

Supporting Information for

Experimental and computational study on rhodium-catalyzed

C4(5)_{aryl}-H activation/annulations of imidazoles with alkynes:

Facile synthesis of six types of *N*-heterocycles

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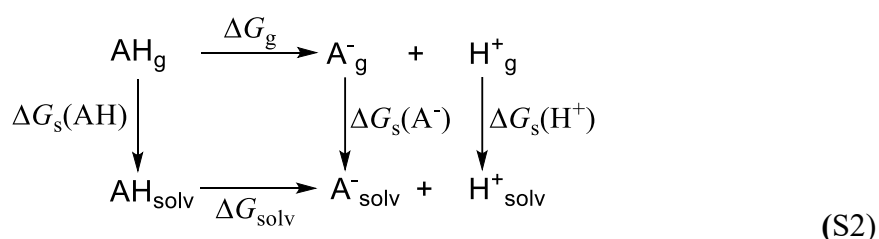
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1. Computational details

All density functional theory calculations were performed with the Gaussian 09 program.¹ Geometry optimizations were carried out at the M06-L²/def2-SVP³ level of theory and frequency calculations were carried out to confirm stationary points as local minima (showing no imaginary frequencies) or transition states (showing one imaginary frequencies) at the same level of theory. For every transition state, intrinsic reaction coordinate (IRC) calculations were employed to confirm the connection between two corresponding minima. Single-point energy calculation is performed to refine the relative energy results at the M06-L/def2-TZVP level of theory. The solvation effect of MeOH was simulated by the SMD⁴ continuum solvent model. The 3D optimized structural figures in this paper were displayed by the CYLview⁵ visualization program.

$$\text{p}K_a = \frac{[\Delta G_g + \Delta G_s(A^-) + \Delta G_s(H^+) - \Delta G_s(AH)]}{2.303RT} \quad (\text{S1})$$

The $\text{p}K_a$ of various substrates were calculated using equation S1 according to the following thermodynamic cycle at the M062X/def2-TZVP/SMD(H₂O)//M062X/def2-SVP level of theory.⁶ The standard free energy of proton in aqueous solution was estimated to be -270.3 kcal/mol (the gas phase Gibbs energy of a proton ($-6.3 \text{ kcal mol}^{-1}$, corresponding to 1 atm in the gas phase and the experimental $\Delta G_s(H^+)$ is -264.0 kcal/mol).⁷



2. Reference

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3. The DFT calculated energies of all transition states

Table S1. The DFT calculated energies of all transition states.

Species	Hc hatree	Gc hatree	H(gas) hatree	G(gas) hatree	Esp + G _{SOL} hatree	G hatree
1a-TS_{aryl}	0.640983	0.523151	-2456.424	-2456.542	-2459.481	-2458.958
1a-TS_{vinyl}	0.641094	0.526724	-2456.425	-2456.54	-2459.481	-2458.954
12-TS_{aryl1}	0.605001	0.493192	-2379.121	-2379.233	-2382.058	-2381.564
12-TS_{aryl2}	0.605319	0.495132	-2379.12	-2379.23	-2382.06	-2381.565
10-TS_{aryl}	0.82549	0.689774	-2994.112	-2994.248	-2997.904	-2997.215
10-TS_{vinyl}	0.824608	0.685578	-2994.123	-2994.262	-2997.911	-2997.225
15-TS_{aryl}	0.630065	0.515058	-2342.987	-2343.102	-2345.871	-2345.356
15-TS_{vinyl}	0.63186	0.518643	-2342.99	-2343.103	-2345.872	-2345.354
10	0.557501	0.462944	-1532.811517	-1532.906074	-1535.045890	-1534.582946
10-C2_{styryl}-H	0.542021	0.447912	-1532.210780	-1532.304888	-1534.497790	-1534.049878
10-C4(5)_{aryl}-H	0.541422	0.446472	-1532.188388	-1532.283338	-1534.479741	-1534.033269
12	0.336112	0.270010	-918.015250	-918.081352	-919.366925	-919.096915
12-C2_{aryl}-H	0.320302	0.255255	-917.411065	-917.476112	-918.817126	-918.561871
12-C4(5)_{aryl}-H	0.320787	0.255560	-917.397679	-917.462906	-918.809545	-918.553985
14	0.374678	0.303211	-882.287453	-882.358921	-883.645329	-883.342118
14-C4(5)_{aryl}-H	0.359323	0.287932	-881.670062	-881.741453	-883.091866	-882.803934
14-C4(5)_{styryl}-H	0.358816	0.287326	-881.660734	-881.732223	-883.094183	-882.806857
1a-D	0.372010	0.299442	-995.287547	-995.360115	-996.763689	-996.464247
1a-D-C4(5)_{aryl}-H	0.356772	0.285626	-994.671771	-994.742917	-996.205965	-995.920339
1a-D-C2_{styryl}-H	0.356878	0.284936	-994.694788	-994.766731	-996.221477	-995.936541

- The **H_c** and **G_c** designate the thermal correction Enthalpy and Gibbs Free Energy.
- The **H(gas)** and **G(gas)** designate Enthalpy and Gibbs Free Energy in gas phase at M06-L/def2-SVP level.
- **E_{SP}** designates the single point energy at M06-L/def2-TZVP level. **G_{SOL}** designates the solvation free energy calculated by SMD continuum solvent mode. The **E_{SP} + G_{SOL}** designates the sum of single point energy at M06-L/def2-TZVP level and the solvation free energy.
- The Final G designates the sum of **E_{SP} + G_{SOL}** and **G_c**.

4. The Cartesian coordinates (xyz) for all optimized structures

10-TS _{aryl}				H	5.86241800	2.10053500	-1.45760000	H	-0.81289400	-4.62568800	-1.16521300
				H	4.64932700	2.35468500	-0.19540900	C	-4.17110700	-5.07709600	-0.93075800
C	-1.24001600	-2.07464000	-0.30719500	H	5.77777600	0.98988600	-0.08011700	H	-5.60525800	-3.56364800	-0.42481300
C	0.15618700	-1.99746400	-0.19945900	C	5.51417500	-1.50979200	-1.44884000	H	-2.52519000	-6.37081400	-1.48740400
N	-1.69434400	-0.74624200	-0.30920800	H	6.27645300	-1.42614100	-2.23949500	H	-4.93180400	-5.84737200	-1.07051500
C	-0.59453600	0.08687700	-0.41479700	H	5.99454400	-1.20126800	-0.51142400	C	-0.51280000	1.50226900	-0.64221800
Rh	2.53630700	-0.27818500	-0.68369400	H	5.24990000	-2.57045200	-1.36488900	H	0.40326100	1.94139000	-0.23405900
N	0.49567300	-0.67110300	-0.32320300	C	2.87454000	-2.45174200	-3.00771400	C	-1.38959300	2.28449700	-1.31508700
C	4.22201900	0.74119100	-1.54429200	H	1.79568400	-2.63666400	-3.09344300	H	-2.25084300	1.81639000	-1.80464500
C	4.34709300	-0.66084600	-1.79114100	H	3.31234400	-2.60343600	-4.00692900	C	-1.28747500	3.72635700	-1.44855100
C	3.15757400	-1.08297400	-2.50786600	H	3.29006000	-3.22070400	-2.34320800	C	-2.09846600	4.40027600	-2.38056900
C	3.01436400	1.23264800	-2.19465500	C	1.10135800	0.11898300	-3.55908800	C	-0.41363200	4.49044300	-0.64759300
C	2.37266000	0.11138100	-2.79593200	H	1.31021700	0.07815300	-4.63934500	C	-2.01937100	5.78075700	-2.53061300
C	2.35846600	-4.90217900	0.89766100	H	0.47695300	-0.75316800	-3.32156300	H	-2.79826400	3.82289700	-2.99188900
C	1.21904400	-4.22545000	0.46799800	H	0.51053500	1.02299300	-3.36969400	C	-0.33774700	5.86856300	-0.79878500
C	1.26929000	-2.85268100	0.18970100	C	2.55949900	2.64563700	-2.19900000	H	0.18385300	4.00014100	0.12683200
C	2.49343400	-2.13361900	0.42627700	H	2.68882700	3.11444700	-1.21332600	C	-1.13523900	6.51901000	-1.74374000
C	3.61949200	-2.85558000	0.85778500	H	3.13977800	3.24594500	-2.91733900	H	-2.65457500	6.28580700	-3.26127800
C	3.56644600	-4.22784100	1.08559700	H	1.50020000	2.74099100	-2.47139000	H	0.33552800	6.44778800	-0.16303100
H	2.29491800	-5.97195300	1.10842300	C	-2.21143200	-3.10944600	-0.51772900	H	-1.07786200	7.60380100	-1.85460000
H	0.28416100	-4.77875600	0.38368800	C	-3.59190300	-2.77579000	-0.38640100	O	1.78036700	-0.68369400	2.48073400
H	4.54689800	-2.31519900	1.07442300	C	-1.85574100	-4.40478300	-0.93950100	S	1.98154500	0.83283900	2.39077200
H	4.44813600	-4.76574100	1.44071800	C	-4.54845800	-3.79479900	-0.56721600	C	3.54060300	1.06656700	3.37727800
C	5.17029000	1.58240900	-0.77533100	C	-2.82043300	-5.37645700	-1.14676800	F	3.89509800	2.33856500	3.32920800

