H	-2.789842000	-2.677544000	1.604738000
C	-2.631381000	-3.358213000	-0.437172000
H	-3.633315000	-3.773096000	-0.478102000
C	-1.792757000	-3.437319000	-1.572544000
H	-2.161028000	-3.906257000	-2.479287000
C	-0.516038000	-2.928238000	-1.537386000
H	0.128127000	-2.986209000	-2.410061000
C	-0.022030000	-2.310139000	-0.357621000
C	1.268937000	-1.736809000	-0.331353000
H	1.930904000	-1.727704000	-1.182993000
C	0.587817000	1.183405000	-0.613385000
C	1.548075000	1.712276000	0.283884000
H	2.510638000	2.055171000	-0.071863000
C	1.074999000	2.076050000	1.560684000
C	-0.233368000	1.860289000	1.911249000
H	-0.627893000	2.121659000	2.884772000
C	-0.713248000	0.958798000	-0.193678000
H	-1.463236000	0.531052000	-0.849815000
C	-0.389600000	-1.555442000	1.983753000
C	0.941859000	-1.093717000	1.926079000
C	2.874523000	-0.360440000	0.818206000
H	3.169500000	-0.011456000	1.794911000
C	3.819303000	-0.282696000	-0.246662000
O	4.848584000	0.534215000	0.116974000
C	5.843864000	0.753759000	-0.887957000
H	5.370091000	1.175366000	-1.779731000
H	6.288572000	-0.205005000	-1.171887000
C	6.872994000	1.695640000	-0.301512000
H	7.657498000	1.893142000	-1.035302000
H	6.410709000	2.645779000	-0.023798000
H	7.332128000	1.258645000	0.588197000
C	-2.518150000	1.026638000	1.472260000
H	-2.688687000	1.655338000	2.347822000
H	-2.540485000	-0.018762000	1.791800000
C	-3.517895000	1.326946000	0.388019000
C	-3.804649000	2.651684000	0.044449000
H	-3.310177000	3.463110000	0.572320000
C	-4.718609000	2.929313000	-0.965583000
H	-4.940188000	3.958784000	-1.226424000
C	-5.353305000	1.884641000	-1.638980000
H	-6.067668000	2.102738000	-2.425972000
C	-5.070392000	0.564430000	-1.301425000
H	-5.560962000	-0.249920000	-1.824007000
C	-4.152410000	0.285524000	-0.289708000
H	-3.921868000	-0.744006000	-0.027550000
N	1.715007000	-1.136555000	0.790053000
N	-1.118091000	1.314688000	1.035174000
O	3.765018000	-0.775338000	-1.371381000
H	1.379346000	-0.592474000	2.777464000
O	-1.128863000	-1.366182000	2.986531000
C	0.918073000	0.877108000	-1.977152000
N	1.157812000	0.656865000	-3.087867000

H	1.739276000	2.534131000	2.282450000
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A_R^{EDG}

C	-3.975065000	1.998991000	0.452252000
C	-4.939759000	3.025976000	0.452645000
H	-5.075178000	3.589937000	1.369098000
C	-5.675537000	3.290900000	-0.679526000
H	-6.417748000	4.082342000	-0.677041000
C	-5.469390000	2.532522000	-1.855962000
H	-6.055144000	2.749207000	-2.743121000
C	-4.535532000	1.526526000	-1.881811000
H	-4.373237000	0.941442000	-2.781904000
C	-3.766013000	1.239419000	-0.722946000
C	-2.795487000	0.213342000	-0.733736000
H	-2.609199000	-0.412197000	-1.593807000
C	0.563816000	0.816763000	-0.295758000
H	-0.067688000	1.651588000	-0.576586000
C	0.114391000	-0.579964000	-0.639888000
H	-0.315393000	-0.609579000	-1.648582000
C	1.308679000	-1.508865000	-0.554622000
C	2.417042000	-1.184048000	0.162839000
H	3.238761000	-1.883090000	0.278999000
C	1.685435000	1.049831000	0.392588000
H	1.992214000	2.046301000	0.689723000
C	-3.196333000	1.726390000	1.664405000
C	-2.249457000	0.670946000	1.530513000
C	-1.014266000	-1.034966000	0.345655000
H	-0.593820000	-1.088085000	1.348974000
C	-1.525452000	-2.417123000	-0.044175000
O	-0.953092000	-3.343363000	0.712332000
C	-1.205264000	-4.717118000	0.334941000
H	-1.054782000	-4.805094000	-0.743106000
H	-2.248650000	-4.945653000	0.567379000
C	-0.234719000	-5.573561000	1.113054000
H	-0.402393000	-6.625401000	0.872393000
H	0.791857000	-5.314062000	0.844587000
H	-0.368381000	-5.437248000	2.188310000
C	1.253997000	-2.777986000	-1.197864000
C	3.839765000	0.396390000	1.382008000
H	4.314200000	-0.530743000	1.715702000
H	3.612394000	0.976969000	2.280772000
C	4.779288000	1.177762000	0.482571000
C	4.684085000	1.116018000	-0.908056000
H	3.900003000	0.526512000	-1.375539000
C	5.585833000	1.819101000	-1.705340000
H	5.500635000	1.766962000	-2.785859000
C	6.588853000	2.586843000	-1.120170000
H	7.288766000	3.135090000	-1.742051000
C	6.685532000	2.653723000	0.269081000
H	7.459895000	3.255936000	0.733034000

