

Supporting Information

A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of *Pseudo(mono)radical* Azomethyne Ylides with Phenyl Vinyl Sulphone

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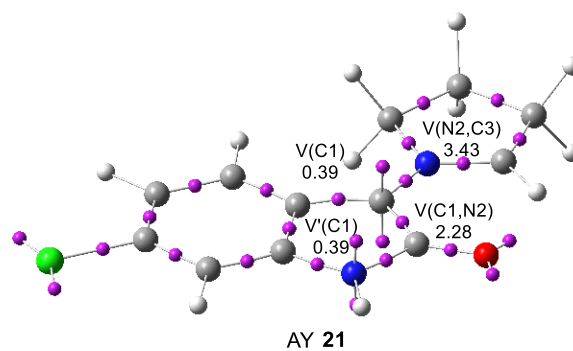


Figure S1. ω B97X-D/6-311G(d,p) ELF basin attractor positions together with the most relevant valence basin populations of AY 21. Valence basin populations are given in average number of electrons, e.

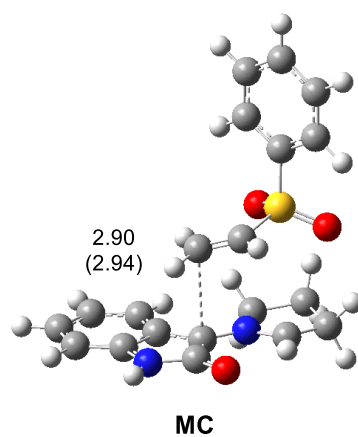


Figure S2. ω B97X-D/6-311G(d,p) geometries of **MC**. The distance between the two frameworks is given in angstroms, Å. The distance in methanol is given in parentheses.

Table S1. ω B97X-D/6-311G(d,p) total electronic energies, in a.u., of the stationary points involved in the 32CA reaction of AY **22** with phenyl vinyl sulphone **20**, in gas phase and in methanol.

	gas phase	methanol
AY 22	-649.158324	-649.174596
20	-858.175486	-858.188771
MC	-1507.360219	-1507.379157
TS-on	-1507.345933	-1507.367662
TS-ox	-1507.335137	-1507.361476
TS-mn	-1507.349936	-1507.368977
TS-mx	-1507.338739	-1507.364747
26	-1507.416376	-1507.437909
27	-1507.416284	-1507.437853
24	-1507.418708	-1507.438884
25	-1507.422023	-1507.445182

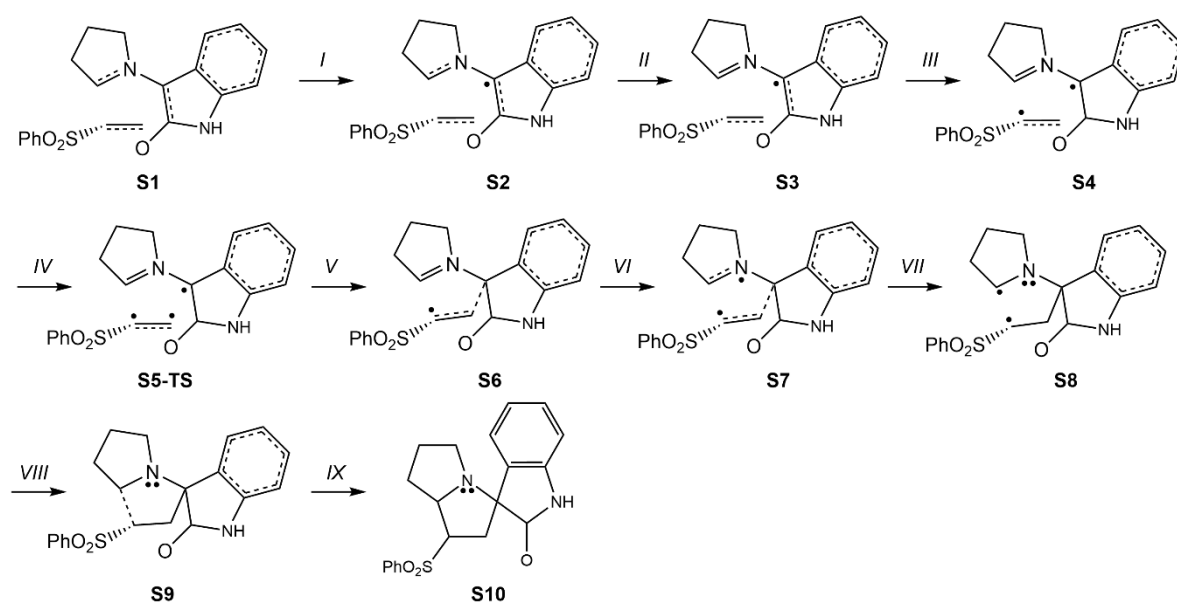
Table S2. ω B97X-D/6-311G(d,p) total enthalpies (H, in a.u.), entropies (S, in cal·mol⁻¹K⁻¹) and Gibbs free energies (G, in a.u.), computed at 65 °C in methanol, of the stationary points involved in the 32CA reaction of AY **22** with phenyl vinyl sulphone **20**.