F	3.35310500	0.69256100	4.62467400	H	-2.08967000	2.89725100	3.10022500	C	1.44453100	0.15992400	-3.87153200
F	4.49804000	0.32145200	2.82532400	H	-5.23024400	3.69182400	0.25315400	H	0.57269500	0.81189200	-3.72843400
O	0.93112400	1.61178400	3.00462600	H	-3.83244400	4.42850300	2.17658400	H	1.84336400	0.36588500	-4.87776800
O	2.41008600	1.19858000	1.00796400					H	1.09078600	-0.87904100	-3.86488700
H	2.17628600	-1.25305900	1.51818400					C	2.23612500	2.97708500	-2.68046000
C	-3.96846400	-1.42258400	-0.02383500	10-TS_{vinyl}				H	2.68844400	3.30752200	-3.62970100
C	-3.02933200	-0.42477200	0.02202100					H	1.15742500	2.88659000	-2.85998000
C	-5.37293800	-1.11907100	0.35793600	C	-0.72164700	-0.18450800	-0.46372400	H	2.39325000	3.77474800	-1.94444900
C	-6.38326000	-1.09547800	-0.61338200	C	-0.54531400	1.99790500	-0.19105700	C	4.58247900	2.49981600	-0.51850100
C	-5.70228000	-0.82724500	1.68725400	Rh	2.20276100	0.21982200	-0.76456700	H	4.60361500	2.19823000	0.53834100
C	-7.69231400	-0.77088300	-0.26351000	N	0.14558200	0.84462700	-0.39421900	H	5.62965900	2.62253400	-0.83616800
H	-6.13477000	-1.31885100	-1.65532600	C	4.24755200	0.06411900	-1.37020500	H	4.09553300	3.47971600	-0.58244600
C	-7.01197500	-0.50645800	2.03597400	C	3.43913100	-0.57985200	-2.35931200	O	0.97288600	-1.15389800	2.09026300
H	-4.91926400	-0.84107700	2.45012400	C	2.47894600	0.39168100	-2.83243000	S	1.74634600	0.10170400	2.53176600
C	-8.00868200	-0.47329200	1.06160100	C	3.90530400	1.48543200	-1.36004100	C	2.86370300	-0.58258400	3.85216100
H	-8.46891000	-0.74676700	-1.03123300	C	2.84486700	1.69006100	-2.27378500	F	3.65042500	0.39155000	4.27390600
H	-7.25459400	-0.27871800	3.07611200	C	-0.20287500	-1.49471300	-0.67241100	F	2.13673700	-1.04177800	4.84921800
H	-9.03451800	-0.21769500	1.33525400	C	1.15385400	-1.65167600	-0.47237400	F	3.60013600	-1.56089600	3.34371900
C	-3.27812600	0.91686800	0.58892400	C	5.35114800	-0.54311500	-0.58577700	O	0.91972800	1.11895600	3.14132700
C	-2.50399700	1.33516200	1.68180600	H	6.32778500	-0.24749000	-1.00073700	O	2.68926800	0.49301000	1.44351700
C	-4.26748700	1.77199900	0.08884200	H	5.33552600	-0.21116400	0.46159800	H	1.11534900	-1.33857300	0.95351800
C	-2.70219300	2.58863200	2.25025900	H	5.30796800	-1.63909700	-0.59501600	C	1.79671000	-2.96438300	-0.58147100
H	-1.73256600	0.67533300	2.09053700	C	3.60581800	-1.95055700	-2.89139100	C	1.28819200	-3.99645000	-1.39201100
C	-4.46324500	3.02835800	0.65846700	H	4.25539800	-1.89788000	-3.78003100	C	2.96031400	-3.22391800	0.16807500
H	-4.88075300	1.45271400	-0.75824600	H	4.08124600	-2.63433600	-2.17914400	C	1.92629200	-5.23087900	-1.45852100
C	-3.67934800	3.44131900	1.73526300	H	2.65796300	-2.39961700	-3.21165500	H	0.39209700	-3.81779500	-1.99475400

C	3.59231000	-4.46182300	0.10955700	H	-6.44675800	4.36516900	0.74839700	H	-7.42724700	-2.60187800	1.89677700
H	3.36068300	-2.43123500	0.80912100	C	-1.91106900	1.67616900	-0.08485100	H	-8.98910400	-2.46745500	-0.03836800
C	3.08085200	-5.46919300	-0.71026100	N	-1.99695400	0.29232700	-0.25467200				
H	1.52391500	-6.01502800	-2.10405600	H	-0.86133200	-2.33648000	-0.88923800				
H	4.48773100	-4.64565000	0.70805400	C	-3.20946900	-0.40737000	-0.19105400	12-TS _{aryl}			
H	3.57917700	-6.43928100	-0.76474200	C	-4.37739400	0.30457300	-0.09682700				
C	0.11859800	3.30604600	-0.16414200	C	-3.14996700	-1.88453600	-0.13883200	C	-2.95296300	0.61133600	0.07231900
C	-0.34753400	4.36287300	-0.96539900	C	-3.64392400	-2.67047400	-1.18511900	C	-1.84135100	-0.14384400	-0.27906400
C	1.26067800	3.50897700	0.62418400	C	-2.59778200	-2.50745400	0.99131400	N	-2.45253300	1.87297900	0.31345900
C	0.30245500	5.59184600	-0.96711000	C	-3.57061700	-4.06086200	-1.11065000	C	-1.09957700	1.87816100	0.16944500
H	-1.22429000	4.21010900	-1.60117000	H	-4.08989600	-2.18756200	-2.05858800	H	-2.98977800	2.62983400	0.72365200
C	1.90262800	4.74688000	0.62842300	C	-2.52877800	-3.89530500	1.06293300	Rh	1.09929100	-0.28513500	-0.89607700
H	1.62558300	2.70071500	1.25873100	H	-2.20837500	-1.89622700	1.81179100	N	-0.71481200	0.65895500	-0.19708300
C	1.42888000	5.79018100	-0.16496000	C	-3.01027400	-4.67427500	0.00920400	C	2.99170800	-0.69452700	-1.78437000
H	-0.06941300	6.40087900	-1.59962600	H	-3.95783100	-4.66854100	-1.93130800	C	1.96681600	-1.12166500	-2.68675200
H	2.77519600	4.89831100	1.26849100	H	-2.10005300	-4.37191500	1.94710600	C	1.12482000	0.02157100	-2.96306200
H	1.93086900	6.76011500	-0.15574400	H	-2.95611700	-5.76344800	0.06618800	C	2.88791000	0.75570600	-1.63180100
C	-3.10907400	2.42418800	0.17182000	C	-5.66639900	-0.43511200	-0.06394500	C	1.75822200	1.19491700	-2.36662600
C	-3.09946200	3.78373200	0.54379500	C	-6.56043000	-0.34861800	-1.13955900	C	-2.28999000	-3.70224200	-1.48297200
C	-4.35865200	1.74198800	0.07679400	C	-5.99462000	-1.24749000	1.02870600	C	-2.61666500	-2.38955400	-1.15013900
C	-4.28295200	4.47087600	0.74490100	C	-7.74704200	-1.07888000	-1.13060200	C	-1.62059100	-1.51690200	-0.69509000
H	-2.15106400	4.29556300	0.69994300	H	-6.31501500	0.28754800	-1.99527800	C	-0.26054100	-1.95172000	-0.60979400
C	-5.54879900	2.47203000	0.28039800	C	-7.18371100	-1.97215400	1.03841900	C	0.01973000	-3.29286500	-0.93213800
C	-5.51446500	3.81922800	0.59183000	H	-5.30787900	-1.31350900	1.87678100	C	-0.97843600	-4.16763700	-1.34870700
H	-4.25280300	5.52237300	1.03666300	C	-8.05962500	-1.89422500	-0.04339500	H	-3.07179000	-4.37621000	-1.84020200
H	-6.50640000	1.95283500	0.21303500	H	-8.43154900	-1.01109900	-1.97903800	H	-3.64773000	-2.04370100	-1.25510600

