Manipulations of Phenylnorbornyl Palladium Species for Multicomponent Construction of a Bridged Polycyclic Privileged Scaffold

Lina Yin,*[a] Ting Guan,‡[a] Jie Cheng,‡[a] Dongchao Pan,‡[a] Jinyang Lu,‡[a] Jiahui Huang,[a] Jiaqi Wu,[a] Xiaoli Chen,[a] Taiyun You,[a] Xuting Huo,[a] Yuting He,[a] Jiayun Pang,*[b] and Qingzhong Hu*[a]

[a]	T. Guan, J. Cheng, D. Pan, J. Lu, M. Liu, J. Huang, J. Wu, X. Chen, T. You, X. Huo, Y. He, Prof. Dr. L. Yin, and Prof. Dr. Q. Hu
	School of Pharmaceutical Sciences, Guangzhou University of Chinese Medicine
	232 East Waihuan Road, Panyu, Guangzhou, China PR
	E-mail: huqqzh@gzucm.edu.cn (Q. Hu); linayin@gzucm.edu.cn (L. Yin)
[b]	Dr. J Pang
	School of Science, Faculty of Engineering and Science, University of Greenwich
	Medway Campus, Central Avenue, Chatham Maritime, ME4 3RL, United Kingdom
	Email: j.pang@gre.ac.uk (J. Pang)
‡	These authors contribute equally to this work.

Cartesian coordinates of all the structures reported and their absolute energies in Hartree. For naming of the structures, see the manuscript.

Int_I (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.881339 Hartree
B3LYP-D3 optimization: -2349.008606 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.594400 Hartree

Pd	-0.30594700	-0.43534500	0.51710200
P	-0.21358500	-0.04147700	2.95922900
C	3.30495100	-2.54204500	0.55158000
H	3.96582100	-2.01253200	1.23186300
C	3.31319400	-3.93170200	0.48428200
H	3.99542700	-4.51404500	1.09884000
C	2.41496000	-4.59197600	-0.35657500
H	2.40819800	-5.67572900	-0.36898600
C	1.51172800	-3.87445000	-1.15987000
C	1.54012600	-2.45045400	-1.14046400
C	2.42334200	-1.81794700	-0.25826600
C	0.64252600	-1.66543200	-2.09219800
H	-0.02837800	-2.38910000	-2.54426800
C	-0.25540700	-0.49991700	-1.55926500
H	-1.29316200	-0.70775600	-1.81885300
C	0.24119500	0.75328700	-2.32347600
H	0.04765900	1.69890600	-1.82061700
C	-0.28911600	0.70558000	-3.77902600
H	0.11647900	1.57385500	-4.31675200
C	0.42456700	-0.56006500	-4.36944000
H	0.98356800	-0.31318800	-5.27579300
C	1.43689500	-0.94204300	-3.22232000
H	2.28739800	-1.51496300	-3.59677200
C	1.72234300	0.43570200	-2.59674000
H	2.19154000	1.13532800	-3.30020000
H	2.30728400	0.41108900	-1.68067000
C	-0.71999500	-1.18390400	4.28300700
C	-1.18283300	-2.47104400	4.23277200
C	-1.36521800	-2.89476800	5.58820300
H	-1.37204500	-3.03211300	3.32904400
C	-0.99804500	-1.83851300	6.36796500
H	-1.72151200	-3.85547800	5.93096300
H	-0.96492600	-1.68019600	7.43553600
O	-0.59880300	-0.78884200	5.60027700
C	1.46474600	0.41485400	3.54111700
C	1.98966100	1.43474700	4.28792300
C	3.38223900	1.13469000	4.46167500
H	1.44351100	2.28547200	4.66626200
C	3.60205200	-0.04460800	3.80765900
H	4.11138000	1.70551600	5.02077500
H	4.46968700	-0.67147900	3.66802100
O	2.44853500	-0.49328900	3.24648300
C	-1.12150100	1.48264800	3.42844600
C	-0.94547500	2.80041500	3.09693000
C	-2.07951700	3.50007300	3.63146400
H	-0.13225800	3.19649400	2.49638400
C	-2.86670400	2.56258400	4.23465600
H	-2.27636200	4.56196500	3.57666700
H	-3.80080200	2.60394400	4.77423500
O	-2.30109700	1.32654500	4.12106700
I	-1.91466900	-2.70083400	0.42805500
N	0.58701100	-4.54530500	-1.98767000
H	-0.32264000	-4.09842800	-1.93857800
C	0.44813700	-5.98961400	-1.88377200
H	0.22800800	-6.34321500	-0.86348000
H	-0.36575600	-6.30481600	-2.54159000
H	1.36231900	-6.48608600	-2.22569900
H	2.40517700	-0.73746700	-0.15638700

C	-0.46907000	-1.73817200	-4.68381800
O	-1.62963200	-1.86881600	-4.33569600
O	0.23046700	-2.68805400	-5.32878100
C	-0.40285400	-3.99396500	-5.49893600
C	0.73670200	-4.99928800	-5.51953500
C	-1.24892400	-3.97497400	-6.76534300
H	-1.04028900	-4.16331800	-4.62633100
H	1.29237800	-4.94015600	-4.58046400
H	0.33746700	-6.01250900	-5.62924900
H	1.41381500	-4.80074100	-6.35670300
H	-2.03458600	-3.21963600	-6.68425200
H	-0.62622600	-3.74878000	-7.63702100
H	-1.71944600	-4.95133100	-6.91882300
C	-1.78255600	0.84135300	-3.97857500
O	-2.59723400	1.07586300	-3.09838400
O	-2.09425500	0.80822400	-5.28506200
C	-3.49823500	0.93203800	-5.65947000
C	-4.20662800	-0.40008000	-5.44288400
C	-3.49254700	1.38617800	-7.11131700
H	-3.94440500	1.69994400	-5.01878500
H	-4.14676200	-0.69982100	-4.39578400
H	-5.25906600	-0.31044900	-5.73150200
H	-3.73764200	-1.18148000	-6.04709800
H	-2.95392300	2.33168000	-7.22174400
H	-3.00940200	0.63486000	-7.74410500
H	-4.51898200	1.52613700	-7.46353300
C	1.36058700	2.09829300	0.63513700
O	1.44146300	3.34641300	0.90971000
O	2.36328500	1.32621100	0.49553700
O	0.11793900	1.61528800	0.51191200
Cs	-2.91357900	1.86151500	-0.05161800
Cs	4.44821700	3.23388800	1.44545400

TS1 (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.843977 Hartree
B3LYP-D3 optimization: -2348.972113 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.589668 Hartree
Imaginary frequency: -838.2052 cm^{-1}

Pd	-0.22891100	-0.40749500	0.42892400
P	-0.21012600	-0.05289600	2.85639500
C	2.62275600	-1.79885900	1.18219200
H	2.78143600	-1.15942200	2.04274400
C	3.25016000	-3.03783100	1.10903900
H	3.88052500	-3.38383100	1.92550500
C	3.07678900	-3.85621000	-0.01189900
H	3.57843400	-4.81701000	-0.05283100
C	2.26448700	-3.43658000	-1.08035300
C	1.60821500	-2.18048500	-0.99429700
C	1.79870100	-1.34231300	0.12924400
C	0.65303000	-1.74227200	-2.08162600
H	-0.00397500	-2.58636400	-2.33008800
C	-0.22099300	-0.54091600	-1.63816600
H	-1.26560800	-0.70666200	-1.88814100
C	0.35701200	0.65068000	-2.45352400
H	0.28094100	1.62021700	-1.96645800
C	-0.26006500	0.57550900	-3.87343200
H	0.19390200	1.36786000	-4.48623700
C	0.29868200	-0.78572400	-4.42452300
H	0.79819400	-0.64219900	-5.38540000
C	1.37243400	-1.17357700	-3.33905000
H	2.15677100	-1.82138500	-3.73624000
C	1.79216300	0.20902400	-2.81035100
H	2.25175300	0.84384100	-3.57750800

H	2.45115800	0.17180500	-1.94685000
C	-1.02291400	-1.28601500	3.90698100
C	-1.55311800	-2.50337500	3.57937400
C	-1.99041100	-3.10215100	4.80329600
H	-1.63686200	-2.89794100	2.57778400
C	-1.69388800	-2.20689800	5.78879800
H	-2.46580500	-4.06411100	4.92913900
H	-1.83665200	-2.20690600	6.85897100
O	-1.10176900	-1.09767400	5.26960300
C	1.37730600	0.13011800	3.77803700
C	2.26383800	1.16053900	3.93183800
C	3.35557100	0.64097600	4.70812800
H	2.17661400	2.13976900	3.48013400
C	3.06352300	-0.66786600	4.95733800
H	4.22442500	1.18008900	5.06152200
H	3.56007400	-1.45466700	5.50435800
O	1.86453800	-0.99628800	4.39982000
C	-1.03304800	1.51666700	3.33527800
C	-0.68897600	2.82452800	3.11844300
C	-1.76988900	3.61304400	3.63907700
H	0.20301100	3.16126100	2.60472100
C	-2.69371700	2.73135500	4.12090500
H	-1.84315400	4.69180000	3.65548500
H	-3.65484500	2.84102600	4.59965800
O	-2.25996200	1.45052800	3.94894500
I	-3.04664200	-0.80316700	0.49927600
N	2.12136300	-4.21698400	-2.23198600
H	1.29793300	-3.99487300	-2.77256900
C	2.44092800	-5.63402800	-2.21565400
H	1.95491300	-6.18093600	-1.39225100
H	2.12179400	-6.07737400	-3.16191500
H	3.52231000	-5.78874500	-2.12847300
H	1.88642100	-0.08127300	0.07138400
C	-0.70136000	-1.90635200	-4.59602900
O	-1.78901400	-1.99185700	-4.05841500
O	-0.17679000	-2.87542100	-5.37761900
C	-0.97406400	-4.08244800	-5.57351700
C	0.02105100	-5.18073800	-5.91489600
C	-2.00369100	-3.82854900	-6.66832900
H	-1.48230200	-4.30010900	-4.62906600
H	0.75811100	-5.29901800	-5.11515100
H	-0.50219300	-6.13214800	-6.04823300
H	0.55376100	-4.94408100	-6.84133900
H	-2.67304200	-3.01560700	-6.37779900
H	-1.50389800	-3.56037300	-7.60474200
H	-2.60307200	-4.72832800	-6.83858700
C	-1.73958900	0.86237600	-3.99040100
O	-2.40807000	1.40642200	-3.12582700
O	-2.20406800	0.57094700	-5.21500900
C	-3.62557000	0.78004900	-5.47499300
C	-4.44335600	-0.31056900	-4.79185800
C	-3.75916900	0.77607000	-6.99009600
H	-3.89415800	1.76012700	-5.06623000
H	-4.30416300	-0.27627400	-3.71002500
H	-5.50545800	-0.16957400	-5.01713600
H	-4.13024900	-1.29597800	-5.14597200
H	-3.13413900	1.55323300	-7.43920900
H	-3.45359900	-0.19376100	-7.39595000
H	-4.79998000	0.95737200	-7.27422500
C	1.80795100	2.13244700	0.64180300
O	2.35174900	3.06323500	1.32578800
O	2.56869500	1.15907600	0.16257200
O	0.53777400	2.08634300	0.41690800
Cs	-2.17657900	3.00545000	-0.35999300
Cs	5.19114900	1.54918700	1.42066900

II (5,6-DiCOOiPr NBE)
M06-2X single point: -2684.885268 Hartree

B3LYP-D3 optimization: -2349.021387 Hartree

B3LYP-D3 thermal correction to Gibbs free energy: 0.591371 Hartree

Pd	-0.47523400	-0.82136400	0.67673700
P	-0.19881900	-0.18592300	3.06666800
C	1.94909100	-2.52794300	1.42007600
H	1.81602300	-2.19900500	2.44154500
C	2.93060600	-3.48687200	1.15220700
H	3.54469900	-3.87146100	1.96470400
C	3.12137000	-3.98304900	-0.14010500
H	3.87614800	-4.74136900	-0.31804400
C	2.30851000	-3.52264400	-1.19262000
C	1.32510300	-2.53320200	-0.92214500
C	1.13379600	-2.03104800	0.38237300
C	0.42201200	-1.99641400	-1.99546400
H	-0.15005700	-2.82551400	-2.43522100
C	-0.54439500	-0.91355500	-1.40609200
H	-1.58560500	-1.11624500	-1.65989800
C	-0.05257800	0.40225800	-2.08054400
H	-0.24191200	1.31923200	-1.52900100
C	-0.52388200	0.47320400	-3.55691600
H	-0.05555500	1.36183300	-4.00594400
C	0.17365700	-0.76480100	-4.20794200
H	0.71623400	-0.48595500	-5.11477900
C	1.18985000	-1.19576000	-3.09060500
H	2.06438400	-1.70554200	-3.49491300
C	1.43881200	0.12296200	-2.34089300
H	1.93350300	0.89716700	-2.93684700
H	1.98995300	-0.02377400	-1.41434300
C	-1.06121600	-1.22792500	4.26794100
C	-1.90374300	-2.28282500	4.04310400
C	-2.30374700	-2.76624600	5.32852800
H	-2.20946900	-2.64038500	3.07048700
C	-1.67319700	-1.97385900	6.24294100
H	-2.96923900	-3.59021700	5.54122600
H	-1.65886600	-1.95367800	7.32228300
O	-0.91208400	-1.03234600	5.62262000
C	1.45389600	0.00095900	3.86218500
C	2.34750700	1.03766100	3.87750500
C	3.54177400	0.54021600	4.50009000
H	2.17498900	2.02264500	3.47187600
C	3.29422600	-0.76346000	4.81623700
H	4.45019500	1.08980200	4.70440100
H	3.86385800	-1.53510700	5.31106400
O	2.02867700	-1.10792900	4.43725100
C	-0.85139000	1.49846800	3.38304600
C	-0.62059600	2.69300700	2.75497900
C	-1.42652300	3.66693600	3.43234400
H	0.02141000	2.85869400	1.90098900
C	-2.09125000	2.99605800	4.41616900
H	-1.49358700	4.72420200	3.21627000
H	-2.80668400	3.28902700	5.16915000
O	-1.74597700	1.67801200	4.40696000
I	-3.27960100	-0.12044100	0.96733300
N	2.46937000	-4.00403200	-2.49739300
H	1.64906200	-3.89146900	-3.07647500
C	3.19295300	-5.23752500	-2.75257600
H	2.83577100	-6.08737400	-2.14955700
H	3.08787700	-5.49258500	-3.80982300
H	4.26236100	-5.11024500	-2.54976000
H	0.86711600	1.08498100	0.56829700
C	-0.73250800	-1.92536600	-4.55710400
O	-1.87963500	-2.08128200	-4.18639400
O	-0.05368700	-2.83646500	-5.29013600
C	-0.76984500	-4.05010400	-5.67467200
C	0.29581500	-5.11582300	-5.87723900
C	-1.59279400	-3.76090600	-6.92452000
H	-1.43292300	-4.31982900	-4.84746300
H	0.84646000	-5.29794500	-4.94956200

