

C–H bond cleavage occurring on a Rh(V) intermediate: a theoretical study of Rh-catalyzed arene azidation

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Table of Contents

1. Completes reference for Gaussian 09. Page S2
2. B3LYP and M11-L absolute calculation energies, enthalpies, and free energies. Page S2
3. B3LYP geometries for all the optimized compounds and transition states. Page S4

1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2013**.

2. B3LYP and M11-L absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3LYP})}^1$	$H_{(\text{corr-B3LYP})}^2$	$G_{(\text{corr-B3LYP})}^3$	$E_{(\text{solv-M11-L})}^4$	IF ⁵
1	-1189.451186	0.298477	0.226898	-1189.663720	-
2-PhPy	-479.335204	0.179954	0.135414	-479.352152	-
2	-1668.776201	0.479794	0.387809	-1669.010366	-
3-ts	-1668.730054	0.475873	0.385531	-1668.981967	-331.9
4	-1439.699128	0.411133	0.332101	-1439.915890	-
HOAc	-229.077610	0.067547	0.034692	-229.101916	-

5	-1208.385224	0.478779	0.390787	-1208.630665	-
Cl ⁻	-460.2487316	0.002360	-0.015023	-460.388508	-
6-ts	-1208.353667	0.472593	0.384941	-1208.598860	-1084.4
7	-979.263421	0.408726	0.333437	-979.499260	-
PhI(OAc)OTs	-1366.194930	0.298578	0.215981	-1366.294618	-
8	-1660.696056	0.454647	0.347019	-1661.004890	-
OTs ⁻	-894.819963	0.141933	0.093238	-894.954216	-
9-ts	-1660.651442	0.452941	0.348405	-1660.975237	-61.8
10	-1417.626801	0.354820	0.272589	-1417.898995	-
IPh	-243.053411	0.097115	0.058488	-243.112570	-
11	-1436.434808	0.534364	0.434411	-1436.847458	-
12-ts	-1436.425403	0.530839	0.435996	-1436.842691	-47.9
13	-1207.352267	0.464317	0.37675	-1207.751932	-
N ₃ ⁻	-164.206993	0.013453	-0.007002	-164.341272	-
14	-1371.883503	0.482062	0.388706	-1372.158522	-
PhI(N ₃)OTs	-1301.897143	0.257526	0.178533	-1302.001886	-
15	-1846.654319	0.526776	0.415097	-1846.974502	-
16-ts	-1846.632151	0.525404	0.415023	-1846.972937	-35.1
17	-1603.619178	0.428208	0.342452	-1603.896475	-
18-ts	-1371.870231	0.480737	0.388805	-1372.142921	-329.1
19	-1371.960896	0.484084	0.390229	-1372.218118	-
PD	-642.926336	0.185323	0.134561	-642.9386971	-
20-ts	-1371.867491	0.480615	0.388080	-1372.135222	-405.4
21	-1371.943371	0.483614	0.388146	-1372.205899	-
OAc ⁻	-228.493171	0.053704	0.020696	-228.635091	-
PD'	-707.217562	0.226094	0.170254	-707.230574	-
22-ts	-1603.605828	0.426813	0.342224	-1603.883831	-335.0
23	-1603.695072	0.430123	0.344274	-1603.960669	-
24-ts	-1603.600330	0.426663	0.341017	-1603.877086	-279.0
25	-1603.652362	0.428927	0.341569	-1603.922002	-

PD''	-938.932923	0.171185	0.123336	-938.945522	-
26-ts	-1846.639534	0.524981	0.412777	-1846.970297	-225.1

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to enthalpy calculated by B3LYP in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M11-L in acetone solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

3. B3LYP geometries for all the optimized compounds and transition states.

1				H	3.13841700	-2.19050400	-0.36542000
Rh	-0.20679200	-0.16011700	-0.00026600	C	-0.72525400	0.02900000	-0.00389500
C	1.82863600	-0.36037800	0.73252800	C	-1.41755400	-1.17976300	0.18163400
C	1.83365200	-0.36651000	-0.72058300	C	-1.47203600	1.20334300	-0.19542100
C	1.29806000	0.90625900	1.16299300	C	-2.81002100	-1.20899100	0.19215400
C	1.30442900	0.89518800	-1.16537300	H	-0.84147300	-2.08859700	0.31512900
C	0.96667300	1.69003200	-0.00550300	C	-2.86619400	1.17286600	-0.18783700
Cl	-0.75639500	-2.48529300	-0.00285200	H	-0.96819600	2.14787500	-0.37783300
C	-2.70005200	0.24749400	-0.00005900	C	-3.54169300	-0.03267000	0.01004900
O	-2.04502800	0.20685400	-1.09225900	H	-3.32665500	-2.15325100	0.34363800
O	-2.04474400	0.20352800	1.09195200	H	-3.42440000	2.09213600	-0.34472800
C	-4.20272600	0.29275600	0.00033900	H	-4.62820300	-0.05609500	0.01679200
H	-4.57865600	-0.73702000	-0.00155000				
H	-4.57151800	0.79186700	0.89970600	2			
H	-4.57185100	0.79526500	-0.89699900	Rh	-0.72435400	-0.15088500	0.01488800
C	2.34481200	-1.46937900	1.59847700	C	-1.71258900	-0.91587100	1.84969600
H	3.44323300	-1.46770400	1.60763200	C	-2.63486800	-0.99846400	0.75664700
H	1.99908700	-1.36765400	2.63009100	C	-0.58886000	-1.78881200	1.54388100
H	2.00186100	-2.43924500	1.22820600	C	-2.05488700	-1.83814800	-0.26459600
C	2.35447400	-1.48353700	-1.57322200	C	-0.79536300	-2.35807100	0.25598400
H	3.45288100	-1.48756700	-1.56852200	C	-2.41447800	1.81704400	-1.52556800
H	2.00154400	-2.44915000	-1.20116800	O	-3.10965100	0.93082100	-2.01930400
H	2.02217300	-1.38636100	-2.60965100	O	-1.51821900	1.68074000	-0.58103100
C	1.11934100	1.32522300	-2.58901200	C	-2.53071900	3.26263100	-2.00695200
H	1.97663400	1.92872500	-2.91649600	H	-2.45482700	3.96775700	-1.17348200
H	1.03449400	0.46697500	-3.25961600	H	-1.70112600	3.46900200	-2.69339000
H	0.21597200	1.93017300	-2.70568800	H	-3.47356300	3.40562900	-2.53978900
C	0.46036400	3.10189100	-0.01441100	C	-1.93396900	-0.21398500	3.15743800
H	1.29543800	3.81601200	-0.02258800	H	-0.99137400	0.13597300	3.58991600
H	-0.15403600	3.29987200	-0.89722000	H	-2.59273200	0.65137800	3.04142700
H	-0.14814600	3.31323100	0.86931000	H	-2.40130000	-0.88662500	3.89047100
C	1.10591900	1.34799900	2.58209300	C	-3.99106100	-0.36539400	0.69741700
H	1.00232400	0.49514400	3.25696900	H	-4.74445600	-1.09310600	1.03102800
H	1.96906900	1.94066700	2.91396500	H	-4.05871800	0.50668100	1.35395000
H	0.21055100	1.96674000	2.68694900	H	-4.22493300	-0.04751500	-0.31920700
				C	-2.70958400	-2.23885900	-1.55108000
2-PhPy				H	-3.43697100	-3.04425500	-1.37479900
C	0.76316200	0.03131200	-0.00003300	H	-3.21660900	-1.38044900	-1.99620000
C	1.51077200	1.20317900	0.21201600	H	-1.96802600	-2.59605500	-2.26908100
C	2.90123900	1.13909700	0.19449200	C	0.08219500	-3.34618500	-0.44928600
C	3.52004300	-0.09114900	-0.02296400	H	1.09659500	-3.34562300	-0.04361900
C	2.70013500	-1.20628400	-0.20365200	H	-0.32974000	-4.35980200	-0.35043600
N	1.36682900	-1.15801000	-0.19557400	H	0.15609300	-3.10278500	-1.51230300
H	3.49159200	2.03699000	0.35762600	C	0.50046600	-2.12784000	2.51631000
H	1.01442300	2.14719200	0.40882600	H	0.10870600	-2.81702100	3.27739500
H	4.60110200	-0.18931900	-0.04426000	H	1.34476900	-2.61659200	2.02780100
				H	0.87076900	-1.24160400	3.04091200