H	1.04269900	-3.66714000	-0.81983800	H	-5.07726400	2.14322300	-0.63391700	H	1.89510100	6.24636000	0.91637500
H	-0.74181900	-5.21036500	-1.57209500	C	-6.09730000	-1.17696300	1.09969900				
C	4.05259400	-1.53756800	-1.18101100	H	-3.98542200	-1.59599400	1.23117300				
H	4.97540300	-1.49734600	-1.78111000	C	-7.07651400	-0.26702400	0.69914800	12-TS _{ary12}			
H	4.30885500	-1.19947500	-0.16863300	H	-7.46686600	1.64361500	-0.22912000				
H	3.75102900	-2.59050500	-1.11571900	H	-6.38375000	-2.10595400	1.59690700	C	0.98661700	1.82307700	0.02204000
C	1.83756000	-2.45881600	-3.31049100	H	-8.13202900	-0.48825400	0.86941400	C	2.12666400	-0.05232000	0.03444000
H	2.37280700	-2.44586200	-4.27355800	O	0.07207300	-1.76144000	1.96398200	Rh	-1.10332500	-0.07594300	-0.82494900
H	2.28906200	-3.25568200	-2.70887500	S	1.03018300	-0.64247600	2.39117300	N	0.87438800	0.49920100	-0.11267000
H	0.79722300	-2.72976500	-3.52374700	C	2.20893700	-1.55401200	3.50755000	C	-2.73009400	-0.95366800	-1.87909000
C	-0.05683600	0.04178300	-3.86105600	F	3.12502700	-0.70084300	3.92956200	C	-2.39434300	0.28824600	-2.50746200
H	-0.78785800	0.79990900	-3.55116000	F	1.55299000	-2.05993200	4.53035200	C	-0.99979300	0.22410900	-2.89197200
H	0.23928800	0.27925600	-4.89530600	F	2.78744500	-2.52367000	2.81534300	C	-1.58247600	-1.84819300	-2.00341800
H	-0.57146000	-0.92769400	-3.88104400	O	0.41659800	0.42169000	3.15394300	C	-0.53263000	-1.13497600	-2.64184600
C	1.27847200	2.58450700	-2.55645000	O	1.88993900	-0.27505200	1.22219800	C	-1.35788300	4.76649300	-0.17715700
H	1.51109600	2.91839000	-3.58001000	H	0.03146000	-1.84115000	0.78994000	C	-0.15717300	4.06077200	-0.14651400
H	0.18896100	2.66044000	-2.44047000	C	-0.27807000	3.06107800	0.37953500	C	-0.18114700	2.66545100	-0.05325000
H	1.74135200	3.29338900	-1.86045000	C	1.03411200	2.94926900	0.86584100	C	-1.41312800	1.94393800	0.00025800
C	3.82409900	1.57638900	-0.82701800	C	-0.79831000	4.33600800	0.09547000	C	-2.59892600	2.69859500	-0.02268600
H	3.89566000	1.20854600	0.20690600	C	1.80503800	4.09224500	1.05494600	C	-2.57865900	4.08971600	-0.10235700
H	4.83802300	1.52731700	-1.25299300	H	1.43040300	1.96765400	1.12917500	H	-1.34275400	5.85592100	-0.24773100
H	3.52658000	2.63080000	-0.79361500	C	-0.01928000	5.47225400	0.28271800	H	0.79038900	4.60394500	-0.20518200
C	-4.36629500	0.30036200	0.26154100	H	-1.81024900	4.43852000	-0.30717700	H	-3.56261400	2.18632700	0.06561300
C	-5.35923600	1.21383300	-0.13022000	C	1.28596400	5.35344300	0.76211000	H	-3.51353500	4.65447500	-0.09641400
C	-4.75213200	-0.89719200	0.88699400	H	2.81835300	3.99844300	1.45282400	C	-4.03851800	-1.32939900	-1.28999400
C	-6.70424900	0.92944400	0.08770300	H	-0.43084300	6.45629500	0.05002700	H	-4.64023000	-1.90163800	-2.01379300

H	-3.91425700	-1.96343300	-0.40211300	H	-1.38931600	1.25219200	1.22346000	15-TS_{aryl}			
H	-4.62692200	-0.45074400	-0.99764200	C	2.38623600	-1.48404600	-0.12102900				
C	-3.31570100	1.41026600	-2.79763900	C	1.47729900	-2.43281600	0.37032000				
H	-3.73650800	1.26627900	-3.80573300	C	3.53419400	-1.92840300	-0.79974600				
H	-4.16258100	1.45562100	-2.10353200	C	1.71429000	-3.79418400	0.18575600	C	2.24489000	-0.23495500	0.57325600
H	-2.81139100	2.38382000	-2.79441200	H	0.59576600	-2.10337300	0.92277400	C	1.03167800	-0.67163300	0.00511100
C	-0.23664000	1.28507100	-3.59472200	C	3.76206100	-3.28716000	-0.98659700	N	1.96161200	0.54659900	1.65992600
H	0.83137600	1.25351200	-3.34143300	H	4.24327300	-1.19746000	-1.19819600	C	0.63788600	0.58289100	1.75030500
H	-0.31282700	1.16481200	-4.68701000	C	2.85128600	-4.22577300	-0.49580400	Rh	-1.92597700	-0.57984300	0.24108100
H	-0.61185000	2.28692600	-3.34913700	H	1.00853200	-4.52337300	0.59104200	N	0.02574400	-0.13355300	0.77466500
C	0.79816900	-1.65458700	-3.03278900	H	4.65420500	-3.61779100	-1.52266400	C	-4.07366200	-0.73697400	0.48478500
H	0.79613800	-1.88921100	-4.10934700	H	3.03526800	-5.29302300	-0.63662500	C	-3.55540200	-1.99984200	0.08238900
H	1.59486300	-0.91678600	-2.87132100	C	4.45383400	0.99728000	0.60784600	C	-2.54703400	-2.38165200	1.05630100
H	1.07086700	-2.57041200	-2.49493600	C	5.27576200	2.03745200	0.14195000	C	-3.50856100	-0.38790800	1.78553700
C	-1.56022100	-3.24814300	-1.52163000	C	5.01785500	-0.00429500	1.41628600	C	-2.59463100	-1.40903000	2.14510400
H	-1.93432700	-3.32274400	-0.49111800	C	6.62789200	2.07103400	0.47081500	C	0.85527000	-2.95520400	-3.00185400
H	-2.21447000	-3.87461500	-2.14779500	H	4.85946300	2.81355100	-0.50767000	C	1.39644400	-2.26235800	-1.92702800
H	-0.55329100	-3.68025800	-1.55037700	C	6.36963400	0.03338600	1.73883500	C	0.59039800	-1.42095200	-1.13754200
O	-1.26641200	0.86020500	2.35406800	H	4.38332600	-0.80193800	1.80985200	C	-0.80612300	-1.28090700	-1.44705700
S	-1.56799700	-0.63836400	2.44163300	C	7.17844300	1.06849100	1.26784200	C	-1.31217200	-2.01114700	-2.54127100
C	-3.37163300	-0.64105800	2.88767200	H	7.25681700	2.88120600	0.09631800	C	-0.50069600	-2.82504300	-3.32539300
F	-3.83338800	-1.87881700	2.84262800	H	6.79361500	-0.74562400	2.37565800	H	1.49713300	-3.60660700	-3.60050700
F	-3.54250500	-0.13316500	4.08765700	H	8.23895900	1.09540200	1.52556200	H	2.45017900	-2.39921300	-1.67518100
F	-4.02486200	0.09894600	1.98982400	N	2.28246900	2.13781100	0.24837000	H	-2.35824200	-1.87806700	-2.83422300
O	-0.84682600	-1.34000300	3.47384000	C	3.03042000	0.98002500	0.28786700	H	-0.91440300	-3.34656200	-4.19198000
O	-1.57006600	-1.20931800	1.05887800	H	2.63666000	3.05458600	0.49797800	C	-5.07503700	0.08625800	-0.23935100