H	-0.17006000	-6.05586600	-6.18716800
H	1.00699600	-4.80889800	-6.65049000
H	-2.31956200	-2.96986100	-6.72418500
H	-0.94082900	-3.44456600	-7.74509600
H	-2.13482200	-4.65908800	-7.23619600
C	-1.99212200	0.71072600	-3.81916500
O	-2.78309800	1.13213800	-2.99080400
O	-2.28814400	0.55164200	-5.11944000
C	-3.67279900	0.74897800	-5.53579200
C	-4.51049800	-0.45551100	-5.12198500
C	-3.61378600	0.95670600	-7.04140100
H	-4.04290600	1.65052900	-5.03588800
H	-4.50981800	-0.56818500	-4.03662200
H	-5.54214200	-0.32326100	-5.46366500
H	-4.10208000	-1.36904100	-5.56211700
H	-2.97890600	1.81113300	-7.29297400
H	-3.20893700	0.06604900	-7.53282500
H	-4.61849500	1.14101900	-7.43319700
C	1.81524600	2.71533500	-0.04113600
O	2.98013900	3.09633400	-0.24663900
O	1.74766400	1.49439800	0.67914100
O	0.70776900	3.22862900	-0.34546400
Cs	-2.31486500	3.34553500	-0.68204900
Cs	4.43248600	0.11992300	0.54373600

Int_V ((5,6-DiCOOiPr NBE)

M06-2X single point: -2684.89643848 Hartree
B3LYP-D3 optimization: -2349.02690405 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.595749 Hartree

Pd	0.04734100	0.35682900	0.19130700
P	-0.15063400	-0.16760900	2.56600000
C	4.59615800	2.51048300	-1.28891300
H	5.08807800	3.45364600	-1.50725800
C	5.05341300	1.67911700	-0.27089600
H	5.91455600	1.96277600	0.32967200
C	4.41577500	0.46522400	-0.02098000
H	4.79809800	-0.18093100	0.76130500
C	3.29458300	0.04955400	-0.77707100
C	2.78428600	0.92494900	-1.78949800
C	3.47207800	2.11610000	-2.02482500
C	1.54880600	0.51335300	-2.59240900
H	1.73183800	-0.51222800	-2.93679800
C	0.14061000	0.51174700	-1.87509600
H	-0.33817500	-0.43611300	-2.10603800
C	-0.64400900	1.66579500	-2.55832000
H	-1.40160600	2.13954600	-1.93456900
C	-1.20202100	1.13402000	-3.89776400
H	-1.70472000	1.95921300	-4.42391600
C	0.10705700	0.82757400	-4.70517100
H	0.10557700	1.37110900	-5.65340000
C	1.23565000	1.44979500	-3.79126900
H	2.10804700	1.72336200	-4.38752200
C	0.45880100	2.58909400	-3.09892400
H	0.08906900	3.35272400	-3.79397000
H	1.02092700	3.07056700	-2.30173400
C	-1.57245800	0.60678900	3.39909300
C	-2.42772000	1.56991200	2.93083700
C	-3.41319000	1.77537700	3.94982900
H	-2.32646400	2.08050100	1.98336200
C	-3.08970100	0.92310400	4.96529500
H	-4.24045500	2.47052000	3.93286400
H	-3.52544700	0.72072800	5.93221500
O	-1.97734200	0.20339600	4.65258700
C	-0.45102400	-1.93098500	2.93695100
C	0.39115900	-2.96783600	3.22635800

C	-0.40673300	-4.16012000	3.21046100
H	1.45099500	-2.88756800	3.41838400
C	-1.67566300	-3.76617600	2.91460900
H	-0.07568700	-5.17071600	3.40256200
H	-2.61403000	-4.28877700	2.80874100
O	-1.72470900	-2.41002400	2.74409200
C	1.31147400	0.16430300	3.58230400
C	2.51192500	0.70225000	3.19935300
C	3.33886600	0.72437700	4.36671400
H	2.76182900	1.03902000	2.20293000
C	2.58484000	0.20232600	5.37655600
H	4.35467200	1.08468800	4.44118700
H	2.77009200	0.02288200	6.42502000
O	1.34918000	-0.14796000	4.92514900
I	0.53846800	2.99071500	0.67116600
N	2.73107800	-1.18034400	-0.55245500
H	1.85286300	-1.48643300	-0.99625900
C	3.11142300	-2.03100600	0.55090400
H	3.03135500	-1.52597900	1.52533800
H	2.42485600	-2.88005000	0.54905800
H	4.14075600	-2.41004400	0.45843200
H	3.12278300	2.78690900	-2.80127900
C	0.41497100	-0.61195400	-5.03158400
O	-0.06759400	-1.60160400	-4.50973800
O	1.38468400	-0.66575500	-5.96837400
C	1.94188300	-1.96796200	-6.29931800
C	3.32345200	-1.69299500	-6.87225900
C	1.01239100	-2.69221700	-7.26813500
H	2.03106800	-2.53246300	-5.36529000
H	3.93823200	-1.15370900	-6.14691000
H	3.82034300	-2.63585000	-7.12036100
H	3.24795300	-1.09039200	-7.78265800
H	0.01899400	-2.81413400	-6.83002900
H	0.91531700	-2.12071100	-8.19653100
H	1.41675000	-3.68014000	-7.51240600
C	-2.29293600	0.09483100	-3.78819700
O	-2.90214800	-0.16182300	-2.76290100
O	-2.62686000	-0.41642900	-4.98745300
C	-3.70428800	-1.39576900	-5.01677600
C	-3.18652200	-2.74538600	-4.52973400
C	-4.19493100	-1.42147400	-6.45608500
H	-4.49474000	-1.03968900	-4.34796100
H	-2.78212500	-2.67238900	-3.51656200
H	-4.00014600	-3.47867200	-4.53576900
H	-2.39940300	-3.09334200	-5.20647700
H	-4.53594000	-0.43041800	-6.76787700
H	-3.39068600	-1.73855700	-7.12814100
H	-5.02742200	-2.12446700	-6.55635400
C	-0.54033500	-2.52867200	-0.89768600
O	-1.51108600	-3.31866900	-1.18301700
O	0.62812700	-2.64374300	-1.40681700
O	-0.79299200	-1.56423200	-0.02293500
Cs	-3.71142300	-1.27206500	0.08406700
Cs	0.06072100	-4.63047900	-3.52008100

TS4 (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.88015411 Hartree
B3LYP-D3 optimization: -2349.01035118 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.592283 Hartree
Imaginary frequency: -425.6702 cm^{-1}

Pd	0.09185600	0.35525300	0.24300300
P	-0.14607500	-0.13257600	2.61585500
C	4.74751600	2.27546900	-1.24961200
H	5.32583400	3.15670600	-1.51163800
C	5.11090900	1.46212800	-0.17979400

H	5.99180300	1.69704100	0.41509600
C	4.35674300	0.33335000	0.13710200
H	4.67170400	-0.28554400	0.96951700
C	3.19074200	-0.02975300	-0.59680500
C	2.81168700	0.82517700	-1.69430600
C	3.60279400	1.93400400	-1.98545000
C	1.57926400	0.45844400	-2.52018600
H	1.72637200	-0.57467100	-2.85329100
C	0.16901100	0.50976200	-1.82092000
H	-0.34802800	-0.42307700	-2.03124300
C	-0.57459000	1.67083800	-2.52771400
H	-1.33781000	2.16339100	-1.92611200
C	-1.11621200	1.13442100	-3.87431600
H	-1.63034500	1.95211900	-4.40068100
C	0.20014200	0.84697400	-4.68113100
H	0.21489500	1.45009200	-5.59155200
C	1.32244600	1.40587400	-3.72498500
H	2.21647900	1.65866100	-4.29747800
C	0.56405000	2.56531500	-3.04627300
H	0.22882300	3.34134100	-3.74518300
H	1.13107300	3.02472300	-2.23894400
C	-1.60552300	0.61901400	3.41023000
C	-2.48241600	1.55386500	2.92499700
C	-3.48795500	1.73592700	3.92903300
H	-2.38212700	2.06406300	1.97740100
C	-3.15386900	0.89963400	4.95418100
H	-4.33449100	2.40692400	3.89632900
H	-3.59643300	0.69021600	5.91649600
O	-2.01675300	0.21150500	4.66073900
C	-0.42733200	-1.89050600	3.03054800
C	0.41163400	-2.90481300	3.39716200
C	-0.37021700	-4.10797000	3.38642900
H	1.46023900	-2.80283600	3.63383500
C	-1.62795900	-3.74288500	3.01523900
H	-0.03650100	-5.10624800	3.63126400
H	-2.55387700	-4.28193800	2.88457400
O	-1.68503500	-2.39436800	2.79322700
C	1.27965800	0.26872400	3.65584300
C	2.46854700	0.83819100	3.28337100
C	3.26505500	0.92726400	4.46842500
H	2.73430100	1.14352800	2.28072400
C	2.50598500	0.40982800	5.47696000
H	4.26569300	1.32545900	4.55434200
H	2.67236600	0.26988200	6.53457600
O	1.29465800	0.00059200	5.00895800
I	0.39967100	3.02040100	0.69144800
N	2.43757500	-1.12160000	-0.27904200
H	1.52406100	-1.80471200	-0.94394700
C	2.87109500	-1.96245400	0.81654900
H	2.92342600	-1.43497600	1.78190600
H	2.14295700	-2.77205700	0.92908500
H	3.86430200	-2.42322600	0.65413300
H	3.32635200	2.58406200	-2.80904700
C	0.48169300	-0.57160400	-5.09913000
O	0.13070300	-1.58554900	-4.51966500
O	1.26050700	-0.58123600	-6.20086900
C	1.74207800	-1.86406100	-6.68731900
C	2.97800800	-1.55511100	-7.51790900
C	0.63606800	-2.55808500	-7.47655700
H	2.01902800	-2.46403600	-5.81411900
H	3.72794200	-1.03863200	-6.91310300
H	3.41427400	-2.48317400	-7.89964200
H	2.71762300	-0.91842000	-8.36901200
H	-0.24882200	-2.70357700	-6.85289700
H	0.35432500	-1.95158500	-8.34295900
H	0.98186500	-3.53300200	-7.83561200
C	-2.18342500	0.06834900	-3.78126900
O	-2.80750500	-0.20548600	-2.76899400

O	-2.46826800	-0.46300400	-4.98407600
C	-3.50581200	-1.48461300	-5.03768500
C	-2.94727200	-2.81431700	-4.54043100
C	-3.96230400	-1.52652400	-6.48780600
H	-4.32354400	-1.16003700	-4.38606400
H	-2.55235500	-2.72617300	-3.52516300
H	-3.73730900	-3.57286400	-4.54941200
H	-2.14416700	-3.14262300	-5.20790900
H	-4.33761600	-0.54993000	-6.80562800
H	-3.13012700	-1.80759800	-7.14168800
H	-4.76174300	-2.26382000	-6.60829000
C	-0.41255400	-2.55391500	-0.89341200
O	-1.26541200	-3.39511600	-1.30279200
O	0.81527700	-2.57047500	-1.38884900
O	-0.71227900	-1.67272400	0.00428600
Cs	-3.61798500	-1.25517100	0.08603700
Cs	0.49182300	-4.57769300	-3.58703300

V* (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.89082949 Hartree
B3LYP-D3 optimization: -2349.02284126 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.596554 Hartree