C	2.17549800	1.41028900	0.43185900	H	-4.39949500	1.56633500	-0.91062800
N	0.86320800	1.30586500	0.75982000	H	-1.60632900	-2.38069300	-1.69925400
C	2.88119800	2.60213400	0.66159000	C	-3.56842500	-1.52464200	-2.03936400
C	0.27789900	2.35550600	1.37409400	H	-3.92930600	-2.35996600	-2.62968400
C	2.26196200	3.68229400	1.27846200	H	-5.35818100	-0.32599100	-2.22287800
H	3.92574300	2.64725900	0.37300200	C	-1.87563200	1.60956100	0.24179900
H	-0.77222500	2.23821100	1.60354700	C	-2.61960100	2.43634900	1.09873500
C	0.93215600	3.54569400	1.66676000	C	-0.46302000	1.72357800	0.16800500
H	0.39509800	4.34562400	2.16577600	C	-1.97704400	3.37886700	1.89768300
H	2.80993100	4.60189500	1.46418500	H	-3.69858600	2.32070900	1.16433900
C	2.95268000	0.25690600	-0.10744700	C	0.15449600	2.70077700	0.97458200
C	3.54031700	0.32593000	-1.37808200	H	0.19704800	1.62069300	-0.84182300
C	3.23406300	-0.84188500	0.71265300	C	-0.58400100	3.50945300	1.83518000
C	4.36480700	-0.70268000	-1.82968600	H	-2.55886000	4.01111400	2.56317800
H	3.31983800	1.17090400	-2.02230900	H	1.22417000	2.83938600	0.84810200
C	4.06347100	-1.87117900	0.26169900	H	-0.08297100	4.26259400	2.43862400
H	2.82549900	-0.87457600	1.71670800				
C	4.62657200	-1.80581400	-1.01344200	4			
H	4.79748100	-0.64599200	-2.82460900	Rh	0.43527700	-0.00322500	-0.20409400
H	4.28286500	-2.71333400	0.91342300	C	1.58352600	-0.31166100	1.67575800
H	5.27277000	-2.60493300	-1.36667300	C	2.25032400	-1.19743300	0.71997600
Cl	0.32796800	-0.24030500	-2.14234000	C	1.78419600	1.04153700	1.23814400
				C	2.74469400	-0.40786900	-0.33060800
3-ts				C	2.40748400	0.99161000	-0.05292300
Rh	0.19884900	-0.56576500	0.00813600	Cl	0.16379400	-0.01738700	-2.59860900
C	0.00678200	-2.12871600	1.55673200	C	1.03062700	-0.73950400	3.00545500
C	1.08481000	-2.45401100	0.65405300	H	0.31140500	-0.01197000	3.39191300
C	0.31892400	-0.88694300	2.20981100	H	0.51970500	-1.70511000	2.93621400
C	2.09222200	-1.41025800	0.77708100	H	1.83194200	-0.84503400	3.75077900
C	1.63277500	-0.47277700	1.74900800	C	2.40260600	-2.68150200	0.89284000
Cl	0.81489200	-0.95144500	-2.29228900	H	3.24866400	-2.91319700	1.55452700
C	2.28005700	2.16927500	-1.70751600	H	1.51316900	-3.13094900	1.34716000
O	1.03361700	2.29003500	-1.95307900	H	2.58462100	-3.18565600	-0.06085500
O	2.78872500	1.86279600	-0.59875400	C	3.48043600	-0.85984200	-1.55558400
C	3.20778300	2.39315300	-2.90428100	H	4.48634400	-0.42084400	-1.58497200
H	2.81893800	3.17875100	-3.55880500	H	3.58863200	-1.94742700	-1.58633200
H	4.21922600	2.64120100	-2.57054800	H	2.94578000	-0.54853400	-2.46029000
H	3.24753700	1.46500100	-3.48761500	C	2.86836500	2.15062500	-0.88853900
C	-1.20739600	-2.97052300	1.81212200	H	2.33767100	3.07079900	-0.62724100
H	-2.06962000	-2.36082900	2.09521700	H	3.94265100	2.33738700	-0.74896800
H	-1.48347900	-3.56389400	0.93637500	H	2.69289200	1.95656500	-1.95081300
H	-1.00963800	-3.67037300	2.63520000	C	1.47597100	2.27082000	2.04106300
C	1.23095200	-3.70105500	-0.16242200	H	2.31750900	2.49895700	2.70986600
H	1.90836000	-4.40368400	0.34192500	H	1.31280200	3.14487100	1.40713500
H	0.27252600	-4.20827900	-0.30558100	H	0.58305900	2.14084000	2.65865500
H	1.64213000	-3.47049700	-1.14842400	C	-2.41725000	-0.74127200	0.11301700
C	3.41381400	-1.34824800	0.07494100	N	-1.19918100	-1.32441300	-0.06348500
H	4.20501300	-1.74847100	0.72513900	C	-3.56721900	-1.54158600	0.20512400
H	3.39642800	-1.93138400	-0.84810000	C	-1.10551900	-2.65675100	-0.19838600
H	3.65333400	-0.31220900	-0.18504800	C	-3.46324600	-2.92165300	0.09929100
C	2.44349400	0.67748600	2.25351500	H	-4.53546700	-1.07438700	0.34443700
H	1.86801400	1.31790100	2.92506400	H	-0.11053500	-3.04369400	-0.38583600
H	3.30650500	0.28658500	2.81027300	C	-2.20787800	-3.49733800	-0.11552600
H	2.81252500	1.27304000	1.41092500	H	-2.08208700	-4.56896400	-0.22703700
C	-0.47105700	-0.23187000	3.30380500	H	-4.35157200	-3.54317300	0.16847100
H	-0.09819900	-0.54469200	4.28898300	C	-2.38072200	0.71891600	0.13856000
H	-0.40043600	0.85714400	3.24834200	C	-3.52265400	1.52514200	0.28947300
H	-1.52997600	-0.49979100	3.25069900	C	-1.10473300	1.29738000	-0.07376900
C	-2.53206700	0.55944600	-0.54791300	C	-3.41646300	2.90870100	0.20651400
N	-1.78840300	-0.55220100	-0.76815200	H	-4.49749600	1.07500300	0.46053500
C	-3.83080400	0.65669900	-1.06822800	C	-1.03196000	2.69031200	-0.19708900
C	-2.28263100	-1.55512500	-1.51377700	C	-2.16921500	3.48824300	-0.05231200
C	-4.35575300	-0.39430000	-1.81013100	H	-4.29875300	3.53174900	0.32315200

H	-0.08273900	3.16461800	-0.42926300
H	-2.08414300	4.56845800	-0.14910100
HOAc			
C	-0.09249300	0.12562300	-0.00002700
O	-0.77858800	-1.04668800	0.00001200
O	-0.64580400	1.20195500	0.00000400
C	1.39759000	-0.10974700	-0.00001700
H	1.91743500	0.84850800	-0.00016000
H	1.68537800	-0.69121800	0.88218900
H	1.68538600	-0.69168800	-0.88188000
H	-1.72363900	-0.80299700	-0.00000800

5

Rh	0.88811400	0.04816200	0.08890200
C	1.84718600	-0.25028800	-1.83356800
C	2.71804200	-0.77001700	-0.78854100
C	0.63836400	-1.03886400	-1.82752700
C	2.02110800	-1.81684000	-0.10918000
C	0.72062000	-1.98237300	-0.75113300
C	1.30917500	1.15216400	2.35106200
O	0.59396000	0.10204500	2.26506600
O	1.82272700	1.60026600	1.26738500
C	1.51424700	1.86120300	3.65749800
H	2.46598500	2.39713700	3.65666200
H	0.70941800	2.59309800	3.79741900
H	1.47493100	1.15097800	4.48650300
C	2.22093800	0.79686400	-2.83894200
H	1.34076500	1.30778400	-3.23785000
H	2.88615900	1.55010500	-2.40774100
H	2.74865500	0.33734300	-3.68540600
C	4.09923900	-0.27176400	-0.49842900
H	4.80599800	-0.71294000	-1.21371300
H	4.16231300	0.81562000	-0.59409000
H	4.42808100	-0.54167300	0.50723800
C	2.53462700	-2.65604000	1.02017400
H	2.93087000	-3.60288200	0.63014000
H	3.33905000	-2.15656600	1.56474400
H	1.74159800	-2.89555400	1.73348600
C	-0.27031000	-3.05560500	-0.42619100
H	-1.28378300	-2.78114000	-0.72404100
H	0.00207400	-3.97820900	-0.95726100
H	-0.28406900	-3.28072100	0.64270100
C	-0.48145400	-0.92071400	-2.81418200
H	-0.25782500	-1.54274500	-3.69117200
H	-1.42918800	-1.26255100	-2.39416700
H	-0.60821100	0.10680000	-3.16470100
C	-2.08042300	1.23449200	-0.19801600
N	-0.74274400	1.48286400	-0.16237600
C	-2.97404600	2.24862400	-0.58167700
C	-0.30058600	2.72519200	-0.47122300
C	-2.51102300	3.51399000	-0.92025500
H	-4.03597000	2.03079500	-0.57760800
H	0.76845600	2.87703500	-0.39215100
C	-1.14042700	3.76060700	-0.85580300
H	-0.72107700	4.73265300	-1.09169200
H	-3.20667400	4.29562300	-1.21035800
C	-2.63830200	-0.08903700	0.18783500
C	-2.32495200	-0.68617600	1.41964400
C	-3.59565300	-0.69978800	-0.64289300
C	-2.95737900	-1.86934900	1.80620100
H	-1.60590800	-0.21791900	2.08160300
C	-4.21121600	-1.89154500	-0.25942000

H	-3.85632500	-0.24136500	-1.59348700
C	-3.89731800	-2.47637500	0.97044000
H	-2.72294300	-2.30862000	2.77173800
H	-4.94424300	-2.35417900	-0.91386900
H	-4.39030800	-3.39390100	1.27826900

Cl-

Cl	0.00000000	0.00000000	0.00000000
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6-ts

Rh	-0.56497700	-0.08285500	0.03466800
C	-1.46076000	0.15229600	-1.99256100
C	-2.32914500	-0.65704200	-1.16869400
C	-1.32955300	1.44451400	-1.38265000
C	-2.77690700	0.17046700	-0.06847300
C	-2.16124000	1.45546700	-0.18508600
C	-0.04839000	-1.35458300	2.68664800
O	0.86233500	-0.48767600	2.82848100
O	-0.77462400	-1.44890400	1.63923300
C	-0.30071500	-2.32508200	3.81622400
H	0.63942900	-2.80784100	4.09878800
H	-0.65534800	-1.76934800	4.69088000
H	-1.04013400	-3.07527100	3.53349600
C	-0.84593400	-0.27769700	-3.28946300
H	0.06586300	0.28060100	-3.51483000
H	-0.60379000	-1.34400900	-3.29333900
H	-1.55502400	-0.09957500	-4.10866900
C	-2.81894100	-2.04264300	-1.46862600
H	-3.77444200	-2.00338200	-2.00875600
H	-2.11579600	-2.59669700	-2.09698400
H	-2.98253300	-2.61595400	-0.55155200
C	-3.73731500	-0.26943600	0.99224000
H	-4.74743000	-0.34323700	0.56903800
H	-3.46603900	-1.25243700	1.38819500
H	-3.77428800	0.43593900	1.82522500
C	-2.45231800	2.65300700	0.67025400
H	-1.65349500	3.39466800	0.61148600
H	-3.37793500	3.13597500	0.32995000
H	-2.58979400	2.38224400	1.72088600
C	-0.61962900	2.63178400	-1.96152600
H	-1.32869800	3.25499200	-2.52242100
H	-0.17019600	3.25264800	-1.18302400
H	0.17365800	2.33271500	-2.65089400
C	2.33501400	-0.55630200	-0.49829600
N	1.14445500	-1.21428900	-0.51623000
C	3.50774600	-1.21771000	-0.88437900
C	1.09246500	-2.51097500	-0.86679300
C	3.45153500	-2.55228400	-1.27296300
H	4.45595800	-0.69345100	-0.85028400
H	0.11465000	-2.97786400	-0.82322500
C	2.22366600	-3.21774600	-1.25727700
H	2.13946900	-4.26274400	-1.53468800
H	4.35710700	-3.07331600	-1.56820700
C	2.26752000	0.82672300	-0.00149300
C	3.25116900	1.78340500	-0.27467600
C	1.13124000	1.15337800	0.79302700
C	3.12928200	3.07373200	0.24442700
H	4.10374800	1.53945300	-0.90223600
C	1.04877000	2.45903300	1.31222100
H	0.86520900	0.28709300	1.74965900
C	2.03449000	3.41116400	1.04650200
H	3.89468900	3.81358000	0.02966100
H	0.22400200	2.71701600	1.97139500