H	-6.08033200	-0.04516800	0.19260500	C	-0.09482500	1.38974800	2.77780200	F	-0.45821900	4.26754000	-0.79175500
H	-4.83448500	1.15626700	-0.18030000	H	-1.12707300	0.99789100	2.81241800				
H	-5.13631000	-0.18188100	-1.30167200	C	0.55037200	1.24585100	4.14844900				
C	-4.03872700	-2.83141100	-1.04799000	H	1.58698700	1.60914500	4.11761500	15-TS_{vinyl}			
H	-4.89071200	-3.44612700	-0.71473700	H	0.00682400	1.82546100	4.90916400				
H	-4.39468300	-2.22590900	-1.89179200	H	0.59086100	0.19872800	4.48106900	C	1.98244200	0.43938100	-0.21851000
H	-3.27117200	-3.51842000	-1.42463500	C	-0.18062000	2.85682600	2.36351500	C	2.08516500	-1.73993700	-0.29595800
C	-1.76313600	-3.64348700	1.06582600	H	-0.75518500	2.97961600	1.43770100	Rh	-0.77332400	-0.40010900	-0.90815300
H	-0.80432800	-3.51331900	1.58530900	H	-0.66954700	3.45979300	3.14358100	N	1.23427200	-0.70260500	-0.43527500
H	-2.31066800	-4.45081200	1.57922100	H	0.82487600	3.27154300	2.19716300	C	-2.75820300	-0.87807100	-1.63177700
H	-1.53797000	-3.98652300	0.04723100	C	6.07968500	-0.25752100	0.39948900	C	-2.27031300	0.25550500	-2.34261700
C	-1.79095000	-1.52613500	3.38878700	C	7.10983600	0.20627400	1.24169900	C	-1.01209100	-0.13441000	-2.95014000
H	-2.05610700	-2.44916700	3.92719100	C	6.46060700	-0.91171700	-0.79110600	C	-1.90749700	-2.02848200	-1.93146400
H	-0.71359600	-1.57791100	3.17322700	C	8.45026500	0.02117700	0.91883300	C	-0.85066300	-1.57504100	-2.75260800
H	-1.95171200	-0.68412000	4.07270500	H	6.83793000	0.72060500	2.16793300	C	1.21251900	1.62783100	-0.13501900
C	-3.86239800	0.83793000	2.54828000	C	7.79859900	-1.09539300	-1.11358700	C	-0.16585700	1.51128200	-0.20628600
H	-3.63609200	1.75009900	1.97612800	H	5.69326900	-1.27807100	-1.47749600	C	-3.98629100	-0.93905500	-0.79871600
H	-4.93875200	0.86315700	2.77995600	C	8.80421200	-0.63222800	-0.26113800	H	-4.84481600	-1.30252000	-1.38704100
H	-3.31877900	0.90258700	3.49896500	H	9.22611800	0.39159300	1.59360900	H	-3.86250300	-1.62626200	0.04890300
C	3.59127700	-0.48651000	0.13607400	H	8.06429000	-1.60524600	-2.04331000	H	-4.25658900	0.04595800	-0.39612500
C	4.69620400	-0.04768700	0.78790200	H	9.85594700	-0.77791100	-0.51831600	C	-2.96504800	1.55089000	-2.53834100
H	4.52900800	0.51887600	1.71051700	H	3.70394900	-1.06244900	-0.78716500	H	-3.50742300	1.53004800	-3.49782700
O	-1.25884000	1.04278200	-2.61977600	C	-0.19441800	3.19685500	-1.52818100	H	-3.70195500	1.75437300	-1.75251700
S	-1.75269700	2.19317300	-1.71767000	O	-2.71656900	3.04752800	-2.37323100	H	-2.27711200	2.40566800	-2.57188300
O	-2.05762700	1.67119300	-0.36338200	F	0.22689600	3.57646500	-2.72324000	C	-0.15421200	0.71028200	-3.81984000
H	-1.06733200	0.08539100	-2.03882900	F	0.73905800	2.47119900	-0.93698000	H	0.90442700	0.43153700	-3.72966100

H	-0.43398300	0.60452700	-4.88103300	C	-2.71759500	4.96853300	-0.20681900	H	3.62175700	-3.98807900	-0.74789300
H	-0.23866000	1.77338800	-3.56003200	H	-1.14656300	5.93592700	-1.32973400	H	2.28774800	-5.06112300	-1.23065800
C	0.25433200	-2.36340400	-3.35344900	H	-4.09344200	3.73567400	0.91494400				
H	0.17862800	-2.34582500	-4.45201300	H	-3.36770700	5.84631600	-0.20114200				
H	1.23762500	-1.94456900	-3.09463600	H	1.69137600	2.59079300	0.08472200	1a-TS _{aryl}			
H	0.24435000	-3.41334300	-3.03753700	C	4.51479400	0.77628500	0.28532900				
C	-2.13890000	-3.40178500	-1.41353700	C	5.64364200	0.12390000	0.81483900		C	-1.74211500	2.41793100
H	-2.16385000	-3.42157300	-0.31388100	C	4.60753000	2.15521100	0.02495300	C	-1.71923000	1.03733700	-0.37878700
H	-3.10273700	-3.80349500	-1.76437200	C	6.80948600	0.82826600	1.09061400	N	-0.41315000	2.79468400	-0.21212100
H	-1.35495500	-4.09939600	-1.73413600	H	5.57311500	-0.94890400	1.00500400	C	0.38650700	1.69661600	-0.31453700
O	-0.38354700	0.68888000	2.38914000	C	5.77510200	2.85828100	0.30482400	H	-0.09282300	3.72668900	0.02660200
S	-0.87485200	-0.77807800	2.54927300	H	3.76284500	2.67784800	-0.42995600	Rh	-0.05366700	-1.44146400	-0.74875200
C	-2.52332900	-0.49434700	3.36343400	C	6.88143600	2.20043700	0.84282500	N	-0.40360200	0.62955200	-0.43061900
F	-3.04428600	-1.66993000	3.68325200	H	7.67291500	0.30336300	1.50766100	C	0.93248400	-3.25603600	-1.32218800
F	-2.37117400	0.23707000	4.45119200	H	5.82577800	3.92906900	0.09203800	C	-0.26938300	-3.12990200	-2.08227400
F	-3.34945100	0.12657500	2.52493700	H	7.79789000	2.75363900	1.06195600	C	-0.21056400	-1.86355300	-2.78642500
O	-0.08773600	-1.52247800	3.50265400	C	3.30620900	0.00700100	0.01578600	C	1.81426900	-2.14322100	-1.66091100
O	-1.19957600	-1.35370700	1.22971300	N	3.33515900	-1.35229100	-0.02963500	C	1.11967000	-1.30197000	-2.56963900
H	-0.27299100	0.97768300	1.36565700	C	1.66070200	-3.17439200	-0.34276800	C	-4.89820800	-0.98167300	-0.75421000
C	-1.03134000	2.69416500	-0.22083800	H	0.65007300	-3.18669100	-0.79135800	C	-4.05443600	0.12655600	-0.74930600
C	-0.64234100	3.89898900	-0.84247300	C	1.54618000	-3.74174000	1.07040400	C	-2.69623800	-0.03382700	-0.45413200
C	-2.29679800	2.66699800	0.39851500	H	1.20100200	-4.78626000	1.04975900	C	-2.15655400	-1.33310600	-0.18253900
C	-1.47265200	5.01713200	-0.83505100	H	2.52487800	-3.71977300	1.57136700	C	-3.05044600	-2.41835300	-0.16960500
H	0.32575800	3.94504200	-1.35068100	H	0.84724800	-3.16443000	1.68822100	C	-4.40597500	-2.25183400	-0.44108800
C	-3.12313900	3.78518600	0.41338900	C	2.61349100	-4.01133500	-1.18476500	H	-5.95629300	-0.85200300	-0.99229000
H	-2.62459400	1.74157000	0.88126700	H	2.70415900	-3.63809700	-2.21460100	H	-4.45293600	1.11586600	-0.98747700

H	-2.68240700	-3.41517900	0.09252700	H	-1.86621400	4.90476400	-1.27657600	F	-0.21502400	-1.24617100	4.94260000
H	-5.08344800	-3.10805700	-0.40750300	C	-4.93283100	4.03912700	0.93917300	F	0.07300400	-2.97822100	3.68110600
C	1.28778100	-4.35953500	-0.39804500	H	-3.99033200	2.12418600	1.25532100	O	0.59577100	0.66033600	2.73345800
H	1.91159400	-5.10872200	-0.91085700	C	-4.83680200	5.29455700	0.33690500	O	0.86183300	-1.42165000	1.32569100
H	1.86185700	-3.99381400	0.46253500	H	-3.64841800	6.58498200	-0.92318400	H	-1.62781400	-1.17222100	1.15768800
H	0.40064300	-4.87814300	-0.01516800	H	-5.79119300	3.79915600	1.56992900				
C	-1.33513100	-4.15151900	-2.21134200	H	-5.62610200	6.03428600	0.48443600				
H	-1.07605100	-4.82936900	-3.04035800	C	1.81542600	1.65203100	-0.27269100	1a-TS_{vinyl}			
H	-1.43229400	-4.77456900	-1.31411700	H	2.20949400	0.63776300	-0.14774300				
H	-2.31535000	-3.71919700	-2.44317700	C	2.65117000	2.71311600	-0.37329200	C	0.83263400	1.72667700	0.89994200
C	-1.23593000	-1.33097400	-3.71788500	H	2.22003600	3.70642700	-0.55307300	C	2.30231600	0.34331700	0.03157800
H	-1.21559400	-0.23401000	-3.75620800	C	4.09964300	2.67495900	-0.29931200	Rh	-0.91437300	0.16604700	-0.87579800
H	-1.06530300	-1.69690000	-4.74286600	C	4.83959600	3.81204600	-0.67481000	N	0.97050300	0.66544600	0.08977800
H	-2.24939900	-1.63420100	-3.42404000	C	4.80409100	1.53560600	0.14012900	C	-2.42215500	-0.41317100	-2.27173800
C	1.61859200	-0.05975800	-3.20757200	C	6.22950500	3.80552400	-0.63716800	C	-2.36649800	1.01554900	-2.24868900
H	1.84806500	-0.25327500	-4.26706900	H	4.30734600	4.70874300	-1.00423000	C	-1.00906500	1.40519500	-2.56213500
H	0.86781700	0.74185300	-3.18928600	C	6.19148200	1.53231300	0.17907300	C	-1.13991700	-0.90957700	-2.76513200
H	2.53300000	0.32170600	-2.73729300	H	4.25322300	0.65794100	0.48863800	C	-0.28255100	0.20497900	-2.96223600
C	3.18388000	-1.96078200	-1.12035800	C	6.91054900	2.66467100	-0.21416900	C	-0.45708000	2.24743700	1.19917400
H	3.19661900	-2.01703800	-0.02229200	H	6.78615300	4.69657200	-0.93419500	C	-1.52879300	1.47651900	0.79947700
H	3.85372600	-2.75369100	-1.48760400	H	6.72301300	0.64634800	0.53321800	C	-3.60071800	-1.26193200	-1.96999700
H	3.62376400	-1.00125200	-1.41875400	H	8.00174200	2.65960200	-0.17763700	H	-4.07093100	-1.61646500	-2.90091100
C	-2.81195300	3.39284100	-0.04269900	O	-1.35396300	-0.84787100	2.25051100	H	-3.32121600	-2.15326800	-1.39144100
C	-2.72047800	4.66298700	-0.63736900	S	0.16381600	-0.68527200	2.42413600	H	-4.36460000	-0.71479100	-1.40408600
C	-3.92929800	3.09414200	0.75519700	C	0.46537600	-1.73843700	3.92811100	C	-3.50287300	1.93887000	-2.04128300
C	-3.72703800	5.60497200	-0.44828700	F	1.75885800	-1.72541700	4.19819400	H	-3.97927300	2.12161000	-3.01804400