Pd	0.02094800	0.55712600	0.40065800
P	-0.12307800	0.30898800	2.92288700
C	4.89301200	1.14791800	-1.14724300
H	5.75327900	1.72845700	-1.46799100
C	4.94143200	0.37455000	0.00815400
H	5.84841700	0.33570300	0.60715300
C	3.82000200	-0.35201100	0.41484800
H	3.87520100	-0.93162600	1.32813300
C	2.61148300	-0.31391900	-0.31584900
C	2.58053100	0.44179100	-1.52877900
C	3.71454400	1.15600200	-1.90863000
C	1.34108500	0.31383800	-2.40435500
H	1.41760700	-0.68659300	-2.84268100
C	-0.05389400	0.37596000	-1.69621200
H	-0.53794100	-0.59836500	-1.74095800
C	-0.82033800	1.43778800	-2.50409500
H	-1.69684700	1.84851300	-2.01034800
C	-1.16218000	0.90183900	-3.92105900
H	-1.77363300	1.65939900	-4.43145200
C	0.22845000	0.89216400	-4.65397400
H	0.22416600	1.65782200	-5.43222800
C	1.19330200	1.38419200	-3.52115600
H	2.12922400	1.74171600	-3.95021500
C	0.29949100	2.43866000	-2.83927000
H	-0.00701400	3.25184000	-3.50714100
H	0.75326600	2.85849100	-1.93938100
C	-1.33785600	1.12405600	4.02506600
C	-2.55663900	1.70516800	3.79401400
C	-3.13329500	1.98339800	5.07499100
H	-2.96774100	1.93743200	2.82423000
C	-2.22886600	1.55183800	5.99857000
H	-4.08431000	2.45564200	5.27549900
H	-2.20407200	1.56326700	7.07779900
O	-1.13674600	1.01971000	5.38567100
C	-0.41315500	-1.42660100	3.42969600
C	0.10895400	-2.29610200	4.34682100
C	-0.49866800	-3.57063800	4.09506600
H	0.85208500	-2.05190000	5.09075600
C	-1.35140600	-3.39050600	3.04693800
H	-0.31411600	-4.49700200	4.62014600
H	-1.99452500	-4.04424100	2.47935400
O	-1.32053100	-2.09118200	2.63576400
C	1.48237000	0.68118100	3.67714900

C	2.57391600	1.26177400	3.08825200
C	3.59971800	1.31172700	4.08442200
H	2.63779500	1.58111900	2.05852200
C	3.06267300	0.75734100	5.20833300
H	4.60005600	1.70418700	3.97366700
H	3.44325600	0.57752200	6.20253200
O	1.77641500	0.36757700	4.98724000
I	-1.30584400	3.01058500	0.57265400
N	1.45676300	-1.00371700	0.06919200
H	0.77433500	-2.15091000	-1.02242300
C	1.64022100	-2.00289300	1.11770600
H	1.95301200	-1.59843800	2.08926000
H	0.70009000	-2.54189700	1.23635900
H	2.40880200	-2.72925300	0.80855800
H	3.70339000	1.73620200	-2.82540600
C	0.68054400	-0.38270900	-5.31760800
O	0.59475100	-1.50792900	-4.85386500
O	1.26637300	-0.11651200	-6.50138000
C	1.83712400	-1.22924300	-7.24794700
C	2.86731800	-0.61418000	-8.18240300
C	0.72368000	-1.97590600	-7.97476500
H	2.32799700	-1.89279200	-6.52824800
H	3.62744900	-0.07064400	-7.61488000
H	3.35991200	-1.39900500	-8.76427800
H	2.38694300	0.08204700	-8.87670500
H	-0.01115300	-2.35497100	-7.26208000
H	0.21643800	-1.30695900	-8.67704700
H	1.13853400	-2.81846200	-8.53731800
C	-2.04372400	-0.32779000	-3.97565000
O	-2.65911800	-0.78907600	-3.02871600
O	-2.18167200	-0.77627500	-5.23453200
C	-3.08794400	-1.89898400	-5.46499900
C	-2.39276300	-3.20964400	-5.11934600
C	-3.49267900	-1.79441400	-6.92772800
H	-3.95583300	-1.75774800	-4.81339500
H	-2.07060800	-3.24108400	-4.07561000
H	-3.08111400	-4.04397900	-5.29108900
H	-1.52295600	-3.34654900	-5.77014400
H	-3.96990100	-0.83207900	-7.13270300
H	-2.61481100	-1.89106900	-7.57507600
H	-4.19656000	-2.59362200	-7.17831400
C	-0.66465300	-3.49671600	-1.34827600
O	-1.02762200	-4.38033600	-2.16856100
O	0.55544400	-2.90064600	-1.65510000
O	-1.25562400	-3.09954500	-0.31194600
Cs	-3.26768700	-0.95254800	0.09054600
Cs	1.33820100	-4.43317700	-4.13209600

V (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.877769 Hartree
B3LYP-D3 optimization: -2349.01768 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.586927 Hartree

Pd	1.16559000	0.00574100	1.09235700
P	0.86667600	0.34616900	3.49844300
C	6.07662400	-1.11037800	-0.46961100
H	7.09441800	-0.90811000	-0.78900200
C	5.82111300	-1.87808500	0.66149000
H	6.64204200	-2.29396800	1.24032600
C	4.50619700	-2.11658100	1.07114800
H	4.33388500	-2.71760000	1.95627100
C	3.40632500	-1.58700800	0.35850600
C	3.67464600	-0.81463100	-0.81582800
C	4.99337600	-0.60009700	-1.20181500
C	2.49244400	-0.36945100	-1.67564200
H	2.26112300	-1.24251300	-2.29509700

C	1.20650100	0.06146100	-0.92745200
H	0.34180400	-0.54587700	-1.17697200
C	0.99002800	1.53606400	-1.28943700
H	0.40580400	2.13449000	-0.58280900
C	0.37771800	1.59401700	-2.70821300
H	0.21089500	2.64567200	-2.96941900
C	1.54752900	1.04167900	-3.60210100
H	1.84193800	1.78511500	-4.34477500
C	2.73108900	0.87795600	-2.57173200
H	3.69542600	0.90852300	-3.07851200
C	2.42354200	2.01887200	-1.58195300
H	2.46580700	3.01744000	-2.02728500
H	3.07438000	1.98574100	-0.70325200
C	-0.30311900	-0.73975100	4.36298200
C	-1.19049800	-1.65090000	3.84850500
C	-1.90664800	-2.18855700	4.96671500
H	-1.32375600	-1.89940600	2.79974900
C	-1.40354000	-1.57459800	6.07614000
H	-2.68582000	-2.93691500	4.94211800
H	-1.61443100	-1.65652000	7.13186300
O	-0.42962700	-0.68752000	5.73422200
C	2.41061000	0.24710800	4.44388600
C	3.67201600	-0.04949000	3.99606800
C	4.53530400	0.02015100	5.13476700
H	3.94093000	-0.29903800	2.97872400
C	3.74099600	0.35605100	6.19139500
H	5.60104300	-0.15502400	5.16063500
H	3.93279600	0.52480400	7.24031000
O	2.44665200	0.49949100	5.79549200
C	0.21314500	2.01655300	3.80005100
C	-0.03781400	3.02768900	2.90647900
C	-0.60387700	4.10800200	3.65478500
H	0.14086800	3.01950300	1.83912600
C	-0.65621600	3.68253100	4.94929200
H	-0.92749700	5.06246900	3.26624200
H	-0.99698000	4.13650600	5.86761700
O	-0.16679400	2.41518000	5.06154000
I	-1.66086700	4.40763500	-0.61041100
N	2.07774000	-1.83235300	0.70973200
H	-4.57743200	-2.99613100	0.90172600
C	1.83947300	-2.73269700	1.83065800
H	2.24968600	-2.38858500	2.79448100
H	0.76205600	-2.86692300	1.94811800
H	2.28415300	-3.71916500	1.62073400
H	5.20143400	-0.02287800	-2.09714800
C	1.26398100	-0.24866200	-4.33755700
O	0.52870000	-1.14397100	-3.94273800
O	1.98257900	-0.32638500	-5.46464600
C	1.91583100	-1.56953700	-6.23342900
C	2.86270800	-2.58671200	-5.60665800
C	2.28054400	-1.19148700	-7.65958800
H	0.88529700	-1.93348500	-6.18088600
H	2.57125000	-2.79998100	-4.57521400
H	2.83871300	-3.52165000	-6.17490900
H	3.88797200	-2.20392100	-5.60954000
H	1.58922500	-0.43888400	-8.04800500
H	3.29671400	-0.78754400	-7.70286000
H	2.23111800	-2.07520000	-8.30254400
C	-0.97527400	0.93991300	-2.89145600
O	-1.64316700	0.40912500	-2.01871900
O	-1.37699700	1.06345300	-4.16470600
C	-2.63346200	0.42626100	-4.54773600
C	-2.48193700	0.08008400	-6.02064500
C	-3.78393700	1.37829700	-4.24688100
H	-2.73428000	-0.48379800	-3.94849800
H	-1.62419500	-0.58234600	-6.16888700
H	-3.38266000	-0.42565600	-6.38130700
H	-2.33130200	0.98628400	-6.61558800

H	-3.80909200	1.61947400	-3.18152900
H	-3.66752100	2.30794100	-4.81238100
H	-4.73674600	0.91692700	-4.52570800
C	-2.71450600	-2.87033200	0.52045000
O	-1.69111300	-2.16851200	0.73520300
O	-2.84376600	-3.90021100	-0.17235300
O	-3.87269500	-2.38141400	1.15243100
Cs	-2.83175300	0.79883300	0.92275300
Cs	-0.03295400	-3.42339800	-1.63873100

TS2 (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.841741 Hartree
B3LYP-D3 optimization: -2348.981176 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.584856 Hartree
Imaginary frequency: -310.5202 cm^{-1}

Pd	1.30719800	0.08116600	1.30091700
P	0.84803300	0.66620100	3.46672400
C	6.23677900	-1.44595400	-0.53118800
H	7.28323700	-1.34952500	-0.80340800
C	5.86553900	-2.15178000	0.61395100
H	6.62911700	-2.61156100	1.23629400
C	4.52103300	-2.27061600	0.98654300
H	4.24207100	-2.81280800	1.88446000
C	3.53074200	-1.65846000	0.19700300
C	3.90693600	-0.99008000	-0.98670700
C	5.24143900	-0.87760900	-1.34416100
C	2.70285900	-0.60771000	-1.82717500
H	2.53708200	-1.43440300	-2.52679800
C	1.45756300	-0.43887000	-0.93324200
H	0.60293300	-1.05494700	-1.16248700
C	1.11768500	1.08844400	-1.08465700
H	0.52275400	1.58236100	-0.30784700
C	0.42778700	1.26594700	-2.46803000
H	0.18830500	2.33310900	-2.54813000
C	1.56737200	0.94676800	-3.49427100
H	1.74880200	1.80129400	-4.14865500
C	2.80889400	0.75221500	-2.55249500
H	3.75437300	0.90080800	-3.07573400
C	2.48502700	1.72322300	-1.40213900
H	2.40379100	2.76863400	-1.71309500
H	3.19960000	1.64599400	-0.57890000
C	-0.35932300	-0.43235500	4.28465300
C	-1.08204100	-1.47430600	3.76097700
C	-1.92321100	-1.95908000	4.81382300
H	-1.04471900	-1.83864100	2.74156900
C	-1.64906600	-1.18805000	5.90475600
H	-2.63405500	-2.77025900	4.75276900
H	-2.01880200	-1.17544000	6.91924400
O	-0.70395400	-0.25362600	5.60741900
C	2.32827900	0.55536600	4.52386800
C	3.58353900	0.10873900	4.19967200
C	4.37029100	0.19466900	5.39211900
H	3.89444400	-0.24192300	3.22485600
C	3.54124700	0.68708200	6.35638000
H	5.41075700	-0.07054000	5.51285500
H	3.67663900	0.92762200	7.40015000
O	2.29661100	0.91156300	5.85263800
C	0.17068300	2.32646900	3.79165900
C	-0.16970600	3.30254600	2.88961500
C	-0.71024200	4.39162300	3.64510500
H	-0.06430400	3.25483500	1.81402900
C	-0.65944000	4.00588800	4.95217600
H	-1.08210000	5.32928400	3.25815600
H	-0.94270200	4.48214500	5.87895500
O	-0.13079000	2.75549800	5.06609200

I	-1.68809000	4.03746500	-0.85537800
N	2.17374800	-1.69549100	0.44251000
H	-4.32112900	-3.30616100	1.61083800
C	1.56442300	-2.84898400	1.08515600
H	1.75744100	-2.87995000	2.16930900
H	0.48013500	-2.81513200	0.95307500
H	1.95439300	-3.78184300	0.64288000
H	5.51957500	-0.37149300	-2.26530300
C	1.33400800	-0.26324700	-4.37051200
O	0.64654800	-1.23070400	-4.06812400
O	2.03026400	-0.17663600	-5.50733800
C	1.99662500	-1.31985300	-6.42257300
C	2.97112000	-2.38069800	-5.92456700
C	2.34785000	-0.75865900	-7.79048200
H	0.97566100	-1.71365800	-6.41581900
H	2.68140900	-2.73563700	-4.93252700
H	2.97763700	-3.23349300	-6.61028700
H	3.98420000	-1.97030400	-5.87111100
H	1.63743100	0.01892700	-8.08341800
H	3.35370900	-0.32772600	-7.78269200
H	2.31874900	-1.55715500	-8.53763100
C	-0.90236300	0.58884700	-2.69084800
O	-1.50077500	-0.09876300	-1.87633300
O	-1.37180600	0.88724900	-3.90798600
C	-2.65262700	0.31792300	-4.31739100
C	-2.54427700	0.10297700	-5.81880700
C	-3.76532300	1.26963600	-3.89945300
H	-2.76923200	-0.63926100	-3.80094400
H	-1.70697700	-0.56280000	-6.04794100
H	-3.46623100	-0.34563800	-6.20078300
H	-2.38364100	1.05581000	-6.33241900
H	-3.74998900	1.42359000	-2.81772600
H	-3.63921300	2.24172600	-4.38505400
H	-4.73866900	0.85777200	-4.18486300
C	-2.65977600	-3.07805600	0.70716300
O	-1.66470800	-2.31193700	0.61394500
O	-2.91630200	-4.12917500	0.08396800
O	-3.61649400	-2.64281400	1.64065900
Cs	-2.80898100	0.61687000	1.05993400
Cs	-0.75399400	-3.44589300	-2.19062800