H	1.95996800	4.40851300	1.47075500
7			
Rh	0.40859900	0.00978000	-0.16039300
C	1.93753700	-0.09096300	1.33562300
C	2.29095700	-1.19388900	0.44087800
C	2.11414700	1.16383100	0.61371900
C	2.51190800	-0.64728400	-0.83176000
C	2.37443200	0.82324300	-0.73876100
C	1.69498100	-0.21316400	2.80638300
H	1.11070500	0.62711100	3.18913600
H	1.17237700	-1.13981500	3.05813700
H	2.65721600	-0.22144300	3.33861000
C	2.40411700	-2.63081800	0.85609000
H	3.37632600	-2.80894000	1.33370900
H	1.63518700	-2.90903900	1.58330100
H	2.33441500	-3.31174700	0.00322700
C	2.86657400	-1.37350700	-2.09241300
H	3.92878900	-1.22390100	-2.32798100
H	2.69420800	-2.44915300	-2.00888000
H	2.29245900	-1.00132200	-2.94723500
C	2.63274200	1.76410500	-1.87537900
H	2.21775400	2.75598100	-1.68324600
H	3.71431100	1.87646200	-2.03192100
H	2.20379400	1.39348700	-2.81120900
C	2.13305400	2.52481400	1.24157700
H	3.08061100	2.66408000	1.77848100
H	2.06430700	3.31974500	0.49556800
H	1.32120500	2.65876100	1.96123200
C	-2.45847200	-0.74551600	-0.04154100
N	-1.22987000	-1.33716300	-0.09679300
C	-3.61157500	-1.53688700	-0.01788400
C	-1.12961700	-2.67773900	-0.14721200
C	-3.50416000	-2.92398600	-0.06132500
H	-4.58750400	-1.06867200	0.03052900
H	-0.12453400	-3.07957000	-0.19884900
C	-2.24022600	-3.51206700	-0.13231600
H	-2.11226200	-4.58790400	-0.17369900
H	-4.39848500	-3.53943400	-0.04311600
C	-2.42275600	0.72415200	-0.03365900
C	-3.57758000	1.51555500	-0.03226500
C	-1.13328300	1.32278000	-0.06116600
C	-3.47348800	2.90698100	-0.06585000
H	-4.56400600	1.06160200	-0.01281500
C	-1.05928700	2.72069900	-0.10244600
C	-2.21580300	3.50933000	-0.10894600
H	-4.37243700	3.51573700	-0.06379900
H	-0.09554900	3.21797700	-0.13698200
H	-2.13195200	4.59200300	-0.14502200

PhI(OAc)OTs

I	-1.44966500	-0.83879600	-0.07196700
C	-1.81749800	1.29958500	0.01221400
C	-2.67976600	1.77649200	0.99104500
C	-1.16376600	2.09754000	-0.91770800
C	-2.90886200	3.15606300	1.01967300
H	-3.15811500	1.10764800	1.69715300
C	-1.41163600	3.47236500	-0.85814900
H	-0.46575200	1.68375100	-1.63847000
C	-2.28079100	3.99783200	0.10023300
H	-3.57681400	3.56460700	1.77255800
H	-0.91762000	4.12719300	-1.57010200
H	-2.46512600	5.06782500	0.13370300

O	0.70357000	-0.26022800	0.19534900
S	1.64721500	-0.55813500	-1.04557500
O	1.44685000	0.47015100	-2.08171800
O	1.51352500	-1.97013700	-1.43243600
C	3.24768600	-0.30297300	-0.29383400
C	3.89093300	-1.37541300	0.32704300
C	3.83380500	0.96200700	-0.33578000
C	5.13503100	-1.16758900	0.91741100
H	3.42798200	-2.35642900	0.32622100
C	5.07932700	1.15091100	0.26080600
H	3.32674600	1.77491800	-0.84410500
C	5.74545400	0.09587000	0.90002600
H	5.64442800	-2.00131200	1.39473000
H	5.54462300	2.13287200	0.22423500
C	7.08179200	0.31455100	1.56929400
H	7.59832100	1.18785800	1.15847100
H	6.95884500	0.48317000	2.64750500
H	7.73652300	-0.55557700	1.45084700
C	-4.33373200	-1.29073100	0.68752300
C	-5.74450900	-1.72620100	0.32649000
H	-6.17840600	-1.02649500	-0.39459200
H	-5.71941400	-2.71185100	-0.14864900
H	-6.35586900	-1.76195900	1.22944400
O	-3.56490400	-1.20412800	-0.39853400
O	-3.96958400	-1.04712500	1.82568600

8

Rh	-2.12206700	0.06771400	-0.20618000
C	-3.82558100	-0.51179000	0.99001800
C	-2.74345700	-0.12897700	1.88291900
C	-4.17967700	0.65409500	0.21019100
C	-2.41129600	1.24072500	1.62658900
C	-3.29233400	1.72723300	0.57338900
C	-1.50948000	-1.75843300	-1.86504900
O	-1.00394900	-1.75612300	-0.68546700
O	-2.35111200	-0.84553400	-2.14006000
C	-1.09699700	-2.77143900	-2.89236300
H	-1.93900900	-3.00784000	-3.54748900
H	-0.30046100	-2.34595400	-3.51497700
H	-0.72098900	-3.67775300	-2.41273000
C	-4.53673900	-1.83069300	0.98469300
H	-4.99618700	-2.03530200	0.01437500
H	-3.85810000	-2.65457800	1.22105900
H	-5.33587400	-1.83065900	1.73808200
C	-2.10716200	-1.03236400	2.89270100
H	-2.74100700	-1.09071200	3.78758300
H	-1.99041700	-2.04729900	2.50236600
H	-1.12456400	-0.67051400	3.20342100
C	-1.38450000	2.06489100	2.34018400
H	-1.86271900	2.64116700	3.14316600
H	-0.60878300	1.44224400	2.79232700
H	-0.90033800	2.77095600	1.66108100
C	-3.31780600	3.12671400	0.03916900
H	-3.74112600	3.16627500	-0.96713600
H	-3.93232300	3.76483900	0.68807300
H	-2.31374800	3.55597200	-0.00195100
C	-5.26489500	0.70774500	-0.81839200
H	-6.23392800	0.85365700	-0.32291300
H	-5.11895700	1.53164400	-1.52003000
H	-5.31750400	-0.22124800	-1.39236400
Cl	-0.14928000	1.30143000	-1.04068000
I	1.88633400	-0.57962600	-0.36320000
C	3.27035400	1.06522100	-0.33603400

C	3.67843300	1.56210400	0.90017900
C	3.71859300	1.56271400	-1.55788100
C	4.58960600	2.62078500	0.89718700
H	3.32477400	1.13042600	1.82870200
C	4.62426000	2.62543600	-1.52906800
H	3.37705300	1.15222000	-2.50142200
C	5.05673300	3.14983400	-0.30866400
H	4.93303700	3.02682500	1.84384500
H	4.99047300	3.03650900	-2.46478600
H	5.76360800	3.97383300	-0.29735400
C	4.78227400	-3.23774500	1.48840600
H	5.68491500	-2.99014400	0.92136600
H	4.39481800	-4.18315400	1.09843400
H	5.02163000	-3.33398100	2.54815700
C	3.75202600	-2.13903200	1.31788800
O	3.30987100	-1.44147900	2.20442300
O	3.39352100	-2.03071600	0.01535700

OTs-

O	2.30914800	-0.00003400	1.46381600
S	1.99230700	0.00000100	0.01035400
O	2.36736600	-1.25372500	-0.69807500
O	2.36737600	1.25375400	-0.69802800
C	0.16954000	-0.00000200	-0.03708100
C	-0.53866300	1.20402600	-0.03601400
C	-0.53866000	-1.20402300	-0.03601600
C	-1.93409200	1.20147100	-0.02125600
H	0.02069400	2.13398900	-0.07056400
C	-1.93409600	-1.20147000	-0.02126200
H	0.02067500	-2.13399900	-0.07056600
C	-2.65604500	-0.00000300	-0.00662600
H	-2.47507100	2.14774600	-0.02849600
H	-2.47506100	-2.14775400	-0.02850700
C	-4.16821600	0.00000400	0.04336300
H	-4.54298300	-0.00004200	1.07764900
H	-4.58744500	0.88615300	-0.44871900
H	-4.58745700	-0.88609500	-0.44879900

9-ts

Rh	2.01625400	-0.03005800	-0.35603500
C	4.15729800	-0.16433400	0.10207900
C	3.49091600	0.01601900	1.35871600
C	3.67307300	-1.40992800	-0.49054000
C	2.60377600	-1.11162700	1.56468900
C	2.72413600	-1.98961600	0.42443200
C	1.71733500	2.18411900	-1.54220600
O	1.29062700	2.00536100	-0.35398000
O	2.34653100	1.20368200	-2.07201700
C	1.47344300	3.45249800	-2.29688600
H	2.30954100	3.66124800	-2.96921900
H	0.57112800	3.33228600	-2.90818100
H	1.32094400	4.28421900	-1.60539100
C	5.21880700	0.70766400	-0.48969300
H	5.10211200	0.79861700	-1.57268500
H	5.20977200	1.71047500	-0.05743000
H	6.20551300	0.26687900	-0.29389900
C	3.69905500	1.12969300	2.33320800
H	4.29828600	0.76337400	3.17806100
H	4.23322700	1.96896800	1.88315400
H	2.74266800	1.48642400	2.72266300
C	1.83528400	-1.38085100	2.81442000
H	2.51346800	-1.82637700	3.55705800
H	1.42712300	-0.45662000	3.22829400

H	1.01554600	-2.08164900	2.64458700
C	2.04091600	-3.30975100	0.26031400
H	1.86930100	-3.54640500	-0.79167100
H	2.67066200	-4.09944000	0.69171100
H	1.07648300	-3.32882400	0.77171400
C	4.16628500	-2.00970600	-1.76937000
H	5.09613600	-2.56410700	-1.58337200
H	3.43813700	-2.70272500	-2.19576000
H	4.37979300	-1.23924300	-2.51502600
Cl	0.27363800	-1.01302100	-1.61839600
I	-2.49531100	-0.29174000	-0.21747200
C	-4.61800300	-0.26646500	-0.19881800
C	-5.31676800	-1.35263000	0.35561900
C	-5.29968200	0.83510600	-0.74421900
C	-6.70840000	-1.34203900	0.33501700
H	-4.78138000	-2.19344000	0.78438200
C	-6.69136100	0.82998700	-0.75707800
H	-4.75139300	1.67322600	-1.16193300
C	-7.39498300	-0.25433200	-0.21851500
H	-7.25925400	-2.18051600	0.75012800
H	-7.22894400	1.66989200	-1.18652100
H	-8.48077900	-0.25045900	-0.22790500
C	-1.70337100	2.34309300	2.28620600
H	-2.60186300	1.80120500	2.60008900
H	-1.90899200	2.80818300	1.31631300
H	-1.47428600	3.11721600	3.02072600
C	-0.52586800	1.40560300	2.16916700
O	-0.56980100	0.39146300	1.34864100
O	0.51063400	1.56058700	2.82750100

10

Rh	-0.01459100	0.03798000	-0.15252400
C	2.22818800	-0.80446100	-0.25547300
C	2.24610000	0.63781800	-0.38236400
C	1.56677000	-1.15521000	0.98259400
C	1.68059000	1.18667100	0.81011700
C	1.24551100	0.06917100	1.65970500
Cl	-0.11061300	-1.28452900	-2.08681900
C	-1.58250700	1.96426900	-0.31437900
O	-0.93581400	1.53443900	-1.32322100
O	-1.23069900	1.42857500	0.81017500
C	-2.66446100	2.97450300	-0.40174200
H	-3.60693200	2.42512700	-0.51630300
H	-2.71378400	3.57376400	0.51104700
H	-2.52006400	3.60927300	-1.27944000
C	2.86854900	-1.75506700	-1.19730700
H	3.88419300	-1.96300300	-0.82471100
H	2.33108600	-2.70356500	-1.25208900
H	2.95577000	-1.34126000	-2.20293300
C	2.82961800	1.38522400	-1.53874300
H	3.92568100	1.33015300	-1.50808900
H	2.49991900	0.95397400	-2.48912400
H	2.54501500	2.43883000	-1.52615600
C	1.63475200	2.62746600	1.19631900
H	2.53082300	2.86645600	1.78611000
H	1.62896200	3.28394500	0.32319800
H	0.76209400	2.85093000	1.81337800
C	0.66478000	0.19106900	3.02797300
H	1.47538900	0.37640600	3.74687800
H	-0.03852500	1.02528100	3.09306900
H	0.14909000	-0.72412700	3.32482200
C	1.32324000	-2.53102700	1.51140000
H	0.25936800	-2.66351900	1.73702000