H	-4.27285300	1.53269600	-1.37496300	C	-4.65180300	3.55220700	1.32835200	C	7.09673300	1.54846100	1.99958300
H	-3.19018900	2.91295300	-1.64845200	H	-2.57558300	4.01003500	0.98601300	H	6.78969400	3.68546500	1.93126100
C	-0.50066300	2.79503900	-2.66924200	C	-5.23341300	1.20918700	1.40184600	H	7.10152700	-0.61167500	1.99366100
H	0.56980400	2.85478300	-2.43308800	H	-3.60171700	-0.17745100	1.12392900	H	8.14370300	1.62809800	2.29886300
H	-0.62787800	3.18090400	-3.69326800	C	-5.61426700	2.55062600	1.47111300	C	3.00511600	1.23679900	0.85109800
H	-1.03392400	3.47665700	-1.99441400	H	-4.94636500	4.60285300	1.37732800	N	2.05616700	2.09609700	1.35203300
C	1.09040400	0.20764300	-3.51978500	H	-5.98054100	0.42191700	1.52488700	H	2.23568300	2.80538100	2.05413100
H	1.05511000	0.54783400	-4.56722200	H	-6.66027900	2.81596600	1.63773800	H	-0.54819100	3.16192000	1.79826500
H	1.75164800	0.90196700	-2.98458800	C	2.83619300	-0.71255800	-0.82960900				
H	1.55927400	-0.78331800	-3.50767400	C	4.03922900	-0.50510400	-1.52820400	10			
C	-0.83693300	-2.33877100	-3.00623800	C	2.14908100	-1.92239100	-1.00983800				
H	-1.12877000	-2.96185400	-2.14970600	C	4.53988800	-1.48082400	-2.38217400	C	1.75132900	2.12839500	-0.53387100
H	-1.40611500	-2.70364500	-3.87560900	H	4.57582500	0.44049700	-1.41377000	C	2.59232900	0.98893800	-0.48702400
H	0.22691300	-2.50885100	-3.20668200	C	2.66084900	-2.90061000	-1.86130900	C	3.93799100	1.11171300	-0.88481300
O	-1.08901000	-0.53257600	2.38596800	H	1.22399800	-2.10750600	-0.46199700	C	4.45170500	2.33786400	-1.27123100
S	-0.67801600	-1.85379200	1.72535600	C	3.85311800	-2.68461000	-2.55081600	C	3.63603300	3.47727700	-1.26762000
C	-1.93880200	-3.03337800	2.41804800	H	5.47068900	-1.30001600	-2.92394300	C	2.30363900	3.37023000	-0.90698100
F	-1.66886900	-4.24745100	1.97436100	H	2.12744000	-3.84762800	-1.97525700	H	4.57285700	0.22770400	-0.90834100
F	-1.88779000	-3.00700900	3.73273700	H	4.25145400	-3.45468200	-3.21482500	H	5.49486800	2.41121200	-1.58161800
F	-3.14676900	-2.66994100	2.00608500	C	4.40974000	1.33839900	1.22809200	H	4.04457800	4.44636100	-1.55654300
O	0.63208900	-2.33781200	2.09725000	C	5.00378200	2.59813200	1.41580400	H	1.66835100	4.25572200	-0.91022600
O	-1.02753300	-1.78129300	0.27146400	C	5.18160700	0.18299000	1.44118700	C	0.34835100	1.99541100	-0.14741300
H	-1.28377000	0.30476700	1.55857000	C	6.33792900	2.70050700	1.79808500	C	2.01123300	-0.27722800	-0.09214900
C	-2.91724700	1.87072600	1.03564000	H	4.42443700	3.50783300	1.23104500	C	-0.48475200	3.22556800	0.00525500
C	-3.31840100	3.21722400	1.11739900	C	6.51412800	0.29248300	1.82167100	C	-0.84098700	3.69327000	1.27416600
C	-3.90209700	0.87394400	1.17938600	H	4.72299700	-0.80209500	1.32635400	C	-0.92471000	3.92506300	-1.12507200

C	-1.63352500	4.83143900	1.41091700	H	4.60094500	-0.44503100	1.41977600	10-C2styryl-H			
H	-0.50311900	3.14750900	2.15718300	C	5.44761700	-3.88053400	-0.16467200				
C	-1.71622100	5.06420400	-0.98872300	H	3.38823900	-3.89175200	-0.83581900	C	1.38985200	2.13478800	-0.74989800
H	-0.64729100	3.56354700	-2.11818200	C	6.43086000	-3.17681900	0.53108000	C	2.40529400	1.15248300	-0.59688700
C	-2.07406800	5.51843000	0.28046000	H	6.88169000	-1.39206400	1.66044600	C	3.70931400	1.44913000	-1.03981000
H	-1.90985800	5.18206100	2.40636900	H	5.67772800	-4.85482500	-0.59882700	C	4.02002500	2.69047400	-1.57282000
H	-2.05797100	5.59699200	-1.87747200	H	7.43165900	-3.59696900	0.64208300	C	3.03166100	3.67547400	-1.68167200
H	-2.69598900	6.40829900	0.38802500	N	1.43105400	-2.42418800	0.23931300	C	1.73518400	3.39387400	-1.27753500
N	0.62009200	-0.37222200	0.00266200	C	0.32471000	-1.72023400	0.14372800	H	4.47729000	0.67910400	-0.98682500
C	-0.18763000	0.77440500	0.12945600	C	-0.99248700	-2.35032400	0.07592900	H	5.03728500	2.89091800	-1.91394900
C	-1.55024900	0.60864900	0.70524300	H	-1.09612000	-3.23377700	0.71096600	H	3.27302500	4.65756300	-2.09164700
C	-1.68933300	0.01394500	1.96406600	C	-1.98087000	-1.97084300	-0.74863900	H	0.96235900	4.15767600	-1.36879900
C	-2.69089000	1.03111300	0.01765200	H	-1.79431900	-1.14751100	-1.44447500	C	0.03360500	1.83694100	-0.28748700
C	-2.95342600	-0.17992000	2.51380100	C	-3.33169500	-2.54421800	-0.80102500	C	2.02527800	-0.14227400	-0.07167400
H	-0.79896100	-0.31735000	2.50393400	C	-4.16734300	-2.23279000	-1.88404500	C	-0.94063200	2.96239700	-0.16386100
C	-3.95624500	0.83273200	0.56657000	C	-3.83769200	-3.37024900	0.21583900	C	-1.21019300	3.54586100	1.07918700
H	-2.58378000	1.50122100	-0.96168500	C	-5.45960200	-2.74556800	-1.96325600	C	-1.60162400	3.45400900	-1.29573000
C	-4.09091300	0.22083600	1.81139600	H	-3.79010800	-1.57991100	-2.67450000	C	-2.13040700	4.58620900	1.19101700
H	-3.05222100	-0.64966100	3.49357000	C	-5.12751500	-3.88439300	0.13630000	H	-0.70787300	3.15384200	1.96562900
H	-4.84179100	1.14742300	0.01289600	H	-3.22044900	-3.59280900	1.08763500	C	-2.51883300	4.49839400	-1.18686500
H	-5.08246900	0.05466800	2.23461600	C	-5.94398000	-3.57626400	-0.95379900	H	-1.40097300	2.99315100	-2.26557800
C	2.48266300	-1.57335600	0.11408600	H	-6.09200100	-2.49493100	-2.81638300	C	-2.78741500	5.06596000	0.05828400
C	3.85977000	-2.09166600	0.23699200	H	-5.50455200	-4.52368400	0.93618300	H	-2.34094000	5.01963100	2.17035400
C	4.84624100	-1.40308600	0.95638400	H	-6.95688400	-3.97739900	-1.01109000	H	-3.03446900	4.86246900	-2.07741300
C	4.16999800	-3.34510100	-0.30695600					H	-3.51222300	5.87730400	0.14645400
C	6.12448900	-1.93858400	1.09591200					N	0.65779600	-0.43016200	0.03035700