C	5.782338000	1.956185000	1.064913000
H	5.854057000	2.016324000	2.147812000
N	-2.094737000	-0.030175000	0.375918000
N	1.173493000	-3.803995000	-1.737073000
N	2.582131000	0.034754000	0.737227000
O	-2.278221000	-2.639228000	-0.963177000
H	-1.616026000	0.392238000	2.360093000
O	-3.346442000	2.369120000	2.724915000

A_S^{EDG}

C	3.779932000	-1.702971000	0.558967000
C	4.779035000	-2.689081000	0.676471000
H	4.886904000	-3.185900000	1.634662000
C	5.581848000	-2.999012000	-0.397485000
H	6.350722000	-3.758889000	-0.304650000
C	5.409899000	-2.328561000	-1.631150000
H	6.047711000	-2.580563000	-2.471879000
C	4.442912000	-1.363917000	-1.771839000
H	4.305936000	-0.847459000	-2.717022000
C	3.605582000	-1.031496000	-0.674577000
C	2.599923000	-0.049101000	-0.796098000
H	2.409195000	0.491554000	-1.714726000
C	-0.864387000	-0.755975000	-0.232966000
C	-0.402864000	0.576473000	-0.792622000
H	0.003680000	0.449442000	-1.802379000
C	-1.581677000	1.518758000	-0.822757000
C	-2.649499000	1.333017000	-0.040446000
H	-3.481376000	2.028039000	-0.012061000
C	-1.971890000	-0.853210000	0.547146000
H	-2.259693000	-1.792853000	1.007603000
C	2.934733000	-1.380149000	1.713594000
C	1.962099000	-0.365338000	1.469099000
C	0.721604000	1.191010000	0.075901000
H	0.334001000	1.425497000	1.068698000
C	1.280888000	2.471378000	-0.545475000
O	2.023308000	3.137387000	0.326201000
C	2.661002000	4.337104000	-0.170874000
H	1.881685000	5.018373000	-0.521124000
H	3.286632000	4.062341000	-1.023939000
C	3.465107000	4.919238000	0.967806000
H	3.965402000	5.829659000	0.631722000
H	2.816260000	5.169819000	1.809497000
H	4.223632000	4.210162000	1.305487000
C	-4.064284000	0.011061000	1.475357000
H	-4.276923000	0.923202000	2.040641000
H	-3.910939000	-0.784548000	2.209964000
C	-5.237359000	-0.325268000	0.572488000
C	-5.060074000	-0.743517000	-0.746191000
H	-4.061524000	-0.809467000	-1.169214000
C	-6.164100000	-1.070035000	-1.533607000

H	-6.014651000	-1.391748000	-2.559150000
C	-7.450164000	-0.982978000	-1.009869000
H	-8.307825000	-1.236340000	-1.624211000
C	-7.631870000	-0.562996000	0.307794000
H	-8.631853000	-0.487304000	0.722417000
C	-6.531628000	-0.233301000	1.091686000
H	-6.675358000	0.099702000	2.116461000
N	1.836554000	0.235578000	0.261647000
N	-2.806711000	0.199657000	0.762969000
O	1.085024000	2.803096000	-1.691211000
H	1.281075000	-0.049593000	2.246420000
O	3.055000000	-1.944145000	2.819752000
C	-0.099638000	-1.931437000	-0.488802000
N	0.536002000	-2.875775000	-0.718826000
H	-1.531035000	2.391763000	-1.460993000

TSc^{EDG}

C	-0.828499000	3.166870000	0.403521000
C	-0.705779000	4.561296000	0.343053000
H	0.196158000	5.015324000	0.739192000
C	-1.718950000	5.319541000	-0.215852000
H	-1.629396000	6.399857000	-0.261286000
C	-2.866962000	4.694480000	-0.730995000
H	-3.657133000	5.295117000	-1.168926000
C	-2.997780000	3.318417000	-0.678880000
H	-3.884637000	2.831857000	-1.074092000
C	-1.979777000	2.540915000	-0.100885000
C	-2.060302000	1.095131000	-0.068273000
H	-3.022691000	0.639301000	-0.278755000
C	-0.953715000	0.289666000	-1.566588000
H	-1.614664000	0.645723000	-2.349226000
C	-1.078196000	-1.131387000	-1.048041000
H	-1.952822000	-1.625824000	-1.475612000
C	0.161998000	-1.915801000	-1.350255000
C	1.373312000	-1.292228000	-1.405877000
H	2.304227000	-1.840362000	-1.492732000
C	0.331677000	0.842538000	-1.462736000
H	0.522104000	1.862733000	-1.779793000
C	0.253806000	2.335364000	0.965175000
C	-0.049537000	0.944999000	1.095347000
C	-1.312238000	-1.003990000	0.551677000
H	-0.504678000	-1.502949000	1.088945000
C	-2.619476000	-1.663693000	0.946388000
O	-2.520148000	-2.972346000	0.727259000
C	-3.700899000	-3.759936000	0.991714000
H	-4.525795000	-3.353542000	0.400908000
H	-3.953837000	-3.657254000	2.050074000
C	-3.373461000	-5.186412000	0.615038000
H	-4.242290000	-5.822353000	0.796331000
H	-3.105970000	-5.252162000	-0.441746000