1b (by-product) (5,6-DiCOOiPr NBE)

M06-2X single point: -2684.937608 Hartree
B3LYP-D3 optimization: -2349.0693 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.590915 Hartree

Pd	1.84300900	-0.30726100	2.04158100
P	1.01650700	0.51609800	3.92212400
C	6.48294800	-1.73475100	-0.76597800
H	7.53209800	-1.79863100	-1.03841300
C	6.08871800	-1.99803700	0.55210000
H	6.83461400	-2.26512000	1.29481300
C	4.74543000	-1.91165000	0.92817000
H	4.43137700	-2.09488300	1.95126100
C	3.81173600	-1.55903900	-0.04444100
C	4.19088400	-1.30293100	-1.36185000
C	5.53286100	-1.38300700	-1.72997400
C	2.98908200	-0.93399000	-2.19236300
H	2.81528800	-1.67043600	-2.98006800
C	1.83757800	-0.87144600	-1.12717400
H	0.95591000	-1.43885000	-1.40412100
C	1.49218500	0.63790600	-1.06666500
H	1.02964900	0.93159800	-0.12259300
C	0.68201100	1.04637400	-2.31550300
H	0.48741400	2.12254200	-2.23632400
C	1.69089400	0.82814800	-3.49933400

H	1.81231100	1.74193400	-4.08299900
C	3.02579000	0.51794100	-2.73105100
H	3.91659900	0.74174500	-3.32118200
C	2.82960400	1.32043800	-1.42475000
H	2.72733800	2.39752100	-1.58303800
H	3.62217300	1.14614500	-0.69402400
C	-0.33562700	-0.51943400	4.59532000
C	-1.00693900	-1.56030500	4.00432300
C	-2.05347500	-1.93970100	4.90488800
H	-0.80739100	-1.98717000	3.02964600
C	-1.94109900	-1.11457800	5.98475500
H	-2.78547400	-2.71838900	4.74965300
H	-2.48467800	-1.02582700	6.91365900
O	-0.90803600	-0.24284800	5.81781700
C	2.13405200	0.73982100	5.34636700
C	3.46721000	0.44202300	5.44958600
C	3.87474100	0.82040700	6.76838300
H	4.07137500	0.00860200	4.66539200
C	2.76215600	1.32491200	7.37417300
H	4.85972400	0.73213700	7.20371500
H	2.57236400	1.73508600	8.35469100
O	1.69485100	1.28600900	6.53050300
C	0.19201100	2.14129600	3.76443900
C	0.14321500	2.98603300	2.68488400
C	-0.71942800	4.07105200	3.04164900
H	0.64646600	2.84032900	1.74010200
C	-1.13634200	3.81401000	4.31421900
H	-0.99882300	4.90459300	2.41430200
H	-1.78632500	4.33350800	5.00248000
O	-0.59783600	2.64789700	4.77347800
I	-1.64784200	3.90656900	-0.92751000
N	2.38140200	-1.45403200	0.15512100
H	-4.15278100	-3.30973500	1.79258600
C	1.80205000	-2.81023600	0.40247100
H	2.25056100	-3.23053000	1.30356200
H	0.72388300	-2.72964400	0.55197700
H	2.02787600	-3.48217500	-0.44197400
H	5.83577200	-1.17293400	-2.75226000
C	1.29499600	-0.28097100	-4.45167200
O	0.69630600	-1.30068600	-4.12823500
O	1.71548400	-0.03304500	-5.69467100
C	1.45146400	-1.04014800	-6.72470400
C	2.51492900	-2.12788700	-6.63697100
C	1.45102300	-0.28491100	-8.04350600
H	0.46306800	-1.46276200	-6.52193900
H	2.47877100	-2.62311400	-5.66353200
H	2.34699000	-2.87879500	-7.41510400
H	3.51101500	-1.69753700	-6.77955500
H	0.69092600	0.50095700	-8.03774700
H	2.42723700	0.17526900	-8.22449900
H	1.23464800	-0.97362600	-8.86545800
C	-0.69581400	0.46683500	-2.50832400
O	-1.27733000	-0.26198400	-1.71580300
O	-1.21813800	0.90542500	-3.65891600
C	-2.56519300	0.50018600	-4.04989800
C	-2.42549400	-0.30821500	-5.33425700
C	-3.38673100	1.77115200	-4.20429100
H	-2.97164000	-0.11935600	-3.24655900
H	-1.77181700	-1.17115500	-5.18112600
H	-3.40688600	-0.65634700	-5.67089700
H	-1.98771700	0.31049400	-6.12446400
H	-3.38126500	2.34318100	-3.27249700
H	-2.96941500	2.40147200	-4.99596000
H	-4.41881500	1.51857100	-4.46825300
C	-2.50519900	-3.17915700	0.84601600
O	-1.45587600	-2.49499700	0.74476100
O	-2.87267100	-4.18077200	0.19345600
O	-3.39889700	-2.70305000	1.82305000

| Cs | -2.44250600 | 0.51611500 | 1.24123600 |
| Cs | -1.15759800 | -3.44772900 | -2.35664900 |

Int_I(a) (unsubstituted NBE)

M06-2X single point: -2071.927353 Hartree
B3LYP-D3 optimization: -1735.945678 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.413907 Hartree

Pd	-0.11656500	-0.37652500	-0.29263600
P	0.96521400	0.54833800	-2.09031300
C	-2.76157700	1.18111900	-1.33846500
C	-3.00495800	2.29355100	-2.17982700
C	-2.61467300	1.42099000	0.03855500
C	-3.07981000	3.58561000	-1.63470600
C	-2.68349200	2.71216300	0.56777000
H	-2.42863900	0.60175900	0.73100400
C	-2.91269800	3.80479100	-0.26931800
H	-3.26891000	4.42496800	-2.30074600
H	-2.55381500	2.85730800	1.63686000
H	-2.96409300	4.81398400	0.13081500
C	-1.05860900	-1.28453500	2.41868900
O	-0.46115100	-1.75671800	3.44723600
O	-0.61177000	-1.70260200	1.22366100
O	-2.02886600	-0.45918300	2.47308500
Cs	-0.83504800	1.12136400	4.71035000
C	-2.72012700	-0.22495200	-1.91993800
C	-3.97809500	-1.07241800	-1.52662300
C	-2.27253400	-2.46042500	-1.01179900
C	-1.55131800	-1.21180700	-1.54864300
C	-3.49371400	-1.86406400	-0.29258600
H	-4.22011400	-2.62545900	0.01944100
H	-3.21236800	-1.26500000	0.57420300
C	-4.13541700	-2.20187300	-2.57193600
H	-5.09484700	-2.71437600	-2.44056400
H	-4.10427100	-1.82576400	-3.60073400
C	-2.93883900	-3.15137200	-2.23705700
H	-3.29294500	-4.15179700	-1.96187000
H	-2.24629200	-3.26947300	-3.07816200
H	-4.87576900	-0.46185000	-1.39209600
H	-1.64060800	-3.11633200	-0.41472900
H	-0.98315300	-1.46784300	-2.44415400
H	-2.68809400	-0.10089000	-3.00373300
Cs	2.14572200	-2.75407300	1.80864400
I	1.77213900	1.30677300	1.51222900
C	2.75687600	0.19746400	-2.00028300
C	3.87282400	0.89371400	-2.37360700
O	3.12815600	-0.98450700	-1.40026100
C	5.00023200	0.10243000	-1.98187900
H	3.87800500	1.85689300	-2.86177500
C	4.49160800	-1.02118200	-1.40206100
H	6.04580800	0.34116400	-2.11401900
H	4.94192500	-1.90355000	-0.97286200
C	0.54145500	-0.06143900	-3.76386700
C	-0.44966400	0.28077600	-4.64184800
O	1.17140600	-1.20690200	-4.19065500
C	-0.42103000	-0.70450300	-5.68339400
H	-1.15467500	1.09402200	-4.52095200
C	0.57429700	-1.57739300	-5.36147500
H	-1.05982900	-0.75183300	-6.55379300
H	0.97788900	-2.45852100	-5.83624500
C	0.89801300	2.33625500	-2.33461200
C	0.27081700	3.29325400	-1.58949000
O	1.53079000	2.92107100	-3.41403300
C	0.52452500	4.54372400	-2.23677300
H	-0.30542200	3.11169100	-0.69567300

C	1.29078400	4.25948900	-3.32882900
H	0.17704700	5.51951700	-1.93005100
H	1.72486400	4.86466300	-4.11046600
N	-3.14654000	2.13389100	-3.59611100
H	-2.95715000	3.02630200	-4.04271300
C	-4.46312300	1.65618500	-4.04697200
H	-5.29310900	2.30019800	-3.71607000
H	-4.47034300	1.60760200	-5.14000900
H	-4.64728400	0.65058200	-3.66389600

TS1(a) (unsubstituted NBE)

M06-2X single point: -2071.885687 Hartree
B3LYP-D3 optimization: -1735.90829 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.408244 Hartree
Imaginary frequency: -1452.3115 cm^{-1}

Pd	-0.41257300	0.44473300	-0.61605700
P	1.25598800	0.37208100	-2.20241000
C	-3.14800200	1.53382800	-0.78675800
C	-3.86177200	2.75569900	-0.86493200
C	-2.31465400	1.26614100	0.33419600
C	-3.74496700	3.69173000	0.17451100
C	-2.20648400	2.25458800	1.33492600
H	-2.11417400	0.05390500	0.94464300
C	-2.90808300	3.45433500	1.26477600
H	-4.30586600	4.62278900	0.11184700
H	-1.52676600	2.08054200	2.16210000
H	-2.80982600	4.20460200	2.04636200
C	-1.08856900	-1.70400300	1.67808100
O	-0.56790600	-2.28440900	2.68954200
O	-0.67785500	-1.88375000	0.47781900
O	-2.09109600	-0.83998000	1.87696700
Cs	-1.10768700	0.02643300	4.62693300
C	-3.12398800	0.59147700	-1.96426000
C	-4.08720000	-0.63896500	-1.92019400
C	-2.05164000	-1.59123200	-2.19391600
C	-1.73391000	-0.08825300	-2.15216400
C	-3.23593600	-1.71106900	-1.21713300
H	-3.70765900	-2.70181500	-1.24678500
H	-2.96721700	-1.47559400	-0.19135400
C	-4.17248700	-1.21209400	-3.35612400
H	-4.96146500	-1.96948400	-3.42076400
H	-4.39770300	-0.44166700	-4.10240300
C	-2.75797100	-1.85508700	-3.55655200
H	-2.83475600	-2.93354500	-3.73774400
H	-2.20853100	-1.42319700	-4.39956700
H	-5.05565200	-0.42190600	-1.46180900
H	-1.20040700	-2.23954900	-1.99545700
H	-1.26666900	0.25233800	-3.07842700
H	-3.34610300	1.19308200	-2.85421300
Cs	2.12575100	-2.74068300	0.87525900
I	1.48062500	1.34812800	1.53799600
C	3.02992200	0.57182400	-1.81098200
C	3.91731700	1.59182200	-2.01038900
O	3.63155800	-0.43045900	-1.08693500
C	5.13959900	1.20166200	-1.37076500
H	3.72000100	2.50898100	-2.54497500
C	4.91306800	-0.02632400	-0.82937300
H	6.06088800	1.76420700	-1.32516700
H	5.52258400	-0.71863700	-0.26913300
C	1.24978300	-1.15484300	-3.21329600
C	0.93913500	-1.43328900	-4.51506200
O	1.42607800	-2.33249800	-2.52022700
C	0.92634500	-2.86229900	-4.63826300
H	0.74189900	-0.70448100	-5.28673100
C	1.22811700	-3.35492200	-3.40585800

H	0.71589400	-3.43918900	-5.52721700
H	1.33916300	-4.35157900	-3.00706400
C	1.03823600	1.65614300	-3.46309600
C	0.13530800	2.68452200	-3.50419300
O	1.84197200	1.70022900	-4.58293900
C	0.39073100	3.40553900	-4.71286100
H	-0.61943600	2.87982100	-2.75527600
C	1.42990600	2.76661100	-5.32316500
H	-0.12945900	4.27976600	-5.07625600
H	1.96969800	2.93681300	-6.24256200
N	-4.62118700	3.10778100	-2.01862100
H	-4.83558700	4.09884200	-1.97935700
C	-5.86229900	2.36713600	-2.27623400
H	-6.52026800	2.29919700	-1.39492700
H	-6.40900900	2.87160600	-3.07844100
H	-5.64470100	1.35358700	-2.61370400

II(a) (unsubstituted NBE)

M06-2X single point: -2071.919655 Hartree
B3LYP-D3 optimization: -1735.944588 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.409869 Hartree