	H	S	G
AY 22	-648.937122	110.4	-648.996582
20	-858.030742	104.2	-858.086842
MC	-1506.980046	181.8	-1507.077931
TS-on	-1506.969563	167.9	-1507.059964
TS-ox	-1506.963476	170.6	-1507.055326
TS-mn	-1506.970888	170.3	-1507.062566
TS-mx	-1506.966761	171.7	-1507.059178
26	-1507.035436	163.5	-1507.123440
27	-1507.035989	164.0	-1507.124286
24	-1507.036811	165.9	-1507.126138
25	-1507.043100	166.1	-1507.132528

Table S3. Most relevant ELF valence basins and their total populations, C–C bond formation distances, IRC values and relative energies, for the structures of the IRC in which there is a relevant chemical change along the *meta/endo* path of the *pmr-type* 32CA reaction between AY **22** with phenyl vinyl sulphone **20**. Distances are given in angstroms, Å, IRC values in a.u, and relative energies with respect to **S1** are given in kcal·mol⁻¹.

Structures	S1	S2	S3	S4	S5-TS	S6	S7	S8	S9	S10
Phases	<i>I</i>	<i>II</i>	<i>III</i>	<i>IV</i>	<i>IV</i>	<i>VI</i>	<i>VII</i>	<i>VIII</i>	<i>IX</i>	
d(C1-C4)	2.842	2.789	2.316	2.176	2.103	2.018	1.982	1.68	1.63	1.544
d(C3-C5)	3.272	3.144	2.736	2.667	2.635	2.597	2.581	2.34	2.156	1.579
IRC	-8.93	-6.19	-1.17	-0.39	0.00	0.46	0.65	2.67	3.72	22.08
ΔE	0.0	0.4	4.6	5.7	5.8	5.5	5.2	-2.1	-7.3	-38.7
V(C1,N2)	2.26	2.26	2.24	2.20	2.16	2.11	2.09	1.88	1.84	1.72
V(N2)							0.81	1.51	1.76	2.24
V(N2,C3)	3.42	3.42	3.48	3.56	3.61	3.67	2.90	2.38	2.15	1.72
V(C1,C)	2.43	2.43	2.40	2.33	2.3	2.25	2.24	2.12	2.11	2.09
V(C1,CO)	3.35	2.95	2.58	2.46	2.39	2.34	2.31	2.17	2.15	2.14
V(C4,C5)	3.43*	3.43*	3.43	3.09	2.88	2.72	2.66	2.17	2.08	1.90
V(C1)		0.38	0.62	0.74	0.80					
V(C3)								0.20		
V(C4)					0.16					
V(C5)				0.41	0.52	0.64	0.69	1.02		
V(C1,C4)						1.13	1.20	1.65	1.72	1.89
V(C3,C5)									1.43	1.91

Superscript * refers to the sum of the populations of two V(X,X) and V'(X,X) valence basins in the X–X region.



Scheme S1. Representation of the molecular mechanism of the *pmr*-type 32CA reaction between AY **22** with phenyl vinyl sulphone **20** by Lewis-like structures based on the topological analysis of the ELF along the *meta/endo* reaction path.