H	1.61301700	-3.29711100	0.79056300
H	1.89449700	-2.68969000	2.43401100
C	-2.66204200	-1.18132500	0.16934600
O	-3.11550900	-0.28495300	-0.51541900
O	-1.38149700	-1.29807200	0.53671500
C	-3.48952800	-2.33956700	0.70692900
H	-3.31804500	-3.21648600	0.07293900
H	-3.20449100	-2.59793400	1.72968400
H	-4.54524700	-2.06666800	0.66341300

Iph

I	-1.57006600	-0.00000100	-0.00000200
C	0.58744000	-0.00003300	0.00002500
C	1.26743700	-1.21651600	0.00000000
C	1.26740500	1.21650200	-0.00000500
C	2.66517000	-1.20747800	-0.00001200
H	0.72556400	-2.15590900	0.00004800
C	2.66511100	1.20751100	-0.00001100
H	0.72548900	2.15587000	0.00006100
C	3.36505900	0.00001700	0.00000500
H	3.20273500	-2.15188700	-0.00002100
H	3.20265500	2.15193000	-0.00001800
H	4.45133300	0.00003400	0.00001900

11

Rh	-0.66793700	-0.24769300	-0.09892900
C	0.08044700	-0.03194700	2.21436900
C	-1.32860500	0.34817800	2.08593000
C	0.25169600	-1.39746400	1.78668900
C	-2.03646700	-0.80739100	1.66959000
C	-1.04800900	-1.91082200	1.51763200
C	-0.92190200	-1.89696300	-1.96298400
O	-1.80345200	-1.73836300	-1.02927000
O	0.14741100	-1.23069900	-1.78556200
C	-1.17059800	-2.76453300	-3.14153800
H	-1.53579400	-2.13557900	-3.96384000
H	-0.23962700	-3.23819100	-3.46527900
H	-1.92940400	-3.51809700	-2.91692100
C	1.11623800	0.79802300	2.86734000
H	2.12710100	0.47577300	2.61977400
H	0.99586800	1.86432300	2.66261600
H	0.98519200	0.67246300	3.95601700
C	-1.93039600	1.61515400	2.60151400
H	-2.22920800	1.45952100	3.64838500
H	-1.22295400	2.44659200	2.58748600
H	-2.81678000	1.89178100	2.02939300
C	-3.50547900	-0.98786600	1.57550200
H	-3.84402800	-1.52242000	2.47778700
H	-4.02990400	-0.03606700	1.51037900
H	-3.77929800	-1.60489500	0.71439800
C	-1.39920000	-3.33761900	1.31958300
H	-0.59646800	-3.90371900	0.84111700
H	-1.54837700	-3.77892100	2.31938600
H	-2.32770300	-3.46744100	0.76297100
C	1.51416800	-2.19830300	1.84447000
H	1.64838200	-2.59474200	2.86070100
H	1.48023600	-3.05014900	1.16169800
H	2.39165500	-1.59924500	1.59568100
C	1.95829600	1.56371400	-0.36338700
N	0.60788800	1.49826300	-0.15042200
C	2.56133600	2.82780300	-0.49743500
C	-0.11312700	2.64793300	-0.06490000
C	1.82462800	4.00144500	-0.41632500

H	3.62857100	2.85446400	-0.68638700
H	-1.17382600	2.54169800	0.10792000
C	0.45241300	3.90549900	-0.18637300
H	-0.18218900	4.78189500	-0.10941000
H	2.30823000	4.96659100	-0.53292400
C	2.87115100	0.38567800	-0.43465500
C	3.89066300	0.27691100	0.53305700
C	2.88969600	-0.47805100	-1.54065600
C	4.85592300	-0.72586000	0.43708600
H	3.94625200	0.99585100	1.34680700
C	3.86297800	-1.47592800	-1.63513500
H	2.17553000	-0.34732900	-2.34230000
C	4.83726000	-1.61167500	-0.64493100
H	5.63478000	-0.79814700	1.19026600
H	3.87608700	-2.12832700	-2.50308600
H	5.59892500	-2.38068300	-0.73054400
C	-2.78941900	1.35541600	-1.32907500
O	-1.60819000	0.78354400	-1.56570200
O	-3.27300500	1.46462100	-0.21110000
C	-3.45033400	1.85068900	-2.59890700
H	-4.02350900	1.02523900	-3.03775800
H	-4.14174400	2.65800500	-2.34933700
H	-2.71629500	2.18313400	-3.33595200

12-ts

Rh	-0.32572800	-0.11333200	-0.11779100
C	0.08480000	0.30765100	-2.31920700
C	-0.43515000	-1.07151500	-2.24617600
C	-0.96348100	1.18172400	-1.92874100
C	-1.78636100	-1.02971000	-1.78808200
C	-2.14553800	0.36211200	-1.66636300
C	-2.82881400	0.35609100	1.49066600
O	-3.33731200	-0.66152500	1.06908700
O	-1.71106200	0.92168500	0.99533700
C	-3.37805400	1.17586700	2.64808400
H	-2.73294100	1.04088200	3.52333000
H	-3.39653700	2.24310800	2.41073900
H	-4.38508900	0.82475700	2.87962500
C	1.38571300	0.69875300	-2.94096000
H	1.71158100	1.69064800	-2.62222700
H	2.18124700	-0.01940900	-2.72946600
H	1.25866200	0.72843300	-4.03261700
C	0.24594700	-2.26993600	-2.80934100
H	-0.03265400	-2.33708900	-3.87278200
H	1.33445300	-2.20422000	-2.76939500
H	-0.08413900	-3.20014600	-2.34157900
C	-2.71855100	-2.18516800	-1.62902600
H	-3.40485300	-2.22669500	-2.48615800
H	-2.18482500	-3.13641000	-1.58484500
H	-3.30847300	-2.07096200	-0.71685000
C	-3.51352700	0.90622400	-1.51579500
H	-3.52931700	1.80066800	-0.88647800
H	-3.84336000	1.22740400	-2.51840900
H	-4.22130700	0.17343400	-1.13299500
C	-0.98018200	2.67445400	-2.00337100
H	-1.46158800	2.98409200	-2.94138000
H	-1.55459000	3.11041300	-1.18210800
H	0.02504100	3.09865500	-1.99099800
C	2.67625500	-0.16948800	0.18150000
N	1.61807000	-1.00423800	-0.03072500
C	3.97546100	-0.68181200	0.25724700
C	1.80712900	-2.33627300	-0.07713400
C	4.18074800	-2.05578800	0.16338900

H	4.80718100	-0.00811900	0.43141400
H	0.91896400	-2.94920300	-0.15827600
C	3.07634800	-2.89794900	0.01267200
H	3.18551300	-3.97669200	-0.02062200
H	5.18296700	-2.46633500	0.23731200
C	2.30477700	1.22345800	0.41575100
C	3.16032900	2.31206700	0.27553000
C	0.95692800	1.41722000	0.87534400
C	2.68943200	3.59992800	0.56920100
H	4.18308500	2.18159200	-0.06485000
C	0.49631300	2.74011500	1.11101400
H	0.66761800	0.68187000	1.74402900
C	1.36719700	3.81562100	0.99044400
H	3.36190500	4.44629400	0.46149900
H	-0.52595800	2.88292000	1.44310500
H	1.03236900	4.82149500	1.22420900
C	-0.23593900	-1.39897600	2.51508800
O	-0.62446500	-1.58287200	1.27406200
O	0.40016100	-0.40965000	2.90772600
C	-0.65051900	-2.50992600	3.45351100
H	-0.15600800	-2.38035000	4.41707300
H	-1.73730900	-2.47417700	3.58742200
H	-0.40650000	-3.48684300	3.02679600

13

Rh	-0.46877200	-0.06336100	0.17060000
C	-1.57983900	-0.14340700	-1.80055400
C	-2.14572300	-1.16565200	-0.91037000
C	-1.90673400	1.13531900	-1.25495000
C	-2.77174900	-0.49391500	0.19750200
C	-2.63634300	0.92188000	-0.01312700
C	-0.98064000	-0.40263200	-3.14507800
H	-0.30787600	0.39930600	-3.45708400
H	-0.43510800	-1.34831400	-3.18059800
H	-1.78764000	-0.46374800	-3.88916400
C	-2.22877000	-2.63081600	-1.17870100
H	-3.23878600	-2.85796600	-1.55426500
H	-1.52569500	-2.96164200	-1.94516000
H	-2.08991100	-3.22599900	-0.27104700
C	-3.47538700	-1.16157900	1.33378500
H	-4.08228000	-1.99865800	0.97364600
H	-2.74596100	-1.56043800	2.05185900
H	-4.12980000	-0.46792500	1.86571100
C	-3.28029300	1.97034800	0.83360800
H	-2.94476000	2.97877000	0.58590100
H	-4.36683800	1.94339800	0.66405500
H	-3.12264000	1.79145500	1.90182300
C	-1.70951000	2.44668400	-1.94501000
H	-2.57226500	2.63086300	-2.60073500
H	-1.64813400	3.28678800	-1.25155000
H	-0.81544300	2.45090800	-2.57301600
C	2.34238500	-0.09761000	-0.72706500
N	1.27274000	-0.93022800	-0.58834700
C	3.54484900	-0.57776800	-1.25132600
C	1.37485300	-2.22962000	-0.91086300
C	3.65264600	-1.92083700	-1.60331500
H	4.38462000	0.09588700	-1.38058100
H	0.50689100	-2.85018500	-0.72489000
C	2.55383400	-2.76369600	-1.42311600
H	2.60440800	-3.82132100	-1.65811100
H	4.58429900	-2.30773000	-2.00389300
C	2.07927400	1.24602100	-0.24270000
C	3.04786400	2.21455700	0.03169900

C	0.72730600	1.52300000	0.11292100
C	2.67618000	3.43352500	0.60476800
H	4.09564800	2.01216400	-0.16799200
C	0.34167900	2.76821600	0.62702700
C	1.33581000	3.69997000	0.92625500
H	3.43468000	4.18394300	0.80513600
H	-0.69131900	3.00058300	0.85592400
H	1.06355300	4.64062000	1.39529200
C	0.82034800	-1.30110300	2.53633000
O	-0.35031200	-1.05175600	1.86248100
O	1.88979900	-0.87437100	2.16358300
C	0.57857600	-2.11212400	3.78703200
H	0.11944800	-3.07328900	3.53288200
H	1.52850100	-2.27503100	4.29787400
H	-0.11163100	-1.58314800	4.45241500