C	-0.30564200	0.57877800	0.11612700	C	-0.72782500	-2.52767900	0.01926800	H	3.84946300	4.75082600	-1.36144300
C	-1.53541500	0.34107500	0.92545700	H	-0.67879900	-3.55375000	0.42393800	H	1.44629000	4.37154200	-0.93319700
C	-1.37504000	-0.04272000	2.25890600	C	-1.75466100	-2.00773200	-0.67600800	C	0.26533600	2.05228900	-0.17397400
C	-2.81738200	0.62592500	0.44284200	C	-3.00405700	-2.67199200	-0.87733900	C	2.07761600	-0.14987700	-0.08993800
C	-2.48360500	-0.13611200	3.10350900	C	-3.36751400	-3.24535800	-2.12626400	C	-0.63480800	3.23454200	-0.02924600
H	-0.37562600	-0.27933400	2.63147300	C	-3.99155400	-2.71409900	0.14496700	C	-1.00492100	3.70686200	1.23452400
C	-3.91753300	0.54407600	1.28695800	C	-4.61518400	-3.81954800	-2.32848600	C	-1.12469300	3.89253300	-1.16420600
H	-2.93867400	0.87745300	-0.61033900	H	-2.63510100	-3.22341100	-2.93636300	C	-1.86094400	4.79930100	1.36173800
C	-3.75448000	0.16706800	2.62439500	C	-5.24374900	-3.27780000	-0.07593600	H	-0.62485000	3.19594600	2.12118400
H	-2.34697900	-0.44539800	4.14152300	H	-3.74108400	-2.29045000	1.12018100	C	-1.97887200	4.98697700	-1.03895900
H	-4.91397500	0.75027000	0.89348600	C	-5.57736500	-3.83899500	-1.31155500	H	-0.83110700	3.53099000	-2.15240600
H	-4.62213900	0.09285400	3.28264200	H	-4.84784200	-4.25967000	-3.30258600	C	-2.35241400	5.44143800	0.22573600
C	2.65471000	-1.35924800	0.18037300	H	-5.97265200	-3.28910300	0.73987300	H	-2.14680800	5.14978800	2.35500100
C	4.08202500	-1.69300600	0.32950100	H	-6.56105700	-4.28116300	-1.47983800	H	-2.35700000	5.48529700	-1.93350400
C	5.00325400	-0.81316700	0.91764500					H	-3.02414700	6.29585700	0.32537300
C	4.52617000	-2.96975100	-0.04842300					N	0.67653200	-0.28680600	-0.01114200
C	6.33720500	-1.18078600	1.08101800	10-C4(5)aryl-H				C	-0.19004900	0.80559100	0.12726800
H	4.65851300	0.16327400	1.26404700					C	-1.50946600	0.57297300	0.77869600
C	5.85823900	-3.33749100	0.11907800	C	1.66732300	2.25928100	-0.51892000	C	-1.54380300	-0.05594900	2.02921500
H	3.79298500	-3.66120000	-0.46518500	C	2.58594000	1.17732100	-0.39911000	C	-2.71196800	0.97111600	0.18758300
C	6.77325100	-2.44282600	0.67676400	C	3.95921500	1.41718300	-0.61233400	C	-2.75844900	-0.30508400	2.66116600
H	7.03770600	-0.48128400	1.54166400	C	4.39531100	2.68643100	-0.95935600	H	-0.60613500	-0.37220600	2.49198600
H	6.18662400	-4.33268100	-0.18746300	C	3.49624600	3.75274200	-1.09227600	C	-3.92851600	0.71909400	0.81883400
H	7.81779200	-2.73193300	0.80687500	C	2.14710200	3.53939800	-0.86229200	H	-2.69070400	1.46384200	-0.78619100
N	1.72363600	-2.34640800	0.30940400	H	4.64541100	0.52444200	-0.46389900	C	-3.95653400	0.07404600	2.05360400
C	0.52784500	-1.80068800	0.17621000	H	5.46313000	2.85160500	-1.12542700	H	-2.77044200	-0.80340500	3.63204900

H	-4.86016500	1.01630200	0.33478600	H	-5.11882700	-5.01651200	0.60834600	C	-2.22546000	3.94266700	0.37554600
H	-4.90986300	-0.13599800	2.54113000	H	-6.68638000	-4.35360600	-1.21295900	H	-0.25824700	3.19315200	0.88597000
C	2.59461200	-1.45858100	0.08960500	C	4.03298800	-3.41284900	0.45283000	C	-3.66534300	2.38970600	-0.77692200
C	3.97387300	-2.02837300	0.16718000	H	3.10882300	-3.97739000	0.58604100	H	-2.83058300	0.44548000	-1.18496100
C	5.13407500	-1.23796900	-0.02380800					C	-3.45170000	3.65172200	-0.22255000
C	6.34501700	-1.95454600	0.10127900					H	-2.04686500	4.93106400	0.80217200
C	5.25862800	-4.05680700	0.56432000	12				H	-4.61428600	2.15981500	-1.26412300
C	6.43272200	-3.31771900	0.38650000					H	-4.23561700	4.40939300	-0.26534300
H	7.29727500	-1.41808500	-0.03250600	C	-1.47107200	-2.85207100	-0.65056300	N	0.95818500	1.10039900	-0.03622500
H	5.29912600	-5.12681800	0.78690500	C	-1.52529500	-1.65151800	0.07261300	C	1.68659300	0.00807600	-0.01775700
H	7.40778100	-3.81172700	0.47063700	C	-2.63204900	-1.40938800	0.90080200	C	3.15449400	-0.03787500	-0.00384500
N	1.53723500	-2.31008400	0.21711100	C	-3.66038800	-2.34199800	0.99150000	C	3.86468800	-1.23856400	-0.12747400
C	0.41532200	-1.63687100	0.11748500	C	-3.59657300	-3.53564900	0.27002600	C	3.86261700	1.16396000	0.13301700
C	-0.86224000	-2.31874200	-0.02002800	C	-2.49755400	-3.78910500	-0.54855000	C	5.25746600	-1.23972900	-0.10349600
H	-0.88429700	-3.28042200	0.50011200	H	-0.62773100	-3.04147300	-1.31865800	H	3.33809600	-2.18662400	-0.25758600
C	-1.90252800	-1.93062200	-0.78044300	H	-2.67396800	-0.48265000	1.47568400	C	5.25296400	1.15902600	0.15368600
H	-1.80173900	-1.02715700	-1.38698600	H	-4.51476100	-2.14056300	1.63934800	H	3.29397100	2.09020000	0.22012100
C	-3.19728300	-2.61120300	-0.87591400	H	-4.40280400	-4.26637800	0.34699000	C	5.95592000	-0.04181000	0.03835300
C	-4.10092300	-2.23939900	-1.88549100	H	-2.44275800	-4.71637700	-1.12079800	H	5.79903900	-2.18162000	-0.20140400
C	-3.59617500	-3.61586800	0.02384600	C	-0.42180500	-0.68393200	-0.00912000	H	5.79486700	2.09980900	0.26120500
C	-5.34163200	-2.85919800	-2.00924700	C	-0.35067600	0.70477100	-0.04257900	H	7.04661200	-0.04325900	0.05586600
H	-3.81308500	-1.45040600	-2.58420000	N	0.88944900	-1.09839600	-0.01274600				
C	-4.83313100	-4.23862900	-0.10236000	H	1.18781600	-2.05878600	0.09708100				
H	-2.93186400	-3.89619500	0.84252100	C	-1.43796900	1.69963500	-0.10791800	12-C _{aryl} -H			
C	-5.71424600	-3.86670400	-1.12007600	C	-1.22488500	2.97609000	0.43015900				
H	-6.02263300	-2.55307200	-2.80572500	C	-2.66500900	1.42178600	-0.72638700	C	-1.01143600	-2.94622200	-0.54786800