ω B97X-D/6-311G(d,p) gas phase Cartesian coordinates of the stationary points involved in the *pmr*-type 32CA reaction between AY **22** with phenyl vinyl sulphone **20**.

20

C	2.66802300	-1.28919100	1.18466500
C	1.89364100	-0.21858600	1.16918600
H	2.88235200	-1.82834600	0.26790000
H	3.11263900	-1.64074400	2.10852900
H	1.63827300	0.38583900	2.03174700
S	1.21632200	0.38166500	-0.36532600
O	1.44387700	1.81638100	-0.40014600
O	1.67695200	-0.49030700	-1.43287700
C	-0.53699700	0.11056300	-0.14449900
C	-1.31801600	1.13585900	0.37215700
C	-1.07759000	-1.12444400	-0.48093600
C	-2.67621800	0.91281000	0.55967500
H	-0.86685500	2.09460400	0.59757300
C	-2.43564200	-1.33451400	-0.28892400
H	-0.44277500	-1.89388000	-0.90336000
C	-3.23089200	-0.31920000	0.23305900
H	-3.30209400	1.70424700	0.95451400
H	-2.87552300	-2.28888000	-0.55295900
H	-4.29164400	-0.48785800	0.37915400

22

C	2.64007400	0.65288100	-0.00008300
N	1.54138900	-0.05293600	0.00000700
C	0.24976800	0.40978200	-0.00004100
C	-0.99404100	-0.31965900	0.00001200
C	-2.00987600	0.67311600	-0.00006300
C	-3.35584300	0.35657000	-0.00004600
C	-3.72114800	-0.98726500	0.00004500
C	-2.74692200	-1.97953100	0.00011500
C	-1.39188900	-1.65882100	0.00009900
C	-0.02548200	1.82306200	-0.00016100
H	-4.10672100	1.13908900	-0.00010200
H	-0.66936200	-2.46465600	0.00014800
C	1.81148300	-1.50630700	0.00014800
H	2.56241100	1.73141100	-0.00022000
H	1.34084600	-1.93533600	-0.88490700
N	-1.41228800	1.91942600	-0.00014300
H	1.34061900	-1.93521700	0.88513700
O	0.74626400	2.78084000	-0.00025300
H	-1.88679100	2.80487400	-0.00028900
H	-4.77059500	-1.25749900	0.00005900
H	-3.04289300	-3.02243800	0.00018300

C	3.34087800	-1.63124100	0.00035800
C	3.87163300	-0.18090500	-0.00002900
H	3.68314100	-2.17795400	-0.87788100
H	3.68293100	-2.17738000	0.87903700
H	4.49029400	0.03622800	-0.87675200
H	4.49049600	0.03661700	0.87645300

MC

C	0.89966700	2.51748900	0.50260800
N	1.55957100	1.60838600	-0.15918200
C	2.30127700	0.57634800	0.36799900
C	-0.03739600	-1.05710100	0.86799600
C	-0.99600900	-0.18397400	1.14471600
H	0.16172500	-1.37640800	-0.14862200
C	3.04220600	-0.46204100	-0.30385500
C	3.62792100	-1.23877500	0.73004000
C	4.41825300	-2.34400400	0.47221000
C	4.64197300	-2.70235800	-0.85439600
C	4.07757200	-1.95999000	-1.88664400
C	3.28248900	-0.84775100	-1.62496900
C	2.45800200	0.42821500	1.79000400
H	4.85243700	-2.91468900	1.28591100
H	2.86726800	-0.29584700	-2.45752200
C	1.43847600	1.79049300	-1.62386900
H	0.92322200	2.49224800	1.58315100
H	1.07542800	0.85732300	-2.05206900
N	3.25736100	-0.70149500	1.94972600
H	2.43409500	2.01262700	-2.01374300
O	1.99294800	1.08871700	2.71900200
H	3.57597300	-1.00551500	2.85284100
H	5.25936100	-3.56376200	-1.08048900
H	4.25909000	-2.24812500	-2.91582500
C	0.43158300	2.93325600	-1.78770200
C	0.27955700	3.53983100	-0.38044700
H	-0.52235500	2.52708300	-2.12123400
H	0.77286900	3.66344400	-2.52098600
H	-0.76446500	3.70485400	-0.11116000
H	0.81122400	4.49295500	-0.27099200
H	0.57195700	-1.47738500	1.65836900
H	-1.24455700	0.18552800	2.13162900
S	-1.99506100	0.47693400	-0.15773200
O	-2.34099900	1.85015000	0.18972200
O	-1.34374000	0.18186400	-1.43068900
C	-3.49745900	-0.48740200	-0.08050700
C	-3.56557100	-1.69140700	-0.77036900
C	-4.55918700	-0.01868600	0.68122200
C	-4.72892900	-2.44290900	-0.68995500
H	-2.72628500	-2.01817800	-1.37205000