N₃⁻

N	1.18178600	-0.14446100	0.00000000
N	0.00000000	0.00026500	0.00000000
N	-1.18178600	0.14419700	0.00000000

14

Rh	0.46484700	-0.18161700	0.05172100
C	1.16104700	-0.40845600	-2.20640600
C	2.31262100	-0.08725900	-1.42482800
C	0.62880700	-1.66661600	-1.73105300
C	2.48714800	-1.13121800	-0.43612900
C	1.47913300	-2.12988100	-0.65960300
C	0.64940500	0.34826100	-3.39155700
H	-0.43127900	0.23504000	-3.50866300
H	0.87749200	1.41463500	-3.32828700
H	1.12100100	-0.03707900	-4.30572900
C	3.22426400	1.08267200	-1.58347800
H	4.24330900	0.73835900	-1.79877200
H	2.91310400	1.74160100	-2.39706500
H	3.26071400	1.65642200	-0.64932000
C	3.59092100	-1.22204300	0.56467200
H	4.38762500	-1.87693900	0.18601700
H	4.02092400	-0.24038800	0.77151400
H	3.22327600	-1.64074100	1.50552600
C	1.43490700	-3.44429800	0.04588300
H	0.60120300	-4.06558500	-0.28484600
H	2.36413300	-3.99500800	-0.14709600
H	1.36235100	-3.29015700	1.12933700
C	-0.44234100	-2.45439300	-2.41587800
H	0.00004900	-3.00483000	-3.25759300
H	-0.90965500	-3.17785100	-1.74676200
H	-1.22815400	-1.80948400	-2.81677600
C	-2.09722700	1.24647000	-0.55679600
N	-0.75503600	1.45058600	-0.51243900
C	-2.94826800	2.28606500	-0.95629600
C	-0.23483200	2.64764200	-0.84211600
C	-2.41635200	3.52044200	-1.30223200
H	-4.01889600	2.12174600	-0.98360400
H	0.83823300	2.74253400	-0.74040600
C	-1.03200400	3.70728800	-1.24718800
H	-0.57513200	4.65859900	-1.49625600
H	-3.07116300	4.33154900	-1.60517600
C	-2.50171700	-0.08989600	-0.15080100
C	-3.83881400	-0.52007700	-0.08284800
C	-1.46671400	-0.97021500	0.22551300
C	-4.14325500	-1.80099800	0.36111700
H	-4.64253000	0.15368100	-0.36400800

C	-1.77898700	-2.24479200	0.69333400
C	-3.11376700	-2.65935900	0.75499100
H	-5.17775600	-2.12403300	0.41853600
H	-1.00306900	-2.91431800	1.04306900
H	-3.34443600	-3.65322200	1.12809100
N	0.63202500	-1.02442600	1.96639200
N	-0.23064200	-0.83618800	2.82091000
N	-0.97272800	-0.74889300	3.69008500
O	1.58398800	1.30938400	0.97448500
C	1.05771500	1.99583700	1.99081100
O	-0.11349900	1.96122100	2.32193400
C	2.10485900	2.83842200	2.70467200
H	1.60453100	3.59068800	3.31688600
H	2.69781300	2.18659300	3.35631800
H	2.78964300	3.31699000	1.99895500

PhI(N₃)OTs

N	4.98315900	-1.90890400	1.20644500
N	4.32874900	-1.73471800	0.28090000
N	3.71158900	-1.57308400	-0.77543200
I	1.56640300	-0.97465900	-0.47631200
C	2.21162900	1.11423100	-0.25689200
C	3.27945100	1.52802600	-1.03997900
C	1.53916600	1.91630000	0.65130500
C	3.70007000	2.85381500	-0.89465100
H	3.78217400	0.85211900	-1.72196300
C	1.98581800	3.23785800	0.77155200
H	0.70498400	1.55122800	1.24282700
C	3.05516400	3.70399900	0.00549000
H	4.53193200	3.21322800	-1.49345500
H	1.48790200	3.89565700	1.47800300
H	3.38918400	4.73203100	0.11144000
O	-0.55534400	-0.13973800	-0.36361000
S	-1.38131500	-0.51203700	0.93445700
O	-1.05593500	0.43571200	2.01582900
O	-1.24782600	-1.95098900	1.20679700
C	-3.04407500	-0.17592700	0.37097000
C	-3.77635600	-1.19276700	-0.24549100
C	-3.58951700	1.09484100	0.55260300
C	-5.06835600	-0.92249100	-0.68852700
H	-3.34248700	-2.18114300	-0.35327000
C	-4.88443100	1.34702900	0.10186500
H	-3.01232000	1.86290000	1.05596800
C	-5.64045300	0.34926300	-0.52869500
H	-5.64631200	-1.71345800	-1.16061300
H	-5.31719100	2.33359000	0.24840400
C	-7.03335500	0.63476000	-1.03821800
H	-7.45783000	1.52752000	-0.56832200
H	-7.02843100	0.80450800	-2.12310200
H	-7.71008300	-0.20520100	-0.84623100

15

Rh	-1.89525400	-0.34003400	0.07819300
C	-3.99537900	-0.34156700	0.66676400
C	-3.89006600	-1.50535700	-0.22157000
C	-3.22322700	-0.62483000	1.85432000
C	-2.96738700	-2.40028700	0.34259800
C	-2.50073700	-1.83279500	1.61733100
Cl	0.27042900	-1.33057400	-0.57787000
C	-4.97948600	0.78051600	0.50813800
H	-4.66838700	1.66805800	1.06536700
H	-5.10010800	1.06738700	-0.54048300
H	-5.96761300	0.48037300	0.88308600

C	-4.69512800	-1.69754300	-1.47233700
H	-5.68572800	-2.09982100	-1.22203800
H	-4.85944900	-0.75469800	-2.00227500
H	-4.22304600	-2.40300400	-2.16214500
C	-2.53599900	-3.73199300	-0.19435100
H	-2.99139100	-4.54207100	0.39048600
H	-2.83543000	-3.86743900	-1.23662200
H	-1.44996500	-3.85408500	-0.13756600
C	-1.58997700	-2.54729800	2.57150000
H	-1.17474900	-1.86905400	3.32189600
H	-2.13437400	-3.33815000	3.10493700
H	-0.75577500	-3.01719300	2.04247300
C	-3.27076400	0.16773900	3.12570200
H	-4.18672300	-0.08769200	3.67503300
H	-2.42676000	-0.05526300	3.78208200
H	-3.28317100	1.24459800	2.94013600
C	-1.30136900	2.08429100	-1.54159400
N	-1.82013700	0.83339000	-1.68340400
C	-1.23125600	2.94314600	-2.64721300
C	-2.22211100	0.40654100	-2.89244800
C	-1.67407600	2.50969100	-3.89133200
H	-0.82842400	3.94248400	-2.52960800
H	-2.59132700	-0.61104000	-2.94041500
C	-2.17101700	1.21130200	-4.02387900
H	-2.51137600	0.82530100	-4.97844600
H	-1.62470100	3.17281200	-4.74972900
C	-0.81764400	2.38044500	-0.18980300
C	-0.18381200	3.58373500	0.16077200
C	-0.96908600	1.33654400	0.75915500
C	0.32543200	3.76118100	1.44554200
H	-0.07593500	4.38441600	-0.56563300
C	-0.43184600	1.53189500	2.03952400
C	0.20811700	2.73017200	2.38367400
H	0.80961000	4.69503400	1.71436000
H	-0.50871900	0.74865900	2.78806100
H	0.60797400	2.85971900	3.38623400
I	2.43907300	0.15713200	0.62642100
C	3.76398200	-1.19670200	-0.39980200
C	4.05946900	-0.94746900	-1.73804000
C	4.30189000	-2.25899300	0.32274900
C	4.94434900	-1.81782200	-2.37870600
H	3.61680700	-0.11541700	-2.27397400
C	5.18662600	-3.11150100	-0.34128300
H	4.04994300	-2.42467800	1.36406300
C	5.50510200	-2.89182000	-1.68360800
H	5.19301200	-1.64919600	-3.42204800
H	5.62386800	-3.94676900	0.19718100
H	6.19381300	-3.56076900	-2.19037600
N	4.16991100	1.25649200	1.62118600
N	4.56222600	2.19430000	0.91507900
N	4.99354200	3.08345700	0.33427100

16-ts

Rh	-1.81907800	-0.24825200	-0.21129600
C	-3.54266300	-1.24813400	0.78591600
C	-3.86359100	-1.18928600	-0.62822500
C	-2.43393900	-2.15808100	0.94069800
C	-2.92663100	-2.00126200	-1.34091700
C	-2.01844400	-2.57116400	-0.37470600
Cl	-0.00921100	-0.00594600	-1.69138500
C	-4.38638300	-0.69872000	1.89878500
H	-3.78285800	-0.44967800	2.77500800
H	-4.92277300	0.20368900	1.59334400

H	-5.13561100	-1.44029300	2.20679400
C	-5.05554700	-0.49291600	-1.20634600
H	-5.93324300	-1.14795100	-1.12022400
H	-5.28715100	0.43248900	-0.67265200
H	-4.92723900	-0.25922900	-2.26580800
C	-2.89811100	-2.28932300	-2.81111200
H	-3.28974600	-3.29655600	-3.00856000
H	-3.51121500	-1.58564500	-3.38006500
H	-1.87773500	-2.24937000	-3.20366800
C	-0.94875600	-3.55645900	-0.72935500
H	-0.45095100	-3.96237400	0.15136500
H	-1.39226900	-4.39360600	-1.28289300
H	-0.18947400	-3.09801400	-1.37141200
C	-1.96809100	-2.72133000	2.24642500
H	-2.65862400	-3.51797300	2.55687400
H	-0.96874800	-3.15315300	2.18279700
H	-1.96943000	-1.96900200	3.03898300
C	-2.33086100	2.65228700	0.08924300
N	-2.41045300	1.65361000	-0.83209400
C	-2.75520300	3.94496700	-0.24920900
C	-2.83184700	1.90976800	-2.08327100
C	-3.22179600	4.20603200	-1.53112200
H	-2.70386200	4.73696300	0.48879600
H	-2.80954000	1.07727700	-2.77583100
C	-3.25031500	3.17421800	-2.47386600
H	-3.57840700	3.34217500	-3.49353900
H	-3.54615100	5.20661700	-1.79998100
C	-1.73016500	2.23493100	1.34907400
C	-1.46893900	3.10005100	2.42243000
C	-1.31879900	0.87964500	1.40689900
C	-0.79676900	2.63018300	3.54718200
H	-1.77533700	4.14129100	2.37839100
C	-0.62315200	0.42679900	2.53258200
C	-0.35959600	1.30218700	3.59114300
H	-0.59742700	3.29945000	4.37838200
H	-0.23203100	-0.58126000	2.56645100
H	0.19836700	0.94298600	4.45178200
I	3.06962500	-0.18380700	-0.32781700
C	5.12185200	0.39534400	-0.37018300
C	5.54124800	1.50240600	0.38045000
C	6.02772300	-0.34575300	-1.14164900
C	6.88251600	1.87826700	0.33869300
H	4.83342400	2.06333900	0.98168800
C	7.36561300	0.04314400	-1.17248900
H	5.69450900	-1.20635900	-1.71220100
C	7.79392300	1.15152000	-0.43462200
H	7.21686500	2.73809300	0.91171700
H	8.07416400	-0.52074900	-1.77188400
H	8.83849800	1.44716500	-0.45970400
N	1.25892400	-1.81356600	1.01794100
N	1.67865900	-2.87790800	1.39511600
N	2.04277000	-3.92529000	1.76154400