Pd	-0.43859400	0.87305200	-0.82754200
P	1.41752700	0.34526100	-2.30682000
C	-3.29811200	1.71782800	-0.84436600
C	-4.38069500	2.57949200	-0.52282000
C	-2.13064200	1.71611500	-0.03888100
C	-4.32655400	3.31604800	0.67491900
C	-2.09868400	2.50306300	1.12635100
H	-2.36559900	-0.32584700	1.35710000
C	-3.19864900	3.28033100	1.49151300
H	-5.16882400	3.95309500	0.94039300
H	-1.18988900	2.54621800	1.71646400
H	-3.17056300	3.88477200	2.39698800
C	-1.21454800	-1.67527600	2.12721500
O	-0.54367200	-1.89318300	3.16684100
O	-1.15012100	-2.23886100	1.01041300
O	-2.14254600	-0.62726800	2.25351500
Cs	-0.82884700	0.91242900	4.57673200
C	-3.24153500	0.87946500	-2.08732200
C	-4.05927900	-0.45912800	-2.06107900
C	-1.95882400	-1.16484800	-2.49242200
C	-1.78076600	0.36056900	-2.34084900
C	-3.06376800	-1.46608400	-1.46817600
H	-3.42967000	-2.49911800	-1.52122100
H	-2.75176800	-1.26775700	-0.44532800
C	-4.16646000	-0.96747600	-3.51885200
H	-4.86452000	-1.80956900	-3.58262500
H	-4.52409300	-0.19343800	-4.20732600
C	-2.70287400	-1.42602700	-3.83261900
H	-2.66536400	-2.49091000	-4.09016800
H	-2.25342800	-0.87440200	-4.66527500
H	-5.01345000	-0.38879500	-1.53883600
H	-1.04673800	-1.74946200	-2.38766700
H	-1.35761300	0.80795600	-3.24638000
H	-3.58528600	1.48700900	-2.93796400
Cs	1.84429100	-2.58149300	0.90477300
I	1.59230400	1.58949000	1.30998400
C	3.19738000	0.40584800	-1.86594300
C	4.18788500	1.31692800	-2.10176100
O	3.67452800	-0.59219200	-1.04782100
C	5.34448000	0.86111900	-1.38664600
H	4.10088200	2.20557300	-2.70878100
C	4.98136500	-0.29516200	-0.76828000
H	6.31463400	1.33489700	-1.34472000
H	5.50079500	-0.99937700	-0.13660600

C	1.33319600	-1.22573700	-3.24863800
C	1.09057500	-1.55334300	-4.55291800
O	1.33799500	-2.37290000	-2.48130500
C	0.93956700	-2.97910400	-4.59978300
H	1.02584600	-0.85797300	-5.37594200
C	1.09983500	-3.42447900	-3.32406400
H	0.73645400	-3.58545100	-5.47070600
H	1.07971100	-4.40104200	-2.86517800
C	1.39414000	1.56686300	-3.64882400
C	0.64456700	2.70453500	-3.78472200
O	2.24262200	1.44231500	-4.72935300
C	1.04587900	3.31707400	-5.01381600
H	-0.10296000	3.04507800	-3.08242500
C	2.01077500	2.51073500	-5.54128700
H	0.66537900	4.23189200	-5.44423800
H	2.60329600	2.55277900	-6.44277500
N	-5.44913600	2.87030200	-1.41074300
H	-5.99189700	3.63414600	-1.02533700
C	-6.35984300	1.84775000	-1.92626900
H	-6.72694600	1.15376000	-1.15358300
H	-7.22397100	2.35682900	-2.36307000
H	-5.89473000	1.26135100	-2.71876000

Int_V(a)

M06-2X single point: -2071.91424476 Hartree
B3LYP-D3 optimization: -1735.93065435 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.414831 Hartree

Pd	0.11065600	0.49937700	0.35823200
P	-0.06542300	0.19350900	2.88172400
C	4.75468000	1.60594500	-1.19199000
H	5.51098700	2.32121600	-1.50181000
C	4.89803800	0.89341900	-0.00612200
H	5.77163700	1.03701500	0.62368500
C	3.90847900	-0.01394600	0.38451100
H	4.02349700	-0.54913900	1.31906000
C	2.76762700	-0.20215700	-0.40436300
C	2.62051000	0.49868700	-1.62638500
C	3.62511500	1.39431400	-1.99257300
C	1.39317400	0.20605500	-2.47052000
H	1.48261200	-0.84617300	-2.77553000
C	0.00808100	0.31236600	-1.73875200
H	-0.47288000	-0.66806400	-1.70010900
C	-0.79360900	1.26836300	-2.63261900
H	-1.66312600	1.71954800	-2.15852100
C	-1.15158100	0.45301600	-3.91187400
H	-1.91043700	0.98434800	-4.49916100
H	-1.53460900	-0.53907400	-3.65634700
C	0.20832600	0.38140400	-4.67135000
H	0.15805700	0.90836400	-5.63072000
H	0.52514500	-0.64663300	-4.87550100
C	1.18003300	1.10925400	-3.71408600
H	2.10223200	1.41835000	-4.21045800
C	0.28685600	2.23456900	-3.14990600
H	-0.07329800	2.92571500	-3.92085400
H	0.75904700	2.80421200	-2.34403500
C	-1.42310400	0.84492500	3.91552000
C	-2.60842200	1.45793100	3.60450500
C	-3.33162000	1.60662400	4.83139500
H	-2.90261100	1.79126600	2.62106200
C	-2.53973100	1.07374300	5.80448200
H	-4.30241200	2.06118900	4.96720500
H	-2.64470500	0.96839500	6.87379400
O	-1.38060700	0.59938300	5.27260900
C	-0.16399900	-1.57862100	3.33240000
C	0.42446500	-2.42046400	4.23606100

C	-0.00310600	-3.74823200	3.89650200
H	1.09179400	-2.12197700	5.03070100
C	-0.82245000	-3.62662000	2.81156700
H	0.26602300	-4.66735000	4.39803100
H	-1.34276000	-4.31381800	2.16435500
O	-0.93574800	-2.31485700	2.46282500
C	1.45494500	0.71618000	3.71800700
C	2.51624700	1.40070400	3.18721200
C	3.47622300	1.54851000	4.23816700
H	2.59809000	1.73859000	2.16423600
C	2.93326300	0.94525300	5.33379800
H	4.43682000	2.03965000	4.18288600
H	3.27287800	0.80526400	6.34902000
O	1.70469800	0.43251700	5.04382100
I	-1.16773600	2.90009800	0.46040900
N	1.68889600	-1.04776100	0.01509000
H	1.29463700	-1.67379900	-0.76366000
C	1.99478200	-2.00569900	1.08364000
H	2.19181400	-1.51016600	2.03360400
H	1.12548600	-2.65444900	1.17594400
H	2.88129300	-2.60279400	0.82304500
H	3.52834400	1.95535800	-2.91485400
C	-0.58375600	-3.06882800	-1.31243600
O	-0.90602600	-3.72296400	-0.23463100
O	0.70124800	-2.90483500	-1.59082100
O	-1.47806000	-2.56218800	-2.07856000
Cs	-3.11716200	-1.32669900	0.10643700
Cs	1.46739800	-5.55468800	-0.34531000

TS4(a)

M06-2X single point: -2071.90814777 Hartree
B3LYP-D3 optimization: -1735.92820931 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.410704 Hartree
Imaginary frequency: -962.2845 cm-1

Pd	0.10563200	0.46162400	0.32976000
P	-0.08646100	0.16648200	2.86569100
C	4.79805800	1.52882600	-1.21524800
H	5.57287400	2.22361700	-1.52629300
C	4.93159000	0.79090900	-0.04452000
H	5.81877700	0.89346200	0.57534400
C	3.91640600	-0.08650400	0.34856700
H	4.03400000	-0.63491000	1.27503600
C	2.74492100	-0.23138600	-0.41657900
C	2.62259800	0.49349400	-1.63454400
C	3.64966700	1.36109900	-2.00106700
C	1.39727900	0.23346800	-2.49238500
H	1.49987500	-0.80378900	-2.83812600
C	0.00953700	0.30934100	-1.76744300
H	-0.46663300	-0.67079500	-1.77193200
C	-0.79403800	1.29394200	-2.63249200
H	-1.66588600	1.72791500	-2.14684600
C	-1.14426300	0.53235900	-3.94462900
H	-1.89465100	1.08943300	-4.51893700
H	-1.54141300	-0.46584800	-3.73713800
C	0.22243700	0.48226400	-4.69427400
H	0.17897000	1.03892000	-5.63708900
H	0.54052600	-0.53889800	-4.92930300
C	1.18675600	1.17833300	-3.70598700
H	2.10837500	1.50905100	-4.18861800
C	0.28719400	2.28046400	-3.10798800
H	-0.06997800	2.99911500	-3.85501400
H	0.75309600	2.82067300	-2.27883400
C	-1.44710900	0.81477200	3.90186800
C	-2.64717700	1.40317200	3.59969700
C	-3.35887000	1.55097800	4.83344900
H	-2.95839400	1.72405600	2.61755800

C	-2.54643900	1.04182700	5.80218800
H	-4.33578400	1.99009200	4.97611700
H	-2.63672700	0.94547000	6.87369700
O	-1.38577900	0.58282100	5.26100300
C	-0.17331200	-1.59474500	3.36744400
C	0.47621100	-2.41578700	4.24685600
C	0.01658000	-3.74932900	3.97835900
H	1.20266500	-2.10058700	4.98076400
C	-0.88275100	-3.64937600	2.95727400
H	0.31392700	-4.65640500	4.48590000
H	-1.46679900	-4.35685900	2.39117200
O	-1.01536300	-2.34721600	2.57941400
C	1.43110300	0.71968000	3.68745100
C	2.49442000	1.38118900	3.13203800
C	3.45280900	1.56788700	4.17801800
H	2.58094100	1.67451600	2.09570000
C	2.90721100	1.00848800	5.29544300
H	4.41437100	2.05478700	4.10486300
H	3.24465100	0.90837500	6.31611400
O	1.67843700	0.48627200	5.02376300
I	-1.22243900	2.86301500	0.48348900
N	1.66127400	-1.05691600	-0.01545200
H	1.18441900	-1.92613500	-0.89157000
C	1.95692700	-1.95491900	1.09969100
H	2.18795700	-1.43632800	2.03361900
H	1.08318700	-2.58948300	1.24520300
H	2.83048300	-2.58606500	0.86272900
H	3.56205000	1.93297700	-2.91791700
C	-0.54480900	-3.06831700	-1.28272900
O	-0.79784300	-3.64244000	-0.16320600
O	0.76648100	-2.81898800	-1.57124700
O	-1.42621600	-2.70936300	-2.11430600
Cs	-3.08642200	-1.32802500	0.07985000
Cs	1.59603700	-5.48312100	-0.16172800

V*(a)

M06-2X single point: -2071.90881698 Hartree
B3LYP-D3 optimization: -1735.93186898 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.412083 Hartree

Pd	0.11393200	0.44917000	0.31230400
P	-0.08344700	0.14608600	2.84768000
C	4.82387800	1.59164700	-1.21371700
H	5.59515500	2.28993600	-1.52588100
C	4.96976300	0.83812700	-0.05441300
H	5.86562800	0.93242200	0.55508600
C	3.95858100	-0.04181300	0.34426400
H	4.08903800	-0.60025100	1.26353800
C	2.76956800	-0.17864900	-0.40357400
C	2.64784600	0.55338400	-1.62284100
C	3.66736600	1.42631400	-1.99118400
C	1.43541100	0.26234000	-2.49058100
H	1.57868800	-0.76824500	-2.84344500
C	0.03856200	0.29560500	-1.78182300
H	-0.41448200	-0.69490600	-1.80731100
C	-0.78334900	1.26906300	-2.64640300
H	-1.66600400	1.68311900	-2.16276000
C	-1.10926500	0.51731600	-3.96851900
H	-1.85755700	1.07270900	-4.54743100
H	-1.50350900	-0.48614300	-3.77882500
C	0.26752300	0.48987400	-4.70159600
H	0.22448800	1.04318300	-5.64635000
H	0.60640200	-0.52591400	-4.93113400
C	1.20884100	1.20429700	-3.70346600
H	2.12502400	1.55945500	-4.17877900
C	0.28024700	2.28213100	-3.10565400

H	-0.08718800	2.99842500	-3.85002600
H	0.72782700	2.82597500	-2.26897500
C	-1.44091800	0.78472000	3.89755700
C	-2.63949200	1.38532400	3.61420200
C	-3.34272200	1.51513700	4.85484800
H	-2.95480300	1.72617200	2.64023600
C	-2.52747500	0.98378200	5.80911100
H	-4.31608000	1.95749500	5.01126600
H	-2.61182900	0.86838100	6.87924300
O	-1.37324400	0.52781900	5.25248400
C	-0.17927700	-1.61234600	3.36601400
C	0.52636600	-2.44669700	4.18674700
C	-0.02244000	-3.76136700	4.00543100
H	1.34095400	-2.15235700	4.83113000
C	-1.02763100	-3.63522400	3.09181600
H	0.28080000	-4.67068900	4.50570000
H	-1.72083300	-4.32588900	2.63836200
O	-1.13933100	-2.33654800	2.69452900
C	1.43419100	0.69890400	3.66951200
C	2.49025700	1.37392600	3.11678300
C	3.44728300	1.56479400	4.16301100
H	2.57583000	1.66869800	2.08079400
C	2.90837200	0.99387700	5.27793800
H	4.40425400	2.06082300	4.09110400
H	3.24790700	0.89136000	6.29770000
O	1.68474600	0.46062900	5.00469300
I	-1.29623700	2.83038100	0.46598400
N	1.69899500	-1.00351900	-0.01938000
H	1.08698300	-2.18419100	-1.09063600
C	1.98880600	-1.89618500	1.09123900
H	2.25156900	-1.39585000	2.03221900
H	1.10538500	-2.51193400	1.26382200
H	2.84571700	-2.55040300	0.84408300
H	3.57443300	1.99961300	-2.90714200
C	-0.63900600	-3.09954500	-1.31945400
O	-0.83227900	-3.47861100	-0.12150400
O	0.69701400	-2.90461900	-1.69388300
O	-1.50985100	-2.88285900	-2.18873000
Cs	-3.11102400	-1.24778900	0.04257400
Cs	1.43079800	-5.46724000	0.20409700