C	-5.71798400	-0.78099800	0.75416800
H	-4.47923900	0.93588100	1.18666800
C	-5.80038900	-1.98971300	0.07312700
H	-4.80164500	-3.38081400	-1.22733300
H	-6.55838300	-0.42703800	1.33911300
H	-6.70726900	-2.58034500	0.13170000

TS-mn

C	0.68323400	2.38446000	0.43662900
N	1.44031000	1.51645600	-0.19241200
C	1.91159600	0.35830200	0.39787600
C	0.09100700	-0.61200300	0.81068900
C	-0.87193000	0.34777600	1.05200200
H	0.08411800	-1.13399200	-0.14059200
C	2.73688300	-0.65454500	-0.26860200
C	3.53977600	-1.23811400	0.72902700
C	4.37724800	-2.30777800	0.47095300
C	4.41275100	-2.80942800	-0.82797500
C	3.61384500	-2.26110400	-1.82468100
C	2.76219100	-1.19305100	-1.54922100
C	2.40414400	0.44933800	1.79535300
H	4.98702300	-2.74190800	1.25490200
H	2.12664100	-0.80011300	-2.33229900
C	1.41822600	1.71616000	-1.65543400
H	0.65773200	2.38644200	1.51320000
H	0.74379100	0.97187500	-2.08068900
N	3.31519500	-0.57967200	1.93290400
H	2.42709900	1.58739800	-2.04695900
O	2.08305600	1.22551300	2.67463900
H	3.78944500	-0.75873200	2.80126700
H	5.06585200	-3.64294900	-1.05847500
H	3.64472000	-2.67298000	-2.82631900
C	0.86413000	3.13518100	-1.81816400
C	0.19601800	3.46364000	-0.46724500
H	0.15569600	3.18001900	-2.64361400
H	1.67423200	3.83738300	-2.02309300
H	-0.89571500	3.43590800	-0.51134100
H	0.47995300	4.44667700	-0.08253200
H	0.47333200	-1.19241900	1.64282300
H	-1.15709000	0.67608500	2.04244000
S	-2.02841900	0.74528200	-0.17560100
O	-2.65026100	2.02568100	0.15560300
O	-1.40640100	0.55570000	-1.49046800
C	-3.32554600	-0.49007000	-0.05838400
C	-3.23359300	-1.65017200	-0.81625700
C	-4.38394800	-0.27743200	0.81515100
C	-4.22069700	-2.61845700	-0.68933000
H	-2.41074700	-1.77321200	-1.50974200

C	-5.36546900	-1.25256800	0.93467700
H	-4.44230400	0.64964300	1.37247200
C	-5.28201700	-2.42210900	0.18742400
H	-4.16445100	-3.52486100	-1.28092400
H	-6.20013100	-1.09562600	1.60797100
H	-6.05128000	-3.17995300	0.28256200