17

Rh	0.48720300	-0.03936200	0.23909300
C	1.24147700	0.89508600	-1.81374000
C	2.32017600	1.02351300	-0.88776600
C	0.93431500	-0.51281100	-1.96574300
C	2.66777300	-0.30487200	-0.42385300
C	1.85258900	-1.25483000	-1.13612200
C	0.60908300	1.99795900	-2.60209000
H	-0.44645500	1.79909100	-2.80469000
H	0.68664000	2.96260000	-2.09606500

H	1.11669600	2.09199500	-3.57181900
C	3.04588000	2.27373000	-0.51541900
H	4.06034100	2.24517200	-0.93446300
H	2.55130500	3.16714200	-0.90246100
H	3.13808100	2.36642600	0.57158000
C	3.77816800	-0.65534900	0.50964200
H	4.64600800	-1.00996200	-0.06335300
H	4.08574500	0.20257400	1.10932700
H	3.46986900	-1.45530400	1.18930200
C	2.05264800	-2.73236800	-1.08288000
H	1.34158000	-3.26967100	-1.71215400
H	3.06490600	-2.97444100	-1.43066400
H	1.96521200	-3.09208500	-0.05064500
C	0.02270700	-1.08223000	-3.00639100
H	0.56622600	-1.15610800	-3.95837200
H	-0.32921700	-2.07958700	-2.73875500
H	-0.85164800	-0.44819300	-3.17232100
C	-2.34238100	0.97106600	-0.01175800
N	-1.08576600	1.41397100	0.26609300
C	-3.40698900	1.88005100	-0.08449600
C	-0.86390400	2.72676700	0.48216500
C	-3.17894900	3.23228300	0.13072200
H	-4.40538700	1.51941600	-0.30140500
H	0.14795800	3.00480700	0.74292700
C	-1.88259100	3.66624200	0.41916600
H	-1.65905100	4.71017700	0.60878100
H	-4.00102600	3.93963200	0.08147500
C	-2.43639200	-0.46885900	-0.19107300
C	-3.64305000	-1.15153400	-0.43244000
C	-1.23741100	-1.19850300	-0.07004600
C	-3.65707900	-2.53567300	-0.54716800
H	-4.57364300	-0.59877600	-0.51716700
C	-1.25882000	-2.58782200	-0.16350600
C	-2.46573000	-3.25238900	-0.40735300
H	-4.59218100	-3.05621000	-0.72747200
H	-0.35668600	-3.16581800	-0.01425400
H	-2.47059300	-4.33691000	-0.47127600
N	0.81704400	-1.65037400	1.57143800
N	0.17255000	-1.63577400	2.61676800
N	-0.38870900	-1.71439200	3.61398900
Cl	1.25919000	1.17262100	2.16044800

18-ts

Rh	-0.44154500	-0.11741300	0.01334800
C	-1.43118400	-0.50629600	1.96600200
C	-2.44116800	-0.79490200	0.97409500
C	-0.37214900	-1.47479400	1.80526800
C	-1.96996600	-1.86650100	0.14170800
C	-0.73680700	-2.34370500	0.71613100
C	-1.57277100	0.48015000	3.08481000
H	-0.60304800	0.78882400	3.48213300
H	-2.11554300	1.37410700	2.76633600
H	-2.13977000	0.02911100	3.90999600
C	-3.78543200	-0.15224900	0.91264900
H	-4.42782400	-0.63421400	1.66424900
H	-3.73789700	0.91138900	1.16009000
H	-4.24669600	-0.26414600	-0.06731900
C	-2.72952500	-2.48621500	-0.99058000
H	-3.54066400	-3.11688400	-0.60317400
H	-3.15762500	-1.70746700	-1.62532600
H	-2.08572200	-3.11439100	-1.61049400
C	-0.07527400	-3.64334000	0.40113500
H	1.00580300	-3.61290000	0.54516000

H	-0.48163800	-4.39805900	1.09026700
H	-0.28723100	-3.98579300	-0.61311600
C	0.80217600	-1.66820800	2.71512600
H	0.56543100	-2.43069500	3.46918400
H	1.68569700	-2.00606600	2.16722500
H	1.05987100	-0.74914300	3.24662200
C	2.27866700	1.10775000	0.43926700
N	0.95726400	1.36289600	0.63281500
C	3.23717700	2.05475700	0.82687500
C	0.56041100	2.52881800	1.17524800
C	2.83228200	3.24588500	1.41519300
H	4.28728700	1.86513900	0.63937400
H	-0.50858900	2.67988400	1.23825600
C	1.46853500	3.49184400	1.59299500
H	1.10853700	4.41571100	2.03176600
H	3.57016700	3.98363900	1.71495700
C	2.56827200	-0.16134700	-0.21666500
C	3.86544000	-0.71119100	-0.30908200
C	1.49953400	-0.88083700	-0.78476700
C	4.08837400	-1.91293900	-0.96363500
H	4.69809900	-0.19127500	0.15491200
C	1.72413000	-2.06261400	-1.49217800
C	3.01340200	-2.58467400	-1.56241600
H	5.09247500	-2.31896100	-1.02802300
H	0.91202200	-2.53781300	-2.02927700
H	3.18252300	-3.50309300	-2.11742500
N	0.13391700	-0.03286400	-2.04089000
N	0.57692000	1.05441300	-2.41006200
N	0.99497400	2.03112500	-2.84285300
O	-1.50455800	1.59936500	-0.46553400
C	-2.42519300	1.58651300	-1.42908600
O	-2.87605500	0.58197000	-1.95494500
C	-2.85335100	2.99272900	-1.82123700
H	-3.76468100	2.94002300	-2.41921500
H	-3.01305100	3.62097700	-0.94028300
H	-2.05850800	3.45420600	-2.41791300

19

Rh	0.65550100	0.06839500	-0.18777600
C	0.60728800	-0.06011800	-2.40632300
C	1.84013400	0.55312000	-1.92843000
C	0.54128600	-1.38244100	-1.88493900
C	2.56886700	-0.45375800	-1.18083300
C	1.75655700	-1.62404300	-1.10494300
C	-0.38361000	0.59068700	-3.32299500
H	-1.37780800	0.14707200	-3.23002100
H	-0.46844900	1.66395200	-3.13262400
H	-0.05959200	0.46644700	-4.36472300
C	2.36594400	1.89856600	-2.32948400
H	2.96354600	1.81400400	-3.24698500
H	1.55760900	2.60708000	-2.53028900
H	3.01019300	2.32429500	-1.55540500
C	3.94019700	-0.29794800	-0.60319300
H	4.68171400	-0.64994900	-1.33319400
H	4.16680300	0.74682300	-0.37768000
H	4.05209500	-0.88020300	0.31272700
C	2.14058400	-2.90958300	-0.43681200
H	1.27748900	-3.56558100	-0.29572200
H	2.86650300	-3.45319700	-1.05564400
H	2.59226400	-2.71775700	0.53963800
C	-0.51985500	-2.40078400	-2.17035700
H	-0.21061200	-3.03437300	-3.01220900
H	-0.69378800	-3.05791900	-1.31461900

H	-1.47185600	-1.93477300	-2.43491300
C	-2.13091100	1.42395800	0.25601300
N	-0.80031000	1.62980600	0.08468000
C	-2.97977600	2.51397100	0.51057300
C	-0.30593800	2.88186700	0.16019000
C	-2.47164700	3.80691600	0.56015700
H	-4.03110200	2.33302500	0.69962000
H	0.76868000	2.96886200	0.06773100
C	-1.10363100	3.99747400	0.37734500
H	-0.65172700	4.98229700	0.42241800
H	-3.13065600	4.64662500	0.75847300
C	-2.71218000	0.05699800	0.20259100
C	-3.99637800	-0.11730600	-0.34452900
C	-2.08646100	-1.07760300	0.76165400
C	-4.65108500	-1.34582500	-0.30786500
H	-4.48591400	0.73077500	-0.81252500
C	-2.74696000	-2.30856700	0.81968000
C	-4.03082000	-2.44091900	0.29478900
H	-5.64087700	-1.44435300	-0.74168100
H	-2.25689900	-3.16723200	1.26994700
H	-4.53368600	-3.40166700	0.34438700
N	-0.73695600	-0.93073300	1.22791000
N	-0.36844500	-1.74060600	2.11726900
N	0.02588500	-2.42928600	2.92259900
O	1.56442800	1.07759100	1.38554600
C	2.23282100	0.36299800	2.26118200
O	2.33811800	-0.86497100	2.21741600
C	2.86924100	1.19394900	3.36331100
H	3.46261700	0.55313200	4.01731100
H	3.50241900	1.97742600	2.93439900
H	2.08991900	1.69253000	3.94988800

PD

C	0.74650700	-0.54277500	0.04934500
N	1.36396000	0.23972500	0.95385500
C	1.45920800	-1.41173300	-0.79373500
C	2.69460900	0.16396900	1.05002600
C	2.84445800	-1.48358000	-0.67614800
H	0.93288800	-2.00468900	-1.53512200
H	3.15350200	0.81623900	1.79118400
C	3.48260100	-0.68386600	0.27074900
H	4.56066000	-0.70509800	0.39729900
H	3.41622100	-2.14662300	-1.31999900
C	-0.74168000	-0.49472200	0.01491000
C	-1.44494600	-1.71116000	-0.01532500
C	-1.49881700	0.70039200	0.07055400
C	-2.83425400	-1.76880400	0.03936400
H	-0.87214700	-2.63388700	-0.04129100
C	-2.89850800	0.63718800	0.14598000
C	-3.56406800	-0.58257600	0.13224900
H	-3.33923400	-2.73020900	0.02893000
H	-3.44572900	1.57294400	0.19605400
H	-4.64876900	-0.60471500	0.18769300
N	-0.99988300	2.02532300	0.05911200
N	0.10542300	2.31737000	-0.40740800
N	1.06934900	2.77501500	-0.81021100

20-ts

Rh	-0.51199700	-0.29984600	0.01081300
C	-2.24223900	-1.35944500	-0.98003700
C	-2.74469700	-0.14952200	-0.35615900
C	-1.28581300	-0.97528900	-1.98111000
C	-2.17798200	0.96609300	-1.05314900