V(a) (unsubstituted NBE)

M06-2X single point: -2071.920539 Hartree
B3LYP-D3 optimization: -1735.938141 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.407383 Hartree

Pd	-0.33367100	1.23977200	0.72375100
P	0.12915600	1.25657300	3.18839500
C	4.59831500	-0.38000900	-0.34750400
H	5.66663600	-0.26874200	-0.51060400
C	4.10752700	-1.25502100	0.61901600
H	4.78956200	-1.84484500	1.22705600
C	2.73094200	-1.35930300	0.83921600
H	2.37577500	-2.02007600	1.62077300
C	1.80886100	-0.58841800	0.09663600
C	2.30553100	0.27910300	-0.92819300
C	3.68605400	0.37165700	-1.10931400
C	1.30466600	0.93642500	-1.87926400
H	0.98101200	0.13431100	-2.55294900
C	-0.01567300	1.56838000	-1.29599000
H	-0.86111700	1.09456300	-1.79671800
C	0.08924400	3.06720100	-1.67936700
H	-0.47980100	3.74278300	-1.04416100
C	-0.28505200	3.17194800	-3.17844100
H	-0.33469500	4.22341600	-3.48685000

H	-1.25701800	2.71781400	-3.39625200
C	0.90201300	2.43493000	-3.87228200
H	1.38940700	3.07497500	-4.61526200
H	0.58407400	1.51962900	-4.38247400
C	1.86934400	2.12641900	-2.69984000
H	2.89758800	1.99740100	-3.04186600
C	1.61134800	3.29973100	-1.73417400
H	1.88566500	4.27778700	-2.14592200
H	2.10428900	3.16580200	-0.76500200
C	-1.13507200	0.97965800	4.46619000
C	-2.48362400	0.78811900	4.32340000
C	-3.01669000	0.61712100	5.64030400
H	-3.01932100	0.80452100	3.38527900
C	-1.95515000	0.71319800	6.49144400
H	-4.04793000	0.44862500	5.91523100
H	-1.85615600	0.64697300	7.56448700
O	-0.80314400	0.93382100	5.80183200
C	1.53239000	0.27499600	3.84528200
C	2.87421000	0.53082100	3.91455100
C	3.49627300	-0.66869700	4.39180900
H	3.35637100	1.46204100	3.65611000
C	2.49374800	-1.57074800	4.57818300
H	4.54892600	-0.83030600	4.57425600
H	2.45975100	-2.58862100	4.93481600
O	1.28868600	-1.01539200	4.24910100
C	0.79081800	2.92111200	3.52368400
C	1.00831000	3.98006500	2.68221400
C	1.58307100	5.02402200	3.47413100
H	0.76549000	4.00755900	1.63022900
C	1.67302400	4.53018300	4.74212400
H	1.88077300	6.00845100	3.14331200
H	2.02735100	4.94056600	5.67571200
O	1.20185800	3.25499400	4.79602200
I	-2.45658200	3.10228400	1.03749300
N	0.43031300	-0.66303200	0.26435800
H	-0.00741500	-1.54079800	-1.29410800
C	-0.05902500	-1.68489900	1.18314700
H	0.28632900	-1.58145200	2.21860500
H	-1.15294700	-1.65794700	1.20513200
H	0.23649600	-2.68606500	0.83174800
H	4.08233700	1.03401300	-1.87124000
C	-0.46503100	-1.97232200	-3.18968300
O	-0.01330600	-2.64648600	-4.13928900
O	0.12994200	-2.27469400	-1.94731300
O	-1.34650000	-1.07448600	-3.18218900
Cs	-3.34555100	-0.44147300	-1.04593500
Cs	2.91964100	-2.98101300	-2.99744300

TS2(a) (unsubstituted NBE)

M06-2X single point: -2071.870446 Hartree
B3LYP-D3 optimization: -1735.886505 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.40482 Hartree
Imaginary frequency: -294.4792 cm^{-1}

Pd	-0.19297600	1.23646400	1.06366600
P	0.36172500	1.58308300	3.22546000
C	4.59409600	-0.41098700	-0.38246300
H	5.67303500	-0.31125600	-0.45577000
C	4.02203500	-1.25117800	0.57639700
H	4.65946700	-1.81357400	1.25442400
C	2.62987500	-1.36763400	0.70239300
H	2.20267100	-2.00222500	1.46996700
C	1.79732800	-0.60766300	-0.13876800
C	2.37637600	0.22505900	-1.12897900
C	3.75409300	0.32365800	-1.24502500
C	1.33403600	0.86374900	-2.02682100

H	1.19460300	0.22383500	-2.90549800
C	-0.01855100	0.94324200	-1.28534900
H	-0.83984700	0.41826700	-1.75265200
C	-0.27904700	2.47832200	-1.17923000
H	-0.98292000	2.82415500	-0.41161500
C	-0.77581500	2.84682000	-2.61479900
H	-1.15982900	3.87213500	-2.59937800
H	-1.58747300	2.19879700	-2.95589300
C	0.51871400	2.72936500	-3.48018800
H	0.76795000	3.68638500	-3.94862100
H	0.42259300	1.98202200	-4.27362700
C	1.59646800	2.33127000	-2.44222100
H	2.62158300	2.51331300	-2.77344100
C	1.13677500	3.09591600	-1.18857400
H	1.11756600	4.18260800	-1.32571500
H	1.72460700	2.85438000	-0.29905800
C	-0.96499300	1.53592600	4.47363500
C	-2.31986700	1.46045500	4.28806800
C	-2.91017400	1.44069800	5.59241100
H	-2.82062000	1.41605100	3.32940000
C	-1.87512200	1.50047100	6.47822700
H	-3.96184800	1.38585700	5.83459500
H	-1.82062900	1.50913800	7.55664900
O	-0.68245100	1.55787600	5.82346500
C	1.55426600	0.36517200	3.91481700
C	2.83459400	0.43622400	4.39266500
C	3.25248400	-0.91090300	4.65426900
H	3.39960700	1.34230600	4.55126100
C	2.19976100	-1.70780100	4.32169500
H	4.20581800	-1.23543100	5.04662600
H	2.02783500	-2.77266100	4.35743700
O	1.15854800	-0.95148000	3.86377700
C	1.25883200	3.12942700	3.59457900
C	1.55099500	4.17530800	2.76020400
C	2.24886500	5.14961800	3.54301300
H	1.28988000	4.22974900	1.71328400
C	2.33348300	4.63023900	4.80069700
H	2.63240400	6.10488600	3.21464900
H	2.76169700	4.98839600	5.72487100
O	1.73971700	3.40587400	4.85640100
I	-3.70661200	0.95000200	0.33805200
N	0.41469200	-0.62602400	-0.17459200
H	0.26293400	-1.71526800	-1.76107100
C	-0.33449200	-1.58664600	0.63678300
H	-0.09167400	-1.53407800	1.70563300
H	-1.40300100	-1.38786800	0.52535000
H	-0.12630600	-2.60789200	0.27546900
H	4.18950900	0.96751300	-2.00530300
C	0.24331500	-2.14301600	-3.68486000
O	0.83112600	-2.86831000	-4.51060800
O	0.53009000	-2.46435600	-2.33754100
O	-0.54752800	-1.17962900	-3.86034400
Cs	-3.32189700	-1.49195100	-2.74633200
Cs	3.45487900	-3.31934400	-2.82740100

1a (by-product) (unsubstituted NBE)

M06-2X single point: -2071.960369 Hartree
B3LYP-D3 optimization: -1735.980983 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.408492 Hartree

Pd	1.55794200	0.36505100	1.84685800
P	0.94614300	1.32167700	3.74014000
C	4.22172700	-2.58211400	-2.36825600
H	4.97977000	-3.11860100	-2.93126700
C	3.85857600	-3.02555000	-1.08967900
H	4.33695700	-3.90435300	-0.66737200

C	2.89226200	-2.34442100	-0.34283900
H	2.61794600	-2.67574600	0.65413300
C	2.29353300	-1.21718700	-0.90573100
C	2.65048200	-0.76085600	-2.17904100
C	3.62132500	-1.44140500	-2.91465400
C	1.85942200	0.46569200	-2.54479700
H	1.25777200	0.32769900	-3.44771900
C	0.95594500	0.69016500	-1.28109100
H	-0.10531600	0.66944400	-1.50962500
C	1.37356900	2.09698300	-0.81347300
H	1.09908500	2.29184500	0.22605300
C	0.79458000	3.09818000	-1.84720400
H	0.85736600	4.12094700	-1.46082800
H	-0.25068300	2.87870400	-2.08568400
C	1.72499700	2.90173000	-3.09024900
H	2.28368600	3.81491700	-3.31924000
H	1.16233400	2.61862700	-3.98466500
C	2.68394000	1.78120800	-2.62694600
H	3.59137700	1.68234800	-3.22882800
C	2.88026500	2.12921600	-1.13641000
H	3.33187000	3.11475800	-0.98094000
H	3.45792900	1.38500200	-0.57905400
C	-0.61489700	0.62726300	4.39608700
C	-1.47371300	-0.29119200	3.84821600
C	-2.57250900	-0.42469400	4.75581700
H	-1.34589300	-0.81379000	2.91133200
C	-2.30231600	0.41065000	5.79936600
H	-3.43630300	-1.06242400	4.63657700
H	-2.81829500	0.64187600	6.71927600
O	-1.12037600	1.05974300	5.60316000
C	1.95660100	1.48155200	5.26132000
C	2.12719700	2.46866200	6.19499800
C	3.08701900	1.97997200	7.13868300
H	1.61746900	3.42099000	6.20636300
C	3.43126600	0.73064900	6.71572700
H	3.46708100	2.49059800	8.01198700
H	4.10714300	-0.02220600	7.09182100
O	2.76013000	0.41066300	5.57461100
C	0.48345900	3.08725000	3.50560300
C	0.87268600	3.98906200	2.54854600
C	0.16678000	5.20862900	2.81041800
H	1.58166000	3.79578100	1.75727600
C	-0.60731600	4.96786900	3.90782000
H	0.23089400	6.13574800	2.25872400
H	-1.30605500	5.56679000	4.47246000
O	-0.42794700	3.68982600	4.34624800
I	-3.78788700	-1.63993800	0.74226600
N	1.24453400	-0.43365500	-0.30560700
H	-2.88578400	-0.91975000	-1.75591700
C	0.02515500	-1.26398900	-0.07769300
H	0.27287000	-2.12837800	0.53830200
H	-0.73226000	-0.68963600	0.44957800
H	-0.42280600	-1.59910100	-1.02070500
H	3.90702300	-1.08598100	-3.90159300
C	-1.88935900	0.25987700	-2.95920800
O	-1.15878500	0.23101400	-3.97392200
O	-2.39543000	-1.00211200	-2.59662100
O	-2.19185400	1.22223700	-2.20810500
Cs	-2.38013800	2.20089500	0.69201500
Cs	-0.21259900	-2.76614700	-3.98813700

IV* (5,6-DiCOOiPr NBE)
M06-2X single point: -2971.44390634 Hartree
B3LYP-D3 optimization: -2635.63336334 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.701993 Hartree

Pd	-0.00937600	0.07184900	0.27734600
P	0.32591300	0.30979500	2.73634700
C	4.94701800	-0.99427700	-0.96262200
H	5.97480400	-0.76430900	-1.22568100
C	4.65909800	-1.73247200	0.17357100
H	5.45847300	-2.09249700	0.81706200
C	3.33458200	-2.00798700	0.49426800
H	3.12187100	-2.57186900	1.39187500
C	2.26867100	-1.53252800	-0.30280400
C	2.55299600	-0.79447300	-1.50597900
C	3.90937700	-0.55111900	-1.80682400
C	1.35381400	-0.50524600	-2.43577600
H	1.20813600	-1.46710400	-2.94679200
C	-0.05320600	-0.12100700	-1.81266600
H	-0.76757200	-0.92756000	-1.96236800
C	-0.46032300	1.15440100	-2.57964700
H	-1.23044700	1.74363100	-2.09070700
C	-0.82057200	0.87025500	-4.06051900
H	-1.08825200	1.82683800	-4.52903700
C	0.55286500	0.44460400	-4.68685500
H	0.84635200	1.14767600	-5.47107800
C	1.53798300	0.63293100	-3.48367000
H	2.55986400	0.73765600	-3.81951500
C	0.90334100	1.83951300	-2.77166300
H	0.87371500	2.74641500	-3.38734300
H	1.39183600	2.06468200	-1.81917200
C	-1.20398300	-0.06596200	3.63486500
C	-2.24692400	-0.84658100	3.21155100
C	-3.17047700	-0.90817700	4.30447800
H	-2.32293500	-1.32981200	2.24536900
C	-2.62535300	-0.16206100	5.30853100
H	-4.11284600	-1.43652600	4.33733000
H	-2.95127400	0.09463900	6.30531000
O	-1.42470300	0.35323000	4.92649700
C	1.56603600	-0.66642300	3.68114300
C	2.93418700	-0.64115400	3.65797600
C	3.37766100	-1.74260700	4.45934200
H	3.54656000	0.06263100	3.11352500
C	2.25132000	-2.36365500	4.90957800
H	4.39810100	-2.02975700	4.66912000
H	2.07202800	-3.21732000	5.54479200
O	1.13811000	-1.72163400	4.44858600
C	0.87719000	1.96718900	3.24304900
C	1.37874200	2.99525700	2.49141000
C	1.81355100	4.00321100	3.40902200
H	1.40140000	3.02576800	1.41251800
C	1.54944900	3.51667100	4.65572000
H	2.25465900	4.96045100	3.17142300
H	1.68630000	3.91086700	5.65139400
O	0.98978200	2.27898800	4.57982800
I	-1.71811600	2.36480600	0.55047500
N	0.94224500	-1.78867100	0.03507700
H	-0.40656600	-2.74402400	-0.90193600
C	0.72337200	-2.71803200	1.14453200
H	1.19873600	-2.43071600	2.08746900
H	-0.35126100	-2.80909800	1.30594300
H	1.11696800	-3.71228800	0.87750800
C	0.63606700	-0.93158900	-5.28863500
O	-0.12880200	-1.85786500	-5.05983200
O	1.69988400	-1.04761100	-6.10000100
C	1.92445100	-2.34428400	-6.73958200
C	3.39228900	-2.37390900	-7.13145500
C	0.98138900	-2.48592800	-7.92931800
H	1.70901200	-3.11788900	-5.99586200
H	4.03274900	-2.29130800	-6.25147800
H	3.62024000	-3.31696500	-7.63704100
H	3.62592900	-1.54974700	-7.81213100
H	-0.05899500	-2.44061500	-7.60145800