TSA-mx

C	0.49583000	2.13301700	0.45731100
N	1.56870000	1.56519400	-0.07355700
C	1.98449600	0.30778600	0.28815900
C	0.06420000	-0.72169800	-0.22439200
C	-0.82798200	0.30476700	-0.42574500
H	0.55917900	-1.18096100	-1.07109000
C	3.01196900	-0.49616900	-0.37184000
C	3.50081200	-1.39111200	0.60236000
C	4.42556100	-2.37416500	0.30104400
C	4.88060800	-2.46605100	-1.01242000
C	4.40120800	-1.60551500	-1.99258500
C	3.45677700	-0.62842800	-1.68243300
C	2.03398600	-0.02927100	1.73057900
H	4.78674800	-3.05200800	1.06587000
H	3.08162300	0.01316100	-2.46960900
C	1.88305500	2.16292500	-1.37852300
H	0.18128700	1.83634200	1.44728600
H	1.40437800	1.55651700	-2.15691600
N	2.89381600	-1.11368000	1.81830700
H	2.96016700	2.15929900	-1.54003100
O	1.47908100	0.50358300	2.66715600
H	3.12072500	-1.53843400	2.70090100
H	5.61170200	-3.22324900	-1.27047400
H	4.75800800	-1.69758500	-3.01150000
C	1.27191600	3.56157000	-1.27861900
C	0.15406500	3.41610900	-0.22749300
H	0.90635100	3.91100500	-2.24384400
H	2.02771300	4.26773800	-0.92963700
H	-0.84759100	3.34126400	-0.65637200
H	0.13002200	4.24815400	0.47950800
H	-0.01773900	-1.32782900	0.67110400
H	-0.99678000	0.73941700	-1.40560000
S	-2.18564800	0.56946300	0.64889400
O	-1.84277000	0.07938300	1.97562400
O	-2.64577400	1.94230500	0.45360100
C	-3.47829400	-0.49526700	0.00362500
C	-3.54975200	-1.81212800	0.43961500
C	-4.36988900	0.00863200	-0.93330900
C	-4.53308200	-2.64111700	-0.08226800
H	-2.85626800	-2.16726200	1.19230900

C	-5.34988000	-0.83000000	-1.44958400
H	-4.30514600	1.04874400	-1.22880400
C	-5.42841800	-2.15214700	-1.02803500
H	-4.60546000	-3.66857100	0.25485700
H	-6.05751000	-0.44757400	-2.17598700
H	-6.19606200	-2.80278500	-1.43126000

TS-on

C	-1.17447500	2.72639800	0.66799400
N	-1.66548800	1.73081900	-0.08601400
C	-1.90196100	0.48936400	0.37567300
C	0.66112200	0.50773200	1.13426600
C	0.79374500	1.86799000	1.10024800
H	1.25020500	2.34005700	0.23687800
H	0.50488900	-0.06211300	2.03965300
C	-2.33524700	-0.69329100	-0.35364900
C	-2.68360900	-1.64478400	0.62559400
C	-3.09627200	-2.92335200	0.30388400
C	-3.17377700	-3.26309300	-1.04267800
C	-2.84079200	-2.34041500	-2.02815100
C	-2.41645600	-1.05921200	-1.69382300
C	-2.11615700	0.23253600	1.81498200
H	-3.34733200	-3.63903700	1.07812700
H	-2.14545900	-0.37426800	-2.48397300
C	-1.61756200	2.05346000	-1.52753100
H	-1.42296300	2.71829900	1.71825600
H	-1.06376500	1.27425400	-2.04415900
N	-2.53190800	-1.08088200	1.88400100
H	-2.64559100	2.10225200	-1.89562900
O	-1.99408400	0.97812200	2.77487600
H	-2.74688300	-1.52482300	2.75946400
H	-3.49387400	-4.25977700	-1.32338500
H	-2.90036000	-2.62380300	-3.07210400
C	-0.88232100	3.39420400	-1.58239300
C	-1.00645000	3.96266500	-0.16159200
H	0.16621900	3.21060400	-1.82374800
H	-1.29508300	4.05552800	-2.34388400
H	-0.13227300	4.54322700	0.14150900
H	-1.88137400	4.61553800	-0.05714000
H	0.85593200	2.40989800	2.03520000
S	1.13568900	-0.47026700	-0.23856900
O	0.86279900	0.28720300	-1.46272300
O	0.61714800	-1.81667900	-0.05428100
C	2.92339900	-0.58368700	-0.11597600
C	3.71690900	0.35200800	-0.76650900
C	3.48065800	-1.59879200	0.65054800
C	5.09712300	0.27144500	-0.63826500
H	3.25265900	1.11229500	-1.38252800

C	4.86211000	-1.66964600	0.77313100
H	2.83622300	-2.33077000	1.12220400
C	5.66809100	-0.73437300	0.13380000
H	5.72821000	0.99054200	-1.14751000
H	5.30986800	-2.46071800	1.36324800
H	6.74613300	-0.79460500	0.23042000