C	-1.29866200	-1.70964700	0.05625100	C	1.68046100	0.30782000	-0.01646800	H	1.06530200	-2.02602200	0.13870900
C	-2.51134600	-1.58176900	0.75615300	C	3.15374400	0.21869600	-0.00402900	C	-1.51132700	1.76807700	-0.01166300
C	-3.41313500	-2.63951400	0.82021600	C	3.66002000	-1.10899200	0.00320000	C	-1.16950000	3.05541400	-0.46136600
C	-3.12112000	-3.85879000	0.20568600	C	3.92935300	1.38510100	0.00142200	C	-2.83633600	1.51361600	0.37557900
C	-1.91112400	-4.00643900	-0.47201200	C	5.06917000	-1.14840500	0.01683200	C	-2.12829200	4.06150800	-0.53799200
H	-0.07133700	-3.06377200	-1.09006300	C	5.31782700	1.26890600	0.01522400	H	-0.13481600	3.24638100	-0.74802900
H	-2.73332600	-0.64113300	1.26248300	H	3.44029900	2.36383800	-0.00643500	C	-3.79008100	2.52795800	0.28853600
H	-4.34838000	-2.51512900	1.36990600	C	5.88547600	-0.00895800	0.02308200	H	-3.08014800	0.50114000	0.75066000
H	-3.82748300	-4.68886800	0.26251200	H	5.58524700	-2.12051000	0.02365000	C	-3.44884000	3.80184800	-0.16631600
H	-1.66494700	-4.95588600	-0.95160400	H	5.95123400	2.15994900	0.01934200	H	-1.84378700	5.05500100	-0.89312700
C	-0.32095800	-0.61991700	-0.00881800	H	6.97654400	-0.11291800	0.03431500	H	-4.81833400	2.31565900	0.59164600
C	-0.41053200	0.77978300	-0.01308000					H	-4.20347200	4.58969800	-0.22775400
N	1.02258500	-0.86920700	-0.03142200					N	0.85740800	1.13476600	0.04035700
H	1.68656500	-1.68390500	0.00503400	12-C4(5) _{aryl} -H				C	1.59021000	0.04600500	0.05488100
C	-1.59332000	1.65650000	-0.07223700					C	3.05194500	0.00604700	0.06823700
C	-1.50117100	2.95351500	0.45917900	C	-1.57606100	-1.71843200	0.02657800	C	3.77500700	-1.19246200	-0.03132300
C	-2.79612600	1.27707700	-0.68915700	C	-2.76665200	-1.59208600	0.78977700	C	3.76477100	1.21203700	0.17970800
C	-2.58555600	3.82470700	0.40921300	C	-3.58759100	-2.74302400	0.70959900	C	5.16823100	-1.18647000	-0.01257600
H	-0.54969000	3.25285200	0.90007800	C	-3.28936400	-3.89577300	-0.02158200	H	3.24941900	-2.14404000	-0.13464500
C	-3.88218800	2.14871300	-0.73361600	C	-2.11464600	-3.95264600	-0.77750500	C	5.15419800	1.21326600	0.19445200
H	-2.87110600	0.29198400	-1.15250900	H	-4.54048300	-2.75270200	1.26119300	H	3.18852300	2.13482800	0.25542600
C	-3.78668400	3.42565500	-0.17969100	H	-3.97557300	-4.75055800	-0.02096600	C	5.86687200	0.01450600	0.10058200
H	-2.49290600	4.82699400	0.83309200	H	-1.87715200	-4.82916700	-1.38594300	H	5.71130400	-2.13028600	-0.09114500
H	-4.80742100	1.83116400	-1.21921900	C	-0.52886900	-0.66579900	0.06226900	H	5.69104700	2.15995300	0.28289800
H	-4.63751200	4.10865100	-0.21773300	C	-0.45475500	0.73909900	0.05342900	H	6.95804900	0.01791900	0.11483900
N	0.84142100	1.33203300	-0.00425500	N	0.78797000	-1.05687700	0.06174900	C	-1.26058100	-2.85574800	-0.75499400

H	-0.35754300	-2.87467200	-1.37836600	C	4.35476600	-1.35679500	0.12784600	H	-3.64606400	-0.26861700	-0.11506500
				C	3.76946700	0.95706100	-0.18908200	C	-1.61265800	0.33919100	-0.08886300
				C	5.70634500	-1.01969000	0.12551300	C	-1.78692000	1.80683800	-0.05718800
14				H	4.05323300	-2.39901800	0.25232600	C	-0.65823500	2.62840100	0.22700000
				C	5.11789000	1.29509500	-0.19124800	C	-3.32252100	3.68472800	-0.25556500
N	-2.66808500	-0.67068800	-0.15022700	H	3.02295700	1.74154200	-0.32266600	C	-0.98162000	4.00445300	0.25654400
H	-3.65930300	-0.47003400	-0.11529100	C	6.09466900	0.30909800	-0.03306000	C	-2.25705000	4.53782800	0.04355300
C	-1.66231500	0.26718400	-0.06375800	H	6.45978500	-1.79955900	0.24754800	H	-4.32316800	4.07888100	-0.45148500
C	-1.93009200	1.70739000	-0.01109300	H	5.41250100	2.33785000	-0.32090100	H	-0.18200400	4.73305200	0.46284900
C	-2.97157100	2.26791400	-0.76805200	H	7.15202000	0.57764800	-0.03654700	H	-2.42691900	5.61947200	0.09723700
C	-1.16287800	2.55237700	0.80625600	C	-2.09135200	-1.90856300	-0.18012600	N	-0.88618900	-1.82524300	-0.15145600
C	-3.23582500	3.63357900	-0.71191300	C	-2.89764700	-3.17647900	-0.22336100	C	-0.49456100	-0.49978100	-0.09473100
H	-3.56173700	1.62879800	-1.42865600	H	-3.58383500	-3.10292000	-1.08564300	C	0.89109500	-0.08370400	-0.04828100
C	-1.42090400	3.92010400	0.84896100	C	-3.74255000	-3.32659400	1.04802000	H	0.98330600	1.00766600	0.03306400
H	-0.37863100	2.12213400	1.43100700	H	-4.42389700	-2.47577100	1.19683800	C	1.94088800	-0.92959000	-0.07458400
C	-2.45806100	4.46599200	0.09275600	H	-4.35230700	-4.23997500	0.99946400	H	1.74647500	-2.00464200	-0.14397200
H	-4.04625800	4.05265700	-1.31027300	H	-3.08858400	-3.39383600	1.92987000	C	3.34447500	-0.51526600	-0.01672000
H	-0.81628300	4.56268600	1.49078900	C	-1.98139100	-4.37790900	-0.42800300	C	4.36413800	-1.48102800	-0.09152700
H	-2.66187300	5.53679300	0.13284500	H	-2.57287700	-5.30201700	-0.48759400	C	3.73532500	0.83370200	0.11448800
N	-0.78849000	-1.81627200	-0.13708100	H	-1.38863900	-4.27097100	-1.34531500	C	5.71072900	-1.12586800	-0.04279200
C	-0.48910000	-0.47541300	-0.06892900	H	-1.27520800	-4.45984800	0.40979700	H	4.08121900	-2.53182400	-0.19128500
C	0.88021700	0.02038800	-0.07078500					C	5.07876900	1.18612700	0.16263700
H	1.00002300	1.10412800	-0.14431100					H	2.96787000	1.60766500	0.18252800
C	1.95106000	-0.78966900	-0.00866500	14-C4(5) _{aryl} -H				C	6.07947400	0.21227000	0.08400100
H	1.75782400	-1.86385400	0.06459800					H	6.47762800	-1.90154100	-0.10456500
C	3.36045900	-0.37802100	-0.02573300	N	-2.67386700	-0.54045300	-0.13846000	H	5.35139700	2.23881500	0.26488400