H	-2.537941000	-5.559473000	1.211113000
C	0.087544000	-3.331662000	-1.467555000
C	2.789263000	0.721495000	-1.323513000
H	2.597428000	1.758823000	-1.041914000
H	3.223723000	0.704355000	-2.328493000
C	3.729468000	0.088698000	-0.326426000
C	4.697134000	-0.826542000	-0.744698000
H	4.791532000	-1.064666000	-1.801455000
C	5.544407000	-1.429918000	0.183150000
H	6.293712000	-2.140061000	-0.150880000
C	5.429969000	-1.115791000	1.534834000
H	6.089665000	-1.583301000	2.258665000
C	4.473992000	-0.191088000	1.955358000
H	4.394775000	0.065788000	3.006943000
C	3.627101000	0.413115000	1.030200000
H	2.897023000	1.157858000	1.344475000
N	-1.286556000	0.415934000	0.840341000
N	-0.002256000	-4.486047000	-1.561608000
N	1.468954000	0.057748000	-1.364377000
O	-3.606251000	-1.105891000	1.362518000
H	0.672072000	0.286217000	1.564830000
O	1.359377000	2.818372000	1.289427000

10a

C	0.820206000	2.457804000	0.272935000
C	1.682822000	3.551312000	0.362362000
H	2.227697000	3.711440000	1.287194000
C	1.836093000	4.398492000	-0.727071000
H	2.504551000	5.250386000	-0.667351000
C	1.127746000	4.146248000	-1.903805000
H	1.245346000	4.807215000	-2.756240000
C	0.262254000	3.058499000	-1.992374000
H	-0.296894000	2.879059000	-2.905875000
C	0.099252000	2.203284000	-0.904509000
C	-0.852665000	1.035798000	-0.965200000
H	-1.680093000	1.259642000	-1.643697000
C	-0.250221000	-0.362034000	-1.266135000
H	0.239766000	-0.491635000	-2.230580000
C	-1.481140000	-1.260641000	-1.043307000
H	-2.120122000	-1.245326000	-1.929348000
C	-1.084924000	-2.667085000	-0.688628000
C	0.071320000	-2.898183000	-0.007206000
H	0.351096000	-3.898576000	0.308680000
C	0.673751000	-0.546290000	-0.054015000
H	1.639845000	-0.068862000	-0.243933000
C	0.700354000	1.491455000	1.395464000
C	-0.126563000	0.269069000	1.051085000
C	-2.199622000	-0.492277000	0.123633000
H	-2.272606000	-1.089301000	1.035130000
C	-3.591938000	-0.009552000	-0.252944000

O	-4.355571000	0.154021000	0.823713000
C	-5.678738000	0.676678000	0.584823000
H	-6.199828000	0.000888000	-0.098409000
H	-5.583475000	1.648967000	0.094131000
C	-6.369218000	0.778315000	1.925409000
H	-7.379009000	1.170672000	1.788605000
H	-6.439411000	-0.203707000	2.397929000
H	-5.822602000	1.450310000	2.590355000
C	-1.934390000	-3.756570000	-1.013106000
C	2.032850000	-2.136414000	1.259495000
H	2.092688000	-3.211334000	1.448366000
H	1.784266000	-1.646064000	2.210720000
C	3.354933000	-1.610309000	0.748577000
C	3.968193000	-2.214054000	-0.352612000
H	3.494647000	-3.071533000	-0.824217000
C	5.173029000	-1.721719000	-0.842277000
H	5.646420000	-2.198587000	-1.694380000
C	5.773400000	-0.616427000	-0.237242000
H	6.713315000	-0.232399000	-0.620102000
C	5.163410000	-0.006017000	0.854718000
H	5.623184000	0.857602000	1.324004000
C	3.955496000	-0.501830000	1.345513000
H	3.469276000	-0.019930000	2.190322000
N	-1.373937000	0.709801000	0.389356000
N	-2.648130000	-4.631519000	-1.290346000
N	0.948872000	-1.919421000	0.301423000
O	-3.953396000	0.233283000	-1.383323000
H	-0.331005000	-0.315135000	1.950938000
O	1.290364000	1.605056000	2.452513000