TS-ox

C	1.86218800	-2.44095500	0.19997400
N	2.31843000	-1.26140400	-0.25507500
C	1.92505300	-0.07438700	0.24790500
C	-0.46041100	-0.81035000	-0.35935100
C	-0.19524500	-2.14279000	-0.51284100
H	0.07154400	-2.51998300	-1.49498800
C	2.06473500	1.25083200	-0.32851800
C	1.86945000	2.15459800	0.73738300
C	1.82456800	3.52150200	0.53554300
C	1.99189000	4.00051900	-0.76135900
C	2.18983000	3.12741000	-1.82571800
C	2.21745800	1.75047300	-1.61840200
C	1.72148800	0.08611600	1.70332900
H	1.66209200	4.19939600	1.36511700
H	2.34415800	1.08931100	-2.46660300
C	2.88513600	-1.41231100	-1.60057300
H	1.55141500	-2.49042800	1.23328900
H	2.09269200	-1.22295300	-2.33465000
N	1.74637300	1.45242800	1.92485700
H	3.68225600	-0.68526300	-1.74936500
O	1.60820000	-0.76896600	2.55894700
H	1.34001100	1.83233900	2.76320700
H	1.96418900	5.06908200	-0.94084700
H	2.31455400	3.51932900	-2.82820000
C	3.35779200	-2.86633500	-1.61931700
C	2.47253200	-3.57513000	-0.57225500
H	3.27554500	-3.30427000	-2.61397900
H	4.40555300	-2.91455300	-1.31758700
H	1.69406700	-4.18913300	-1.03658500
H	3.05422300	-4.23683700	0.07334700
H	-0.62970800	-2.85244900	0.18205700
H	-0.34570300	-0.06911300	-1.14040500
S	-1.53182700	-0.27912300	0.93757100
O	-1.70897300	-1.37958200	1.87298600
O	-1.12458000	1.04258900	1.39614900
C	-3.08576200	-0.04906100	0.06904400
C	-3.96595100	-1.11735100	-0.04188300
C	-3.36942000	1.18903900	-0.49206000
C	-5.15636100	-0.93842300	-0.73323200
H	-3.72314900	-2.06302300	0.42764500

C	-4.56181200	1.35576000	-1.18479600
H	-2.67140600	2.00774400	-0.36443600
C	-5.45113300	0.29411700	-1.30684500
H	-5.85789000	-1.76001300	-0.81959400
H	-4.79975600	2.31812100	-1.62278500
H	-6.38239700	0.42951400	-1.84507000

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C	0.41522500	1.42677900	-0.06891400
N	-0.83967200	1.00661700	0.50421100
C	-1.71432600	0.46194600	-0.49682100
C	-0.71506900	-0.08842300	-1.55858100
C	0.69768500	0.29981400	-1.06176000
H	-0.82586100	-1.16387000	-1.69739700
H	1.33673800	0.61765600	-1.88620900
C	-2.70552200	-0.52974800	0.05590700
C	-3.99781500	-0.11067300	-0.25190300
C	-5.10898100	-0.83370500	0.14063400
C	-4.88762200	-2.00410800	0.86826900
C	-3.60236300	-2.42384100	1.19163800
C	-2.49242500	-1.67984500	0.78683400
C	-2.64697200	1.52638800	-1.14448200
H	-6.11381200	-0.50700100	-0.10088500
H	-1.47963600	-1.97926500	1.03710000
C	-1.23128600	1.93393800	1.54309600
H	0.31408700	2.34527600	-0.67634300
H	-1.78601300	1.41387000	2.32837000
N	-3.93720400	1.09739300	-0.96388800
H	-1.86169200	2.75169000	1.16069900
O	-2.30097200	2.54812200	-1.68883500
H	-4.73144000	1.63360300	-1.27158600
H	-5.73959400	-2.59280700	1.18924300
H	-3.46186200	-3.33339300	1.76328400
C	0.13467000	2.49199100	2.03012200
C	1.20659500	1.75694800	1.19110100
H	0.28629400	2.33424200	3.09845800
H	0.18214200	3.56769300	1.84712100
H	1.49637300	0.83639700	1.69536600
H	2.09526600	2.36279100	1.00791300
H	-0.89046600	0.38830800	-2.52345000
S	1.54544600	-1.18272300	-0.43328700
O	1.57567600	-2.11390300	-1.55361500
O	0.98830200	-1.60149400	0.84549500
C	3.22500200	-0.62811200	-0.14739200
C	3.72085000	-0.59855500	1.14773800
C	4.01319100	-0.27459400	-1.23643900
C	5.02990100	-0.18392000	1.35748600
H	3.08595300	-0.90800500	1.96901700