H	7.13282000	0.49624300	0.12277700	C	-0.86039100	3.95080000	0.58627000	H	-5.02846600	-1.90715200	-0.33525400
C	-2.18908100	-1.81982100	-0.17363200	H	0.18428100	2.09373500	0.93243600	H	-5.18169600	-3.56897100	0.26017600
C	-3.08761400	-3.02539600	-0.19815100	C	-2.00899300	4.56849700	0.08520600	H	-4.52323100	-2.30796600	1.33059000
H	-3.78777900	-2.91078400	-1.04621800	H	-3.90371600	4.24540400	-0.89947100	C	-2.50604500	-4.14353700	0.59747100
C	-3.91746300	-3.11841700	1.08844700	H	-0.07628700	4.55277500	1.04989900	H	-3.07971600	-5.07354600	0.46579800
H	-4.51998900	-2.21292100	1.25299500	H	-2.12689400	5.65175100	0.14583000	H	-1.46961100	-4.29356300	0.27123700
H	-4.60153900	-3.98041900	1.05450700	N	-0.91787600	-1.85153000	-0.16009000	H	-2.48055100	-3.89330000	1.66913700
H	-3.25007900	-3.23669100	1.95519100	C	-0.45573100	-0.55241700	-0.14867400				
C	-2.26289400	-4.28925500	-0.41503000	C	0.96670100	-0.19583400	-0.20213000				
H	-2.91301400	-5.17637400	-0.44803800	H	1.14053200	0.85178400	-0.52097600	1a-D			
H	-1.68745800	-4.22504300	-1.34748600	C	1.97743700	-1.03671100	0.08277400				
H	-1.53658900	-4.40331000	0.40171500	C	3.34665200	-0.66437500	0.02258300	C	1.84768600	2.86212200	-0.65285800
C	-3.07927900	2.31634800	-0.31343600	C	4.03779100	-0.12412800	1.14837100	C	2.10439800	1.68991400	0.07337000
H	-3.91570800	1.65968400	-0.58724800	C	4.14262300	-0.87346100	-1.14346800	C	3.24141900	1.63683400	0.89425500
				C	5.39205100	0.17753300	1.10367200	C	4.10220000	2.72677100	0.97475400
				H	3.46805400	0.04722700	2.06493400	C	3.83754500	3.89035700	0.24990200
14-C4(5) _{styryl} -H				C	5.49556200	-0.56578200	-1.17339400	C	2.70633700	3.95580100	-0.56144200
				H	3.65497600	-1.28945800	-2.02816500	H	0.98027400	2.90689800	-1.31542800
N	-2.67283800	-0.51490000	-0.16897500	C	6.15018300	-0.03786600	-0.05346100	H	3.43964000	0.73201300	1.47140100
H	-3.62659400	-0.21050600	-0.03822500	H	5.87170300	0.59679000	1.99398500	H	4.98241500	2.67183600	1.61693600
C	-1.55538000	0.31208700	-0.13464100	H	6.05811700	-0.73805700	-2.09657700	H	4.51295700	4.74419100	0.31842200
C	-1.69354300	1.76114700	-0.07551800	H	7.21596200	0.19625300	-0.08143400	H	2.49585200	4.85880000	-1.13637900
C	-2.84450700	2.39926500	-0.57864600	C	-2.22353100	-1.79914700	-0.15978200	C	1.17510100	0.55347200	0.00155800
C	-0.70310300	2.57079100	0.51615500	C	-3.13399400	-2.99931600	-0.19579200	C	1.33531200	-0.82980400	-0.02952400
C	-3.00211800	3.78035000	-0.49459700	H	-3.20663000	-3.32099000	-1.25080800	C	-0.78961400	-0.47813500	0.00791400
H	-3.61500600	1.80293400	-1.07358100	C	-4.54503900	-2.67291900	0.29158800	N	-0.18497800	0.74627500	0.00615400

H	-0.63858500	1.64502600	0.10767600	H	-7.02912200	-2.36397300	0.18252600	C	-4.88485500	-3.37360600	0.12864500
C	2.57165100	-1.63188300	-0.09916600	H	-8.50626200	-0.36443800	0.02941600	H	-3.49921700	-4.87513500	0.83627600
C	2.56899900	-2.92850900	0.43317200					H	-6.00109000	-1.67999400	-0.60860800
C	3.73667800	-1.15562800	-0.71648500					H	-5.75521900	-4.03195700	0.18274600
C	3.71359600	-3.71891000	0.37509200	1a-D-C4(5) _{aryl} -H				N	-0.21433500	-1.42987300	-0.04840500
H	1.64954600	-3.30175900	0.88551100					C	2.11625400	-0.69505500	-0.05786200
C	4.88129300	-1.94760900	-0.77038700	C	-1.64942900	2.85137000	0.76574200	H	2.36836200	-1.75794000	-0.06825900
H	3.74127600	-0.16404800	-1.17207900	C	-2.14660200	1.78079300	-0.01671100	C	3.08198700	0.24845800	-0.04717800
C	4.87616100	-3.22963700	-0.22088700	C	-3.34594700	1.84663200	-0.77336300	H	2.79202700	1.30420900	-0.03194600
H	3.69826500	-4.72511900	0.79717000	C	-3.97299300	3.11358800	-0.68727200	C	4.52663200	0.00781600	-0.05066800
H	5.77994300	-1.56444500	-1.25651800	C	-3.49237400	4.20084900	0.04618000	C	5.40753000	1.10354500	-0.02699500
H	5.77303800	-3.84932300	-0.26606200	C	-2.31942500	4.06837900	0.79644600	C	5.09341100	-1.28094500	-0.07658000
N	0.11217600	-1.43653800	-0.01329700	H	-4.91429900	3.27612400	-1.23447100	C	6.78859500	0.92615100	-0.02817600
C	-2.22511700	-0.70093500	0.02471700	H	-4.03467200	5.15330400	0.05253000	H	4.99042700	2.11302600	-0.00744800
H	-2.48581500	-1.75923100	0.07858800	H	-1.94388300	4.89392400	1.40642300	C	6.47196000	-1.45819700	-0.07756300
C	-3.16826800	0.25503400	-0.02745600	C	-1.28194500	0.57637700	-0.06226200	H	4.44261700	-2.15601800	-0.09717200
H	-2.85992000	1.30417100	-0.09900100	C	-1.43852700	-0.82823400	-0.06346700	C	7.33189100	-0.35730300	-0.05328200
C	-4.62254700	0.04993900	-0.00756400	C	0.69229100	-0.47225600	-0.05414300	H	7.44497400	1.79833000	-0.00959200
C	-5.46854600	1.16596700	-0.09205500	H	-0.75186600	2.72536400	1.38428300	H	6.88253600	-2.46960700	-0.09808000
C	-5.21016800	-1.22257300	0.09226900	C	-2.64901400	-1.67288800	-0.00772000	H	8.41347300	-0.50096000	-0.05450000
C	-6.85393300	1.02181500	-0.07920200	C	-2.51562600	-3.00359200	0.42597100	N	0.07693000	0.74760800	-0.05773500
H	-5.02786900	2.16250200	-0.16958400	C	-3.91644200	-1.20583900	-0.38816300	H	0.51282700	1.65857000	-0.11207300
C	-6.59238100	-1.36721100	0.10466700	C	-3.62213500	-3.84483700	0.49372100				
H	-4.57981400	-2.10996900	0.16201100	H	-1.52351800	-3.35980600	0.70525900				
C	-7.42189300	-0.24648600	0.01895500	C	-5.01951700	-2.05661300	-0.31057600	1a-D-C2 _{styryl} -H			
H	-7.49165400	1.90447700	-0.14619400	H	-3.99595600	-0.16313500	-0.75070900				

C	1.42299500	2.87843200	-0.59179300	H	6.06847900	-3.52207400	-0.19079800
C	1.87377500	1.70915900	0.04555300	N	0.22730500	-1.62161200	-0.01032400
C	3.07194700	1.77644000	0.77885300	C	-2.21771600	-0.97593800	-0.00768800
C	3.80147700	2.95884800	0.84645000	H	-2.51060500	-2.03907200	0.00980400
C	3.34622700	4.11135100	0.20229700	C	-3.05009800	0.08347400	-0.00916400
C	2.14935700	4.06422900	-0.51134200	C	-4.47932800	-0.06440400	0.00427600
H	0.49720600	2.84525700	-1.16951300	C	-5.22320400	-0.06384600	1.21359800
H	3.41803400	0.88648800	1.30685900	C	-5.23686800	-0.14918500	-1.19350000
H	4.72867600	2.98544200	1.42239300	C	-6.61031100	-0.15037700	1.21975100
H	3.91687700	5.03959600	0.26298600	H	-4.67387000	0.00671400	2.15519800
H	1.77827600	4.95760500	-1.01738400	C	-6.62420800	-0.23370100	-1.17774500
C	1.07868100	0.48093200	-0.01843600	H	-4.69833400	-0.14745600	-2.14393000
C	1.37981800	-0.88281100	-0.01868600	C	-7.33463300	-0.23410100	0.02649200
C	-0.77135800	-0.75170900	-0.02381400	H	-7.14004100	-0.15507700	2.17688700
N	-0.29333200	0.51783400	-0.04453300	H	-7.16489000	-0.30516300	-2.12608600
H	-0.95993500	1.28941000	0.00449800	H	-8.42433200	-0.29688000	0.03497500
C	2.68405300	-1.56684200	-0.07079000				
C	2.78397900	-2.86718200	0.45026300				
C	3.82168400	-1.00163000	-0.66834300				
C	3.98974000	-3.56137900	0.40990600				
H	1.88320500	-3.31225400	0.87433300				
C	5.02879000	-1.69646900	-0.70371800				
H	3.75141800	-0.01275300	-1.12422000				
C	5.12272300	-2.97771300	-0.15957800				
H	4.04633900	-4.56981500	0.82531100				
H	5.90055600	-1.23699600	-1.17435400				