H	1.15960700	-1.68371000	-8.65214900
H	1.14934500	-3.44579500	-8.42768100
C	-2.02240700	0.00132100	-4.34344500
O	-2.72263800	-0.57193100	-3.52369900
O	-2.30079600	0.00977700	-5.66514100
C	-3.49468900	-0.68192700	-6.12427500
C	-3.18024000	-1.18640300	-7.52392700
C	-4.67264700	0.28367700	-6.06640700
H	-3.68464000	-1.51871800	-5.44623900
H	-2.31571100	-1.85561100	-7.50504800
H	-4.03800500	-1.73095200	-7.93020700
H	-2.95274300	-0.34999900	-8.19189600
H	-4.83335100	0.62376300	-5.03976700
H	-4.48184400	1.15535800	-6.69992900
H	-5.58533400	-0.20898500	-6.41605900
C	-2.34037500	-3.08003700	-0.76945100
O	-3.31184500	-3.49344400	-1.45595000
O	-1.09170100	-3.30069200	-1.34930500
O	-2.37684000	-2.47792200	0.33241600
Cs	-4.34101100	-0.38513400	-0.75696400
Cs	-1.98955100	-4.08906200	-4.17124500
C	4.97295000	1.43181000	-2.77663900
C	5.08395400	-0.67924700	-3.95057400
C	5.16609100	2.14532500	-4.11392500
H	5.95538700	1.32596200	-2.28141800
H	4.33224300	2.03506800	-2.12459800
C	5.25635400	0.09601900	-5.25597600
H	6.08241300	-0.95603000	-3.56499200
H	4.52965600	-1.60640600	-4.13135900
H	5.73238800	3.07178500	-3.97932700
H	4.18225600	2.39535200	-4.54472700
H	5.88315900	-0.46109400	-5.95935700
H	4.26868400	0.25847200	-5.71720400
N	4.32429000	0.14048800	-3.00909500
O	5.90904700	1.34213900	-5.02790700

IV (5,6-DiCOOiPr NBE)

M06-2X single point: -2971.433185 Hartree
B3LYP-D3 optimization: -2635.632298 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.698745 Hartree

Pd	0.63714900	-0.00107200	1.38772900
P	0.39670900	0.39445100	3.79776800
C	5.64549800	-1.23940900	0.07080900
H	6.69117900	-1.13937000	-0.19224800
C	5.28847600	-1.92309000	1.22310800
H	6.05628100	-2.33922100	1.87035400
C	3.94672700	-2.09856800	1.54289100
H	3.68782300	-2.65324000	2.43518400
C	2.92552400	-1.55736500	0.72846100
C	3.28535900	-0.79026400	-0.43096000
C	4.65389100	-0.69965800	-0.77393700
C	2.14640500	-0.24715600	-1.31336400
H	1.95806400	-1.04645800	-2.03744300
C	0.79105300	0.09406100	-0.62365800
H	-0.03684200	-0.52051200	-0.96842100
C	0.54949100	1.58768200	-0.87534400
H	-0.10759100	2.09998300	-0.16297100
C	0.04597300	1.77628500	-2.32363900
H	-0.10191100	2.84922700	-2.49450000
C	1.28483700	1.30629900	-3.16990600
H	1.61337000	2.10223000	-3.84005500
C	2.39719200	1.09318600	-2.07092600
H	3.39947600	1.19374500	-2.46680300
C	1.98217500	2.12752700	-1.01047600
H	2.02787200	3.16397000	-1.35858200

26

H	2.57051300	2.02893300	-0.09283100
C	-0.41595600	-0.80523100	4.89193800
C	-1.34203500	-1.77553500	4.61225000
C	-1.66201200	-2.39593700	5.86303400
H	-1.77048400	-2.01453200	3.64489300
C	-0.90612600	-1.76803400	6.80840500
H	-2.35840700	-3.20543800	6.02912100
H	-0.79304400	-1.89275400	7.87481000
O	-0.14285900	-0.79405600	6.24221800
C	2.02865200	0.65731600	4.54978400
C	3.27352100	0.41858600	4.02823400
C	4.21707300	0.82056000	5.02600900
H	3.48333900	-0.00458600	3.05576800
C	3.48182400	1.28165800	6.07811500
H	5.29475300	0.77619800	4.96382100
H	3.74114700	1.69229100	7.04227500
O	2.15045300	1.19176300	5.81143200
C	-0.50992100	1.94170200	4.10444100
C	-0.86873200	2.93733200	3.23198900
C	-1.59305400	3.90919800	3.99278900
H	-0.65983400	2.99123800	2.17150300
C	-1.62632000	3.43842200	5.27215500
H	-2.02907000	4.82435600	3.61972100
H	-2.05590400	3.80946900	6.19043100
O	-0.97376600	2.24468800	5.36407600
I	-2.19656000	4.40135200	-0.28587600
N	1.57560000	-1.81020700	0.99908700
H	-1.89130700	-4.33273900	2.04167700
C	1.28345900	-2.72779600	2.09551600
H	1.61381400	-2.38356200	3.08936000
H	0.20647600	-2.89662600	2.13790800
H	1.76362700	-3.70189000	1.90869900
C	1.03656300	0.07530700	-4.01368000
O	0.32271900	-0.86610100	-3.69402000
O	1.72702200	0.11030200	-5.16322700
C	1.50973300	-0.97926300	-6.11819900
C	2.30230700	-2.21486200	-5.70784700
C	1.91992700	-0.41833900	-7.46996100
H	0.43956600	-1.20785000	-6.10149000
H	2.02450000	-2.53552300	-4.70211200
H	2.09223800	-3.03329800	-6.40350400
H	3.37631600	-2.01461300	-5.73275300
H	1.33323700	0.47134800	-7.71294900
H	2.98013400	-0.14698100	-7.46686800
H	1.75637600	-1.16840900	-8.24935100
C	-1.29527400	1.16205700	-2.65255300
O	-2.03962000	0.61809000	-1.85654000
O	-1.60021200	1.36124900	-3.94508900
C	-2.89256000	0.87602900	-4.42300600
C	-2.83146900	-0.63305800	-4.63283000
C	-3.17059600	1.65670200	-5.69753200
H	-3.63458700	1.11538000	-3.65489300
H	-2.62111500	-1.13963900	-3.68947800
H	-3.79051000	-0.99155600	-5.02017500
H	-2.04516700	-0.88490100	-5.35071900
H	-3.17738600	2.73152800	-5.49806500
H	-2.40416700	1.44613200	-6.45070600
H	-4.14474500	1.37080400	-6.10524200
C	-2.57061700	-2.86609300	1.01783500
O	-2.58423300	-2.36802900	-0.12886300
O	-1.81790200	-4.05792600	1.11647400
O	-3.09629500	-2.45910300	2.08049300
Cs	-3.31607500	0.58825900	1.02051200
Cs	-0.10430200	-3.41931000	-1.62763400
C	6.37125500	0.58447100	-2.00587300
C	4.91009800	-0.92538200	-3.19111900
C	6.50406200	1.40668800	-3.28446200
H	7.21367600	-0.12956800	-1.97803100

H	6.44535300	1.23361900	-1.12816100
C	5.13683500	-0.09389600	-4.45592600
H	5.62129600	-1.77130100	-3.17291200
H	3.89914900	-1.34212100	-3.21064900
H	7.48815500	1.88156200	-3.33513900
H	5.73061100	2.19174000	-3.30672500
H	5.14779000	-0.74125000	-5.33752400
H	4.31808700	0.63246100	-4.57432400
N	5.06863100	-0.08114300	-2.00072500
O	6.39441500	0.57047900	-4.43254100

TS3 (5,6-DiCOOiPr NBE)

M06-2X single point: -2971.40363 Hartree
B3LYP-D3 optimization: -2635.600379 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.696211 Hartree
Imaginary frequency: -308.0299 cm^{-1}

Pd	0.78250300	0.06123600	1.63603100
P	0.46333600	0.77066900	3.79454400
C	5.73007600	-1.30085700	0.08007400
H	6.79301500	-1.18929500	-0.09583800
C	5.28945400	-2.02155000	1.18723400
H	6.01943000	-2.45533400	1.86593800
C	3.92856500	-2.20105500	1.43976000
H	3.59270900	-2.75976400	2.30637700
C	2.99477000	-1.61211200	0.56799200
C	3.43170300	-0.89074300	-0.56601600
C	4.80059000	-0.74973600	-0.82969900
C	2.26170600	-0.46989800	-1.44553000
H	2.13601600	-1.25651200	-2.20004500
C	0.95470400	-0.38202400	-0.62261300
H	0.14582000	-1.02528800	-0.93254800
C	0.55878600	1.13465900	-0.72627300
H	-0.10969000	1.55832100	0.03112500
C	-0.04980200	1.35365800	-2.13933000
H	-0.32222400	2.41380100	-2.19042800
C	1.16670700	1.12036400	-3.10152200
H	1.35506800	2.00922900	-3.70701100
C	2.35367600	0.93561100	-2.09143900
H	3.32770500	1.14888200	-2.52031600
C	1.91613000	1.83305500	-0.92175200
H	1.81584100	2.88916500	-1.18859700
H	2.58177800	1.74189300	-0.05945600
C	-0.52948200	-0.32930100	4.85744400
C	-1.17541500	-1.50057000	4.55363800
C	-1.80553900	-1.94259700	5.76226700
H	-1.22162200	-1.98928100	3.58976700
C	-1.49629600	-1.01711200	6.71465800
H	-2.40526000	-2.83134200	5.89715700
H	-1.73491400	-0.92004600	7.76323700
O	-0.72257700	-0.02810000	6.18874600
C	2.05989500	0.88668600	4.66834000
C	3.29863800	0.46299800	4.25966500
C	4.20454100	0.75405700	5.32888700
H	3.52384300	-0.00827100	3.31226300
C	3.45653700	1.33447500	6.31027300
H	5.26721300	0.56089500	5.35957100
H	3.69018200	1.72683100	7.28858900
O	2.15176700	1.42275500	5.93214400
C	-0.31404600	2.39877900	4.03569700
C	-0.82380600	3.25603200	3.09426600
C	-1.36069800	4.37590300	3.80532900
H	-0.83217000	3.11410100	2.02211700
C	-1.13984100	4.12457700	5.12721800
H	-1.84369000	5.24351600	3.37975500

H	-1.35816600	4.66899200	6.03377300
O	-0.50752400	2.92931000	5.29228200
I	-2.61496700	3.73420100	-0.53606100
N	1.62420200	-1.71091700	0.70364500
H	-1.48273500	-4.77881200	1.36782100
C	1.01976000	-2.83276900	1.40292600
H	1.20502100	-2.82104100	2.48865100
H	-0.06271700	-2.81502300	1.26961500
H	1.40543800	-3.78281600	0.99682000
C	1.02800600	-0.05067800	-4.04766500
O	0.29258900	-1.01387900	-3.87331500
O	1.84607400	0.06435500	-5.10014900
C	1.76088900	-0.96123000	-6.14687000
C	2.48917400	-2.22871800	-5.71536800
C	2.35155400	-0.31535000	-7.38927400
H	0.69766600	-1.17793000	-6.29051300
H	2.07302000	-2.61842700	-4.78425100
H	2.38029900	-2.99319600	-6.49101800
H	3.55620900	-2.03739600	-5.57645000
H	1.80572700	0.59522300	-7.64921200
H	3.40211000	-0.05705200	-7.22490700
H	2.29364600	-1.01033200	-8.23201900
C	-1.34159100	0.63788700	-2.45361000
O	-1.91017500	-0.15268000	-1.71303200
O	-1.80370600	1.02637600	-3.64540800
C	-3.06386300	0.47476100	-4.13957100
C	-2.75630200	-0.16935700	-5.48487700
C	-4.06205900	1.62118000	-4.20719200
H	-3.40130800	-0.27629600	-3.42148900
H	-1.98548100	-0.93753100	-5.37468800
H	-3.66037800	-0.62605700	-5.89937900
H	-2.39255100	0.58185900	-6.19335000
H	-4.18100900	2.07998300	-3.22163900
H	-3.71543500	2.38988200	-4.90503000
H	-5.03391900	1.25180600	-4.55002700
C	-2.65604600	-3.35435200	0.86861200
O	-3.29385100	-2.87414100	-0.09365500
O	-1.91094800	-4.51342600	0.54122200
O	-2.54080200	-2.94926900	2.04797900
Cs	-3.26243700	0.11013600	1.30384300
Cs	-1.26502900	-3.35679400	-2.42417000
C	6.56633600	0.53903800	-1.97268400
C	5.06586500	-0.84324800	-3.25427400
C	6.73361900	1.43368500	-3.19784800
H	7.37788700	-0.21012200	-1.98096600
H	6.65905400	1.13281100	-1.05833000
C	5.31136800	0.06287600	-4.46097000
H	5.76122000	-1.70092600	-3.28881800
H	4.04897500	-1.23867600	-3.30294800
H	7.73586200	1.87106900	-3.22004600
H	5.99152300	2.24795800	-3.16501600
H	5.29477600	-0.52196300	-5.38559900
H	4.51568000	0.82232200	-4.52048100
N	5.24002100	-0.07693600	-2.01298400
O	6.58996600	0.68222100	-4.39996900