C	5.31586900	0.14873100	-1.01499100
H	3.62049700	-0.35120500	-2.24370200
C	5.82117200	0.19656000	0.28030300
H	5.43161600	-0.16048300	2.36350300
H	5.94079100	0.42962500	-1.85433800
H	6.84090500	0.52316100	0.44874800

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C	-0.23372300	-2.16177100	-0.05480600
N	-1.56507000	-1.64682500	0.30709900
C	-1.50453400	-0.24511900	0.70707000
C	0.00031200	0.00910500	0.91126900
C	0.62224500	-0.89252200	-0.14780900
H	0.28423200	-0.34653700	1.90616800
H	0.57249800	-0.45218900	-1.14785300
C	-2.18098500	0.76724400	-0.20184800
C	-3.21916000	1.38247400	0.50246500
C	-4.01864700	2.35547700	-0.07092600
C	-3.75496700	2.71785700	-1.39087900
C	-2.72000500	2.12682700	-2.10380600
C	-1.92689700	1.14653200	-1.50586700
C	-2.27524400	-0.04336900	2.04366200
H	-4.82112500	2.82438500	0.48655200
H	-1.12037500	0.69000200	-2.06834300
C	-2.55103600	-2.10809800	-0.66601200
H	0.16280200	-2.79339600	0.74626500
H	-3.32183500	-1.35230500	-0.82885800
N	-3.27590000	0.87145500	1.79980800
H	-3.04583600	-3.01175400	-0.29204200
O	-2.04510500	-0.57874100	3.09379000
H	-3.90972400	1.17805800	2.51867900
H	-4.36789000	3.47666100	-1.86359500
H	-2.52780700	2.42646600	-3.12686600
C	-1.74220500	-2.42683900	-1.92761400
C	-0.42619500	-2.96157200	-1.35273400
H	-1.57228500	-1.51030700	-2.50057200
H	-2.23872600	-3.14269800	-2.58505200
H	0.42989400	-2.85621700	-2.02034100
H	-0.52691300	-4.02275500	-1.11209600
H	0.26125600	1.06214800	0.80826300
S	2.37359900	-1.23972800	0.11313200
O	2.54815500	-1.74101800	1.46747400
O	2.82778700	-2.00881400	-1.03738700
C	3.11389200	0.38537300	0.02435400
C	3.31225400	1.10329700	1.19665400
C	3.44734700	0.90689400	-1.21920600
C	3.85123700	2.38056600	1.11564900
H	3.06211700	0.65390100	2.15015600

C	3.98416900	2.18545800	-1.28712800
H	3.30906200	0.30628900	-2.11043600
C	4.18126600	2.92012200	-0.12275400
H	4.01882800	2.95224300	2.02066400
H	4.25683500	2.60512700	-2.24815500
H	4.60274400	3.91710200	-0.18042200