C	-1.25063700	0.46604500	-2.03945400
C	-2.71015100	-2.73880700	-0.65767600
H	-2.19757700	-3.49763000	-1.25301500
H	-2.55676700	-2.95838400	0.40488700
H	-3.78482700	-2.81490700	-0.86560400
C	-3.79157300	-0.09436500	0.71078600
H	-4.79264500	-0.15233300	0.26177600
H	-3.68243100	-0.93080800	1.40595400
H	-3.72244200	0.83411200	1.28095800
C	-2.62494100	2.38431100	-0.89443400
H	-3.62746100	2.48079400	-1.33388100
H	-2.69134900	2.66595600	0.15784700
H	-1.97112800	3.08505600	-1.41567100
C	-0.53010700	1.27600700	-3.06995600
H	0.36720200	0.76561900	-3.42900800
H	-1.18622300	1.44160700	-3.93528500
H	-0.23259000	2.25346900	-2.68519700
C	-0.57084600	-1.90018600	-2.91858500
H	-1.16760400	-2.02846800	-3.83134300
H	0.40395200	-1.50519500	-3.21507500
H	-0.42016900	-2.89011700	-2.48202400
C	2.48524400	-0.50719900	-0.29449400
N	1.37955300	-1.27897800	-0.11611800
C	3.75759800	-1.09500500	-0.31795000
C	1.50347700	-2.61268800	0.02478800
C	3.88388300	-2.47243300	-0.18990400
H	4.63668100	-0.46863300	-0.41464000
H	0.58307700	-3.15653600	0.20004200
C	2.73576100	-3.25017500	-0.02158400
H	2.78858600	-4.32752900	0.08883100
H	4.86622000	-2.93418600	-0.20803800
C	2.22833000	0.91954000	-0.44838500
C	3.15191200	1.82157500	-1.01081600
C	0.97122400	1.42624800	-0.07482900
C	2.84468200	3.16867000	-1.15901700
H	4.11176000	1.44819400	-1.35522900
C	0.65421600	2.77724300	-0.17612500
C	1.59661500	3.64152100	-0.73962500
H	3.57115300	3.84780800	-1.59253400
H	-0.28236700	3.15924000	0.20636900
H	1.35157300	4.69622200	-0.82884300
N	-0.93293700	-1.73019700	1.52213700
N	-0.25220800	-1.67268500	2.53605500
N	0.35431400	-1.67718700	3.51422900
O	0.43418500	0.77501000	1.62126000
C	-0.33695000	1.58234300	2.39174000
O	-1.41452900	2.01596100	2.03378100
C	0.32064100	1.86904100	3.72154800
H	-0.33387100	2.50378400	4.32040000
H	0.52365500	0.93099100	4.24670900
H	1.28130500	2.36938000	3.55717300

21

Rh	1.05612500	-0.15893500	-0.08838500
C	2.65141900	-0.05244600	1.36216600
C	3.09815800	0.58441900	0.12145100
C	1.56455200	0.72765800	1.90596900
C	2.24155800	1.69301400	-0.12598400
C	1.28603700	1.78145000	0.98306400
C	3.31687000	-1.21586200	2.02680000
H	2.63127400	-1.75416800	2.68614500
H	3.72549900	-1.92130800	1.29830300
H	4.15451400	-0.85843700	2.64202100

C	4.25835500	0.14778100	-0.71780100
H	5.16187600	0.69076500	-0.41024300
H	4.45865800	-0.92085600	-0.60884900
H	4.08448600	0.35099100	-1.77679100
C	2.31923500	2.65799400	-1.26774400
H	2.79461200	3.58953400	-0.93182900
H	2.91320500	2.25607700	-2.09134100
H	1.32523100	2.90239300	-1.65105300
C	0.26986100	2.86578400	1.12571000
H	-0.49755100	2.61492400	1.86009500
H	0.77066400	3.78634600	1.45803200
H	-0.21905900	3.07537700	0.17106800
C	0.90071300	0.49657100	3.23059100
H	1.49547600	0.95565700	4.03099200
H	-0.09756300	0.93716500	3.26150200
H	0.80957700	-0.56902200	3.45990600
C	-1.76149200	-1.40400500	0.69594400
N	-0.46422700	-1.63585200	0.36744600
C	-2.62624000	-2.47153100	0.97351100
C	-0.02940400	-2.91686600	0.31023900
C	-2.16963000	-3.78431100	0.91956600
H	-3.65892300	-2.25130300	1.21999900
H	1.00877500	-3.05402900	0.02906900
C	-0.83670000	-4.01132900	0.58365500
H	-0.42423100	-5.01216800	0.51898400
H	-2.84174500	-4.61089200	1.12847800
C	-2.29270500	-0.01638200	0.83466200
C	-2.70516200	0.40957200	2.11117600
C	-2.54747200	0.82821700	-0.25657900
C	-3.31154600	1.64915300	2.30059500
H	-2.55167700	-0.25395100	2.95786600
C	-3.17088400	2.06547600	-0.07730600
C	-3.54466400	2.47756200	1.19927900
H	-3.62119100	1.95592800	3.29487000
H	-3.37593500	2.68971500	-0.93932600
H	-4.03641700	3.43682200	1.32929800
N	1.16368700	-0.81984900	-1.98186700
N	0.50525200	-1.73503700	-2.46065700
N	-0.06384900	-2.58011100	-2.99398400
O	-2.29342100	0.34899100	-1.53775200
C	-1.57853900	1.13096700	-2.42451900
O	-0.97767600	2.12172300	-2.08082300
C	-1.69000700	0.58577200	-3.81937800
H	-0.92712000	1.04316400	-4.45005900
H	-1.59833600	-0.50311100	-3.82999900
H	-2.68085400	0.83472000	-4.21818900

OAc⁻

C	-0.22056600	0.00178000	-0.00001500
O	-0.80821400	-1.10889200	0.00000300
O	-0.69630600	1.16613000	0.00000300
C	1.35422000	-0.05478100	-0.00000500
H	1.75044400	0.47278500	-0.88032400
H	1.75037700	0.47219900	0.88070000
H	1.73341800	-1.08487900	-0.00031000

PD⁺

C	1.13098400	0.63607700	-0.00703000
N	1.46172200	-0.56557200	-0.51746900
C	2.10322400	1.52878400	0.47487000
C	2.75638000	-0.89073400	-0.57630500
C	3.44767200	1.17433600	0.40639200
H	1.80248900	2.47581500	0.91122800

H	2.98015500	-1.86709500	-1.00416000
C	3.78990100	-0.06266500	-0.13644100
H	4.82436400	-0.38354600	-0.21277300
H	4.21325200	1.85066500	0.77736500
C	-0.30861900	1.01520800	0.00860900
C	-0.69335300	2.32460600	-0.32513400
C	-1.32807500	0.11171000	0.35230200
C	-2.03042500	2.71504600	-0.32661900
H	0.07342500	3.03675000	-0.61653700
C	-2.66722500	0.49150500	0.35854600
C	-3.02202000	1.79484500	0.01567500
H	-2.29634400	3.73159400	-0.60193800
H	-3.41774800	-0.24025500	0.63805300
H	-4.06828500	2.08702300	0.01514700
O	-0.98229200	-1.16176300	0.79469900
C	-1.17380500	-2.22119000	-0.06200800
O	-1.75965900	-2.13932000	-1.11026300
C	-0.54814200	-3.46048000	0.52325800
H	-0.83639400	-4.33027100	-0.06811400
H	0.54056600	-3.34435500	0.50529000
H	-0.85090000	-3.59094600	1.56654600

22-ts

Rh	-0.57928000	-0.10690400	0.23665700
C	-1.46584900	0.02334900	-1.85877600
C	-2.39036000	-0.64332400	-0.99456300
C	-1.30067400	1.37480600	-1.38404100
C	-2.79883800	0.30717300	0.04172000
C	-2.12495800	1.53908200	-0.20101300
C	-0.85608100	-0.53288800	-3.10906500
H	0.13066600	-0.10441500	-3.30217500
H	-0.75590500	-1.61987100	-3.06589100
H	-1.49519800	-0.29309200	-3.96924100
C	-2.98931800	-1.99742800	-1.19974000
H	-3.98349600	-1.88474900	-1.65338600
H	-2.38823500	-2.61231800	-1.87382200
H	-3.10733300	-2.52960900	-0.25265900
C	-3.85536600	0.07797600	1.07276700
H	-4.83849300	0.30050400	0.63399200
H	-3.86019300	-0.95583100	1.42218700
H	-3.71708500	0.72976200	1.93848600
C	-2.36268000	2.80150000	0.57311200
H	-1.77496000	3.63559500	0.18692400
H	-3.42082600	3.08162600	0.50473900
H	-2.12620500	2.67145800	1.63465500
C	-0.59731000	2.45181600	-2.14424700
H	-1.24215700	2.77455300	-2.97346700
H	-0.38055900	3.32472900	-1.52938300
H	0.34332000	2.09935700	-2.57582700
C	2.29155300	-0.77931300	-0.39841700
N	1.06958000	-1.36374700	-0.26584800
C	3.41630000	-1.56283600	-0.69265500
C	0.93478700	-2.69360700	-0.44292300
C	3.27581300	-2.93074600	-0.88545000
H	4.39400400	-1.09966000	-0.74913900
H	-0.05643600	-3.09736400	-0.28771700
C	2.00984800	-3.50830300	-0.76916400
H	1.85269000	-4.57220500	-0.90695800
H	4.14394800	-3.54150900	-1.11313500
C	2.31152700	0.66627400	-0.20698200
C	3.41512700	1.47661200	-0.55560300
C	1.16778500	1.29852600	0.31166600
C	3.38390900	2.85013500	-0.37185400

H	4.29507900	1.01583700	-0.99354700
C	1.14282300	2.67447200	0.54094400
C	2.24403300	3.44814000	0.18222300
H	4.24365200	3.45434800	-0.64198600
H	0.30392700	3.12859600	1.05264800
H	2.22246800	4.51806400	0.36908700
N	0.23844800	0.68496400	2.03602600
N	1.05515900	-0.02034800	2.63551300
N	1.82338900	-0.59772900	3.25648300
Cl	-1.24315000	-1.91668300	1.69489400