2b (product) (5,6-DiCOOiPr NBE)

M06-2X single point: -2971.504102 Hartree
B3LYP-D3 optimization: -2635.692435 Hartree
B3LYP-D3 thermal correction to Gibbs free energy: 0.701134 Hartree

Pd	1.21180500	-0.08089200	2.44999500
P	0.42841200	0.77114000	4.33972800
C	6.01102600	-1.25575100	-0.03833800
H	7.08037200	-1.24191200	-0.21374400
C	5.53865800	-1.55294800	1.24473700

H	6.25245100	-1.76075500	2.03654200
C	4.17327500	-1.58004500	1.52460300
H	3.79788500	-1.77542300	2.52381600
C	3.29761600	-1.29692800	0.47628900
C	3.74211600	-1.01642200	-0.81273400
C	5.12231600	-0.97689900	-1.09189700
C	2.57495800	-0.67033400	-1.70401800
H	2.44889100	-1.38946100	-2.51491100
C	1.36193400	-0.66935500	-0.71142400
H	0.52610800	-1.27752500	-1.04334000
C	0.94822000	0.82144300	-0.66375200
H	0.40495200	1.08918500	0.24459000
C	0.21217600	1.20708200	-1.96397400
H	-0.06378300	2.26386200	-1.88123200
C	1.32585700	1.08624700	-3.07282400
H	1.45384500	2.03754000	-3.59131800
C	2.60379300	0.79408200	-2.21299700
H	3.53429000	1.04909000	-2.71973100
C	2.27889900	1.56164700	-0.91177400
H	2.14507900	2.63697500	-1.05940500
H	3.02080700	1.40447000	-0.12597500
C	-0.68461300	-0.35942700	5.25139500
C	-1.20444900	-1.57206800	4.87399700
C	-2.05509700	-2.00259800	5.94378200
H	-1.02193200	-2.08937500	3.94179900
C	-1.98916500	-1.02984700	6.89729200
H	-2.63042400	-2.91606500	5.99347800
H	-2.44031700	-0.91084600	7.87110400
O	-1.16515800	-0.02283800	6.49829700
C	1.67194000	1.23484500	5.59392100
C	3.03428000	1.09629000	5.54948500
C	3.54406100	1.62421200	6.77838100
H	3.59025000	0.66961500	4.72675400
C	2.45704400	2.04998400	7.48298800
H	4.57643200	1.68197700	7.09211100
H	2.33458300	2.51558800	8.44936800
O	1.31129900	1.82365600	6.78393900
C	-0.59638700	2.27431900	4.18096500
C	-0.84317000	3.04473300	3.07389100
C	-1.76327200	4.06548100	3.47355100
H	-0.43544700	2.89742800	2.08440700
C	-2.01147800	3.84926800	4.79659100
H	-2.18465600	4.83272400	2.84093900
H	-2.63088400	4.34655800	5.52803600
O	-1.31524200	2.76696800	5.24844800
I	-2.48369900	3.65300800	-0.50324200
N	1.85497700	-1.23399200	0.59673800
H	-0.87586800	-4.78578900	1.19259200
C	1.29472300	-2.59639100	0.82950500
H	1.75612200	-3.02459600	1.72044800
H	0.22276900	-2.53032200	1.00653400
H	1.50391800	-3.25707700	-0.02622600
C	1.04311900	0.03016500	-4.11963400
O	0.52609000	-1.05847400	-3.89219400
O	1.44213200	0.41565800	-5.33503500
C	1.18422800	-0.48558400	-6.46113700
C	2.30201600	-1.51601600	-6.54714900
C	1.07911000	0.40989900	-7.68453500
H	0.23064400	-0.98338400	-6.26545500
H	2.37154200	-2.08604800	-5.61713300
H	2.10474600	-2.21269700	-7.36776100
H	3.25951400	-1.02350200	-6.73577800
H	0.27633000	1.14145600	-7.55933600
H	2.01798700	0.94700000	-7.85035100
H	0.86482000	-0.19541300	-8.57026800
C	-1.09874900	0.52767800	-2.26929700
O	-1.64780100	-0.30844300	-1.56420100
O	-1.59690600	0.99249800	-3.42021700

C	-2.89240400	0.51705000	-3.90039300
C	-2.63789500	-0.19476100	-5.22364600
C	-3.79868300	1.73260800	-4.02147300
H	-3.28775500	-0.17768100	-3.15530400
H	-1.93174000	-1.01947700	-5.09535700
H	-3.57552400	-0.58752900	-5.62855300
H	-2.21127200	0.50234200	-5.95218700
H	-3.88078700	2.24232800	-3.05791400
H	-3.39329700	2.43965000	-4.75229300
H	-4.79486100	1.42197400	-4.35286000
C	-2.20513400	-3.44807800	0.87949100
O	-3.00514000	-3.01327500	0.02331200
O	-1.42775000	-4.54733800	0.43389100
O	-1.95200900	-3.04081900	2.03636700
Cs	-2.84238700	-0.00044400	1.47300300
Cs	-1.34675600	-3.39135000	-2.60499900
C	6.93571500	-0.10684500	-2.51498000
C	5.25401900	-1.54187700	-3.47682000
C	7.09410000	0.55886600	-3.88050700
H	7.68264700	-0.91524600	-2.42601900
H	7.12714200	0.62521300	-1.72485900
C	5.47480500	-0.85135600	-4.82026300
H	5.89584300	-2.43809800	-3.41581100
H	4.21595600	-1.87073900	-3.40431500
H	8.12649500	0.88825400	-4.02761600
H	6.42974000	1.43641800	-3.93789400
H	5.33520200	-1.56238600	-5.63935300
H	4.74313200	-0.03377500	-4.93305100
N	5.56649400	-0.60714900	-2.38688700
O	6.80076400	-0.35140100	-4.93572900

Int_I (DavePhos+5,6-DiCOOiPr NBE)

B3LYP-D3 optimization: -2727.97232206 Hartree

Pd	-0.48944900	-0.51172700	0.45095800
P	-0.61816700	-0.61123100	3.05175100
C	4.24877600	1.12267000	-1.62101800
H	4.78245900	2.03260200	-1.88647100
C	4.87690000	0.10936200	-0.89634300
H	5.90513600	0.22451900	-0.56001000
C	4.19258400	-1.07608900	-0.62044500
H	4.70021100	-1.86696900	-0.07995200
C	2.87448500	-1.28491200	-1.08288100
C	2.21705400	-0.25072000	-1.82252500
C	2.93103800	0.92361900	-2.06655200
C	0.87313100	-0.56578100	-2.46971700
H	1.00452200	-1.57297900	-2.87701500
C	-0.46531900	-0.58480800	-1.62248100
H	-0.95630900	-1.53741100	-1.80779500
C	-1.30933600	0.56748900	-2.22739900
H	-2.00778000	1.02505300	-1.53342000
C	-1.94412200	0.06228100	-3.54163600
H	-2.52660400	0.88202100	-3.98835000
C	-0.69651400	-0.16042900	-4.46844500
H	-0.78171900	0.44735200	-5.37198000
C	0.48060100	0.42271700	-3.59810600
H	1.31805100	0.72392400	-4.23285500
C	-0.24888900	1.52094500	-2.79662100
H	-0.66538700	2.32035500	-3.42198000
H	0.36040900	1.95457500	-2.00467900
I	-1.03938200	-3.23202900	0.56690400
N	2.24232700	-2.49414500	-0.90256900
H	1.23051300	-2.48190400	-0.86059600
C	2.85131400	-3.61211300	-0.21871400
H	3.16087400	-3.37949800	0.81065800
H	2.11596900	-4.41665800	-0.17047000
H	3.73445800	-3.96982800	-0.76279100

H	2.46587200	1.71053100	-2.64966600
C	-0.42382300	-1.57898300	-4.91181500
O	-0.60727400	-2.58315700	-4.25240200
O	0.13407900	-1.58893900	-6.14570500
C	0.53128400	-2.88214900	-6.67931800
C	1.64393800	-2.59468700	-7.67646100
C	-0.68524900	-3.55996700	-7.30059700
H	0.90320900	-3.48734000	-5.84649200
H	2.47828500	-2.08537000	-7.18617600
H	2.01204400	-3.52949700	-8.11081100
H	1.27762100	-1.95648500	-8.48714000
H	-1.45253500	-3.71945900	-6.54065300
H	-1.10078700	-2.93624000	-8.09895400
H	-0.40671800	-4.53027300	-7.72452400
C	-2.96246500	-1.04426700	-3.37282000
O	-3.51552800	-1.30864200	-2.32372700
O	-3.27596100	-1.62761700	-4.54928100
C	-4.21529100	-2.74057600	-4.50190300
C	-3.53203200	-3.97577000	-3.92254900
C	-4.69179200	-2.92418100	-5.93548000
H	-5.04699500	-2.44251900	-3.85421600
H	-3.21589900	-3.79189600	-2.89427400
H	-4.22802800	-4.82155900	-3.93221000
H	-2.64685200	-4.23237700	-4.50984800
H	-5.14613600	-2.00447200	-6.31575800
H	-3.85258900	-3.18809600	-6.58691400
H	-5.43349200	-3.72740800	-5.98553200
C	-0.25259900	0.86534500	4.19542700
C	-0.91446900	2.17378400	3.71290800
C	-0.52086400	0.69272900	5.70166000
C	-0.86696100	3.28328200	4.79596700
H	-0.41428600	2.52740500	2.81000800
C	0.24422400	1.77561200	6.49895500
H	-1.59468100	0.78928800	5.87912300
C	0.34624400	3.10759700	5.71785100
H	-0.83309000	4.27292000	4.31961300
H	1.25204100	1.41374400	6.73841600
H	1.25823800	3.11439800	5.10382900
C	-2.09386300	-1.43650800	3.87481300
C	-1.86165400	-2.59147600	4.64518600
C	-3.43855200	-0.98262700	3.74851700
C	-2.87493300	-3.25032500	5.33540000
H	-0.86883900	-3.01390700	4.69267700
C	-4.44370600	-1.65323300	4.47325800
C	-4.17716100	-2.76113900	5.26826000
H	-2.64390400	-4.14253700	5.91047000
H	-5.46275000	-1.29707300	4.37810100
H	-4.98565400	-3.25728500	5.79779800
C	0.89579700	-1.69463900	3.46933000
C	2.06187900	-1.17929600	2.58005400
C	1.41281900	-1.83685000	4.91496600
C	3.45283900	-1.61667700	3.09035500
H	1.90001900	-1.52123100	1.55555700
C	2.47787000	-2.95615000	4.99603700
H	1.85501200	-0.88489400	5.23497200
C	3.37451600	-3.00340400	3.73691700
H	4.16324200	-1.60321900	2.25732300
H	1.97901600	-3.92368000	5.12762700
H	2.95178100	-3.70533100	3.00830800
H	0.44129900	3.95203200	6.40973600
H	-1.77476000	3.26440600	5.41230200
H	-0.26066500	1.94371800	7.45790500
H	-0.25613200	-0.29685300	6.06870300
H	-1.95444100	1.96550400	3.43464100
H	0.83504700	0.96988100	4.07108600
H	0.61783300	-2.05466700	5.62956400
H	3.09045300	-2.79710000	5.89221000
H	4.37206600	-3.38027900	3.98826900

H	3.83274000	-0.90042700	3.83349800
H	2.02655100	-0.08526100	2.53318600
H	0.60546200	-2.68184100	3.09329800
C	-3.94062200	0.03787800	2.76513700
C	-4.88340700	1.05686900	3.10091700
C	-3.67199500	-0.19409500	1.41019500
C	-5.48830400	1.78522500	2.05964600
C	-4.27760600	0.53319000	0.38507200
H	-3.01345700	-1.01170400	1.14268400
C	-5.20160800	1.51604000	0.71506200
H	-6.22969100	2.54218700	2.29502000
H	-4.04119400	0.28479400	-0.64223700
H	-5.71558900	2.07533100	-0.06399000
N	-5.28293700	1.27026300	4.45082200
C	-4.24099500	1.65248800	5.38702600
H	-3.95937900	2.71963300	5.28777700
H	-4.58002000	1.48811900	6.41547600
H	-3.35394200	1.04608100	5.22553400
C	-6.52087400	1.98718300	4.68715400
H	-6.80554000	1.86133300	5.73685000
H	-6.45104600	3.07666000	4.49450600
H	-7.32116000	1.58000800	4.06453800
C	-0.60318000	2.50625200	0.44978700
O	-1.81554600	2.40132700	0.10540100
O	0.21533500	1.45702100	0.41742800
O	-0.08094200	3.61163300	0.88992500
Cs	-2.94513000	4.54314300	1.63030700
Cs	2.75118700	2.52490300	1.31720000

broblasts expressing human CYP11B1 with deoxycorticosterone (100 nM) as the substrate;