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C	-0.23310000	2.55671400	0.57339600
N	-1.35049900	1.79304700	0.00469600
C	-1.24363700	0.43263100	0.51700700
C	0.29227100	0.15232100	0.71455800
C	0.93264700	1.54921900	0.73725200
H	1.63419600	1.66677600	-0.09147600
H	0.46017500	-0.39976800	1.63991300
C	-2.18495200	-0.56086200	-0.14536000
C	-3.23583700	-0.83017400	0.73562600
C	-4.29232400	-1.65796000	0.40532700
C	-4.28533400	-2.24137400	-0.85890600
C	-3.24734000	-1.99810600	-1.74704700
C	-2.19292500	-1.15679700	-1.39486100
C	-1.84053000	0.50691100	1.96180400
H	-5.09504000	-1.84905900	1.10785900
H	-1.38322300	-0.99530100	-2.09367900
C	-1.43526900	2.04590300	-1.44893800
H	-0.50655600	2.94917300	1.55267300
H	-1.37595000	1.12978500	-2.03191400
N	-3.02844000	-0.16386300	1.94408600
H	-2.39478900	2.52382800	-1.66984500
O	-1.34712700	1.05590000	2.91698000
H	-3.60326100	-0.25177800	2.76519900
H	-5.09865300	-2.89820300	-1.14554700
H	-3.24728400	-2.47038700	-2.72165500
C	-0.26139400	2.97480300	-1.77629900
C	0.02774000	3.66482400	-0.44163600
H	0.59603700	2.37546000	-2.09332000
H	-0.49676800	3.67643600	-2.57820600
H	1.04172700	4.06389600	-0.36566700
H	-0.67183800	4.48869900	-0.27427200
S	1.03898600	-0.91085400	-0.54516200
O	0.87897400	-0.27310000	-1.85073800
O	0.57917700	-2.27279700	-0.32524400
H	1.48221500	1.71042200	1.66408000
C	2.78010600	-0.85144200	-0.13139700
C	3.63860300	-0.07308300	-0.89525800
C	3.23606500	-1.59837900	0.94791200
C	4.98601600	-0.03478600	-0.56014500
H	3.24944000	0.47435000	-1.74532900

C	4.58315800	-1.54697300	1.27739800
H	2.54917500	-2.22506700	1.50439000
C	5.45425800	-0.76466400	0.52620900
H	5.67050400	0.56316700	-1.15001500
H	4.95493600	-2.12507200	2.11492800
H	6.50622600	-0.73036300	0.78515900

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C	3.11346300	-0.74381300	-0.38987100
N	2.29015600	0.44000900	-0.59616500
C	1.05781600	0.27776500	0.13619600
C	0.73944300	-1.16013500	-0.36211900
C	2.09807100	-1.89709100	-0.41577600
H	2.23043600	-2.54855800	0.44805800
H	0.34701100	-1.04849300	-1.37478000
C	0.01511000	1.32321700	-0.15617500
C	-0.35426900	1.94912000	1.03417800
C	-1.31102900	2.94794200	1.06069100
C	-1.90294100	3.30732800	-0.14966400
C	-1.54542300	2.68876400	-1.34170100
C	-0.57251800	1.68914600	-1.34818200
C	1.24844100	0.42530100	1.68021400
H	-1.59480000	3.43305400	1.98731700
H	-0.27928700	1.20420600	-2.27289400
C	3.17922400	1.57767100	-0.55522700
H	3.58533300	-0.71984200	0.60295000
H	2.72351800	2.45068300	-1.02691000
N	0.36435800	1.39730700	2.09501700
H	3.46871100	1.84718700	0.47373200
O	2.06965500	-0.11981300	2.36958100
H	0.33087600	1.71039800	3.05083200
H	-2.65792900	4.08535300	-0.15658700
H	-2.02206800	2.98558300	-2.26789600
C	4.40803400	1.02682100	-1.33624600
C	4.18498900	-0.51017800	-1.44599800
H	4.48494100	1.48305800	-2.32407700
H	5.33033800	1.25357800	-0.79861200
H	3.79868900	-0.77519500	-2.43358800
H	5.09940500	-1.07757500	-1.26574200
H	2.15844700	-2.50813600	-1.31628200
S	-0.55247000	-2.10611000	0.48145400
O	-0.44297100	-1.92783700	1.92012900
O	-0.52213700	-3.43224000	-0.11693100
C	-2.04976600	-1.29160300	-0.06098200
C	-2.66320800	-0.37446600	0.77890500
C	-2.53945400	-1.56150300	-1.33255300
C	-3.78841000	0.30023800	0.32548300
H	-2.25820000	-0.20129600	1.76823300

C	-3.66411400	-0.88014500	-1.77570600
H	-2.05475800	-2.30712900	-1.95190700
C	-4.28241200	0.05225300	-0.94925800
H	-4.27462000	1.02514900	0.96695300
H	-4.06210400	-1.08134100	-2.76328400
H	-5.15867000	0.58520300	-1.30024400