23

Rh	0.80496100	0.04147000	0.16147200
C	1.33759700	0.15526500	-1.99162500
C	2.44594300	0.56548000	-1.14767400
C	1.01513600	-1.20082800	-1.67993400
C	2.86162700	-0.59285500	-0.37331800
C	1.95818800	-1.65965000	-0.66262300
C	0.68214500	1.00713600	-3.03501300
H	-0.34660500	0.69549400	-3.23070500
H	0.67299100	2.06292300	-2.75192200
H	1.23988700	0.92517900	-3.97727900
C	3.17922900	1.87127500	-1.21405600
H	4.01767500	1.79769800	-1.91958100
H	2.53302400	2.68303200	-1.55868000
H	3.58803400	2.14826700	-0.23888300
C	4.04907200	-0.64474100	0.53464600
H	4.95535700	-0.79964700	-0.06636900
H	4.16397900	0.28366000	1.09787100
H	3.97622300	-1.46317200	1.25356400
C	2.02300500	-3.05008200	-0.10547400
H	1.03705800	-3.52227500	-0.07974000
H	2.66833200	-3.67640300	-0.73549500
H	2.43655500	-3.06127800	0.90596800
C	-0.01024500	-2.05424500	-2.36248000
H	0.45884100	-2.62375700	-3.17584300
H	-0.46342900	-2.77456000	-1.67661300
H	-0.81350200	-1.45442200	-2.79688300
C	-2.02386700	1.37036300	0.02878700
N	-0.69049600	1.59462100	0.17216300
C	-2.92451500	2.44508500	0.10674000
C	-0.24919100	2.85093900	0.38728300
C	-2.46361600	3.74206300	0.30318700
H	-3.98810800	2.24827700	0.04705700
H	0.81663100	2.95578000	0.54399500
C	-1.09416900	3.95174800	0.44350800
H	-0.68004300	4.93864400	0.61830000
H	-3.16500400	4.56824000	0.36725800
C	-2.56757200	-0.00046100	-0.17352800
C	-3.70747900	-0.18196500	-0.97740100
C	-2.06477800	-1.13632800	0.49439900
C	-4.34067000	-1.41867500	-1.08164000
H	-4.10170100	0.66322000	-1.53265300
C	-2.70361900	-2.37580000	0.41085900
C	-3.85086400	-2.51423800	-0.36864700
H	-5.21727300	-1.52363500	-1.71274000
H	-2.29911100	-3.22934400	0.94816700
H	-4.34575900	-3.47834700	-0.43080100
N	-0.83201100	-0.98063100	1.20298800
N	-0.67605200	-1.58273500	2.29111700
N	-0.40839500	-2.07038100	3.27777800
Cl	1.50430700	0.83925000	2.29479200

24-ts

Rh	-0.57584900	0.09044400	-0.10693900
C	-0.99651200	-0.47929300	2.04267500
C	-2.10710100	0.25245800	1.48418800
C	-0.87967800	-1.72146300	1.33947000
C	-2.67287700	-0.55122900	0.41077100
C	-1.89319500	-1.74218400	0.29913100
C	-0.17980900	-0.07507500	3.23114000
H	0.83592100	-0.47486800	3.17633800
H	-0.11717800	1.01076200	3.33319700
H	-0.64209500	-0.46738600	4.14683200
C	-2.68664700	1.53353800	1.98808000
H	-3.64597400	1.33511800	2.48332300
H	-2.03225400	2.02199100	2.71392000
H	-2.87175700	2.22271600	1.15795000
C	-3.91082400	-0.22194800	-0.35927200
H	-4.79271000	-0.53966000	0.21392800
H	-3.99195600	0.85298600	-0.53572900
H	-3.93847800	-0.73560500	-1.32338100
C	-2.19406600	-2.88141200	-0.62725400
H	-1.36805000	-3.59161500	-0.68654000
H	-3.07336500	-3.42799300	-0.26189400
H	-2.41969100	-2.53154800	-1.63840600
C	-0.00081300	-2.85487700	1.75923900
H	-0.43442200	-3.32497000	2.65278900
H	0.08570300	-3.62262000	0.99071100
H	1.00717500	-2.52009900	2.01927000
C	2.29836600	1.02693300	0.14350200
N	1.02014400	1.47499000	0.25599400
C	3.37336300	1.90979600	0.31125600
C	0.78460300	2.76768200	0.54878200
C	3.13133900	3.24058500	0.62967000
H	4.38672000	1.55406500	0.16677300
H	-0.25675100	3.06147300	0.57723500
C	1.81238900	3.67808700	0.75989900
H	1.57483000	4.70832000	1.00079800
H	3.95951800	3.93024200	0.76033000
C	2.44791600	-0.39333600	-0.16302300
C	3.63392600	-1.10876300	0.10160700
C	1.36453000	-1.10652100	-0.70066600
C	3.74117400	-2.46260200	-0.18957100
H	4.46869100	-0.59131300	0.56483500
C	1.46609200	-2.45711200	-1.03142100
C	2.65425400	-3.13474500	-0.75907300
H	4.66657200	-2.99059900	0.01556000
H	0.65837200	-2.96074800	-1.54817000
H	2.73442500	-4.18564600	-1.02230000
N	-1.54941700	1.84518500	-0.84941700
N	-1.65767600	1.96953900	-2.06351600
N	-1.79110900	2.14367700	-3.19185800
Cl	0.22633900	-0.24399100	-2.38343100

25

Rh	-0.90298300	0.04391500	-0.17454000
C	-1.18958400	-0.89796200	1.82624900
C	-2.31441500	-0.05167100	1.42785300
C	-1.07745200	-1.94580200	0.87749800
C	-2.95244500	-0.66826400	0.27703200
C	-2.15019900	-1.78118900	-0.11024300
C	-0.34819200	-0.70136500	3.05043400
H	0.65565000	-1.11440200	2.92340100
H	-0.25258800	0.35630200	3.31039100
H	-0.81223100	-1.20864800	3.90657000

C	-2.86553500	1.10631500	2.20125800
H	-3.57381600	0.74643100	2.96014700
H	-2.07951800	1.65781900	2.72433800
H	-3.40163500	1.80067300	1.54900600
C	-4.18956700	-0.15863400	-0.39228600
H	-4.99332300	-0.04018100	0.34312900
H	-4.00087400	0.81442000	-0.86098600
H	-4.53825400	-0.84358600	-1.16786800
C	-2.41209900	-2.71485100	-1.25289700
H	-1.48147300	-3.07763000	-1.69776500
H	-2.97204900	-3.59094000	-0.89928700
H	-2.99780600	-2.23545500	-2.04017400
C	-0.11835600	-3.09534500	0.91934200
H	-0.59572500	-3.95583200	1.40757600
H	0.18026500	-3.41487600	-0.08227500
H	0.78594200	-2.85408900	1.48272400
C	2.00879600	1.20072300	0.33195600
N	0.67511000	1.46368800	0.31895100
C	2.92923200	2.22757400	0.59153500
C	0.25647600	2.71984400	0.58545400
C	2.48979200	3.51803300	0.86742100
H	3.98925300	2.00580800	0.54942800
H	-0.81431900	2.87690700	0.53624800
C	1.12024100	3.76795100	0.87436000
H	0.71866800	4.75525900	1.07427100
H	3.20461300	4.31207300	1.05970700
C	2.54273900	-0.17128200	0.09908000
C	3.56265700	-0.64069700	0.94993500
C	2.17618100	-1.01661800	-0.96080100
C	4.18943800	-1.86766600	0.74131400
H	3.86123200	-0.02507800	1.79298100
C	2.80281100	-2.23655400	-1.19948100
C	3.81949400	-2.66247100	-0.34367700
H	4.97064800	-2.19482000	1.42004000
H	2.50261200	-2.83928200	-2.05010300
H	4.31289200	-3.61171800	-0.52755400
N	-1.70065000	1.44056900	-1.47248600
N	-0.97829400	2.15761500	-2.15379800
N	-0.36456300	2.86653400	-2.82178400
Cl	0.87440000	-0.55144800	-2.06610800

PD''

C	0.92920700	-0.33004300	0.04658900
N	1.48733000	0.54254500	0.90220100
C	1.69410800	-1.13401000	-0.81224500
C	2.81973800	0.63525100	0.92075800
C	3.08273300	-1.02651000	-0.77957000
H	1.20294800	-1.81541000	-1.50006500
H	3.23469900	1.35207300	1.62776800
C	3.66429700	-0.12246000	0.10693700
H	4.74173500	-0.00200400	0.16828600
H	3.69718400	-1.63351400	-1.43914800
C	-0.55735500	-0.45648200	0.06459800
C	-1.12693900	-1.72902400	0.23705500
C	-1.43769000	0.62961400	-0.07968000
C	-2.50620400	-1.91777700	0.28199600
H	-0.46111200	-2.57861300	0.36084000
C	-2.82117200	0.45320600	-0.03812600
C	-3.35618600	-0.82047400	0.14778200
H	-2.91251800	-2.91450600	0.42737400
H	-3.46900500	1.31480900	-0.15977100
H	-4.43427900	-0.94948500	0.18264600
Cl	-0.84224600	2.25535800	-0.38587600

26-ts

Rh	2.13438900	-0.36875000	-0.02224800
C	4.28847700	-0.08747700	-0.47568600
C	4.25655400	-1.04757300	0.62209600
C	3.68042800	-0.72114900	-1.62367600
C	3.55884000	-2.19565800	0.18986800
C	3.14499600	-1.97670600	-1.19997100
Cl	0.29307900	-1.75790900	0.65759700
C	5.07727600	1.19010800	-0.48249000
H	4.71092300	1.88886600	-1.23972200
H	5.03650900	1.69360600	0.48803300
H	6.13468100	0.98938600	-0.70257900
C	4.90037600	-0.82933800	1.95898200
H	5.98305800	-0.99622800	1.88724100
H	4.75540700	0.19482800	2.31751600
H	4.51300900	-1.51555500	2.71617400
C	3.30025500	-3.45753800	0.95198100
H	2.23081600	-3.69307200	0.96334300
H	3.82777100	-4.29566200	0.47910400
H	3.64518000	-3.38816400	1.98644700
C	2.45855500	-3.00859300	-2.04319900
H	2.10367800	-2.59200000	-2.98933100
H	3.15044200	-3.82820000	-2.27871000
H	1.59864900	-3.43126500	-1.51577300
C	3.74323500	-0.21266600	-3.03308100
H	4.69627000	-0.52384400	-3.48138200
H	2.94649900	-0.62391500	-3.65728600
H	3.69958400	0.87820200	-3.08673100
C	1.17687300	2.13252800	1.24694600
N	1.63357500	0.90213600	1.59705800
C	0.82212800	3.07080600	2.21962600
C	1.70931700	0.56031900	2.88840300
C	0.92921500	2.72743700	3.56678700
H	0.44552000	4.04469400	1.92689900
H	2.03485900	-0.45211700	3.09614300
C	1.37048900	1.45026200	3.90832700
H	1.44313800	1.13363700	4.94303600
H	0.65380500	3.44173700	4.33626400
C	1.04349500	2.31059800	-0.20149100
C	0.88664900	3.52916700	-0.83317100
C	1.06854300	1.06727600	-0.96921400
C	0.70767000	3.57747300	-2.23638900
H	0.89840800	4.45898800	-0.27258800
C	0.86587500	1.18198000	-2.39586100
C	0.72286100	2.41513100	-3.01815700
H	0.55954300	4.54212300	-2.71280900
H	0.80764100	0.26600300	-2.97310000
H	0.57088400	2.47836700	-4.09090700
I	-3.23802300	-1.09739800	0.34598200
C	-5.29655500	-0.55159500	0.06692600
C	-5.91592900	0.28193100	1.00100700
C	-5.98847700	-1.04391100	-1.04191600
C	-7.25863300	0.61935700	0.81948100
H	-5.36883600	0.65746000	1.85917900
C	-7.33068700	-0.69680000	-1.20852700
H	-5.49698500	-1.69061100	-1.76086800
C	-7.96615900	0.13318000	-0.28215800
H	-7.74984500	1.26233500	1.54436900
H	-7.87799500	-1.07986800	-2.06512100
H	-9.01029100	0.39916300	-0.41760400
N	-0.94161100	0.66250700	-0.95236200
N	-1.52586700	1.70907000	-1.20923300