

Supporting Information

Tetranuclear Rollover Cyclometalated Organoplatinum-Rhenium Compound;

C-I Oxidative Addition and C-C Reductive Elimination Using a Rollover

Cycloplatinated Dimer

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Contents	Page
Figure S1. ¹ H NMR spectrum (400 MHz) of complex 1 in CDCl ₃ .	S3
Figure S2. ¹ H NMR spectrum (400 MHz) of complex 2 in CDCl ₃ .	S3
Figure S3. ³¹ P NMR spectrum of complex 2 in CDCl ₃ .	S4
Figure S4. ¹³ C NMR spectrum of complex 2 in CDCl ₃ .	S4
Figure S5. ¹ H NMR spectrum (400 MHz) of complex 3 in CDCl ₃ .	S5
Figure S6. ³¹ P NMR spectrum of complex 3 in CDCl ₃ .	S5
Figure S7. ¹³ C NMR spectrum of complex 3 in CDCl ₃ .	S6
Figure S8. ¹ H NMR spectrum (400 MHz) of complex 4 in CDCl ₃ .	S6
Figure S9. ³¹ P NMR spectrum of complex 4 in CDCl ₃ .	S7
Table S1. Crystal Data and Structure Refinement for 5 .Hexane	S8
Espenson's Approach for determination of higher and lower rate constants	S9
Table S2. Rate Constants (k_2 and k'_2) and Calculated ϵ_A Values at 375 nm for Cases I and II	S10
XYZ Cartesian coordinates of optimized structures	S10

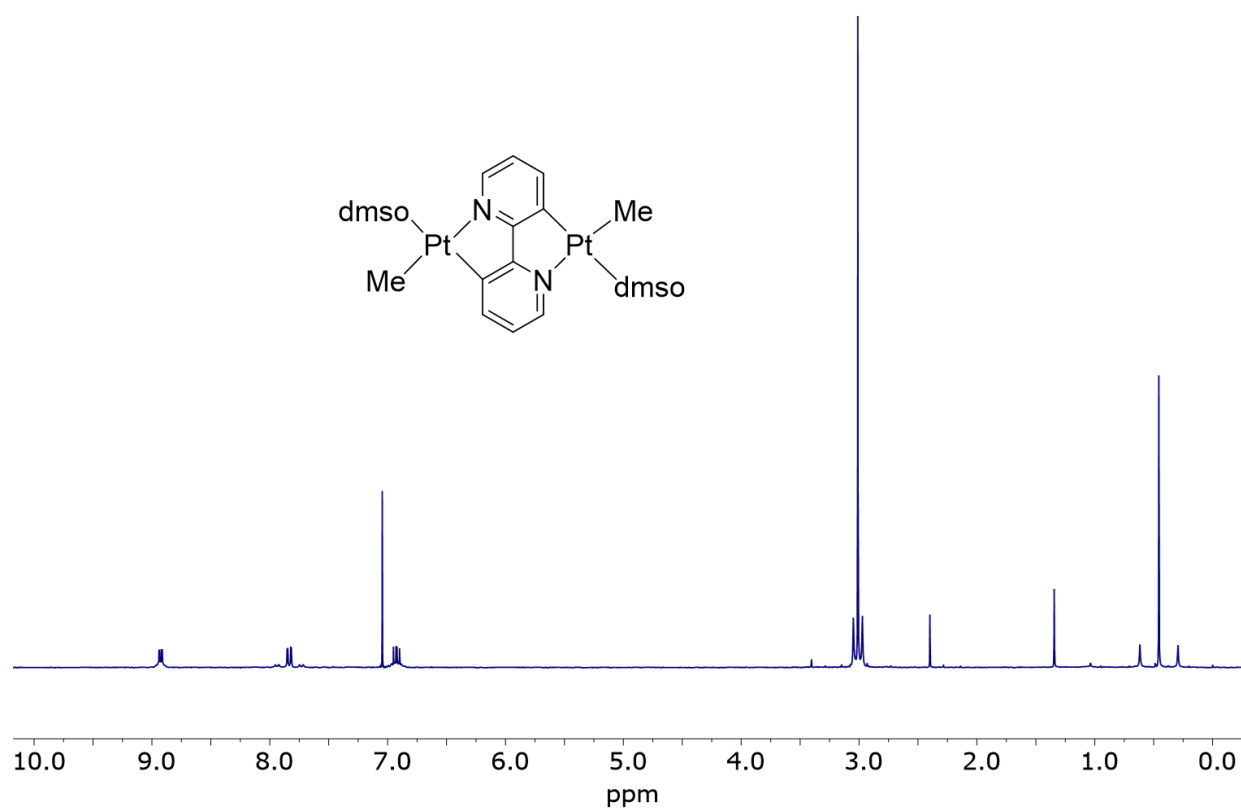


Figure S1. ^1H NMR spectrum (400 MHz) of complex **1** in CDCl_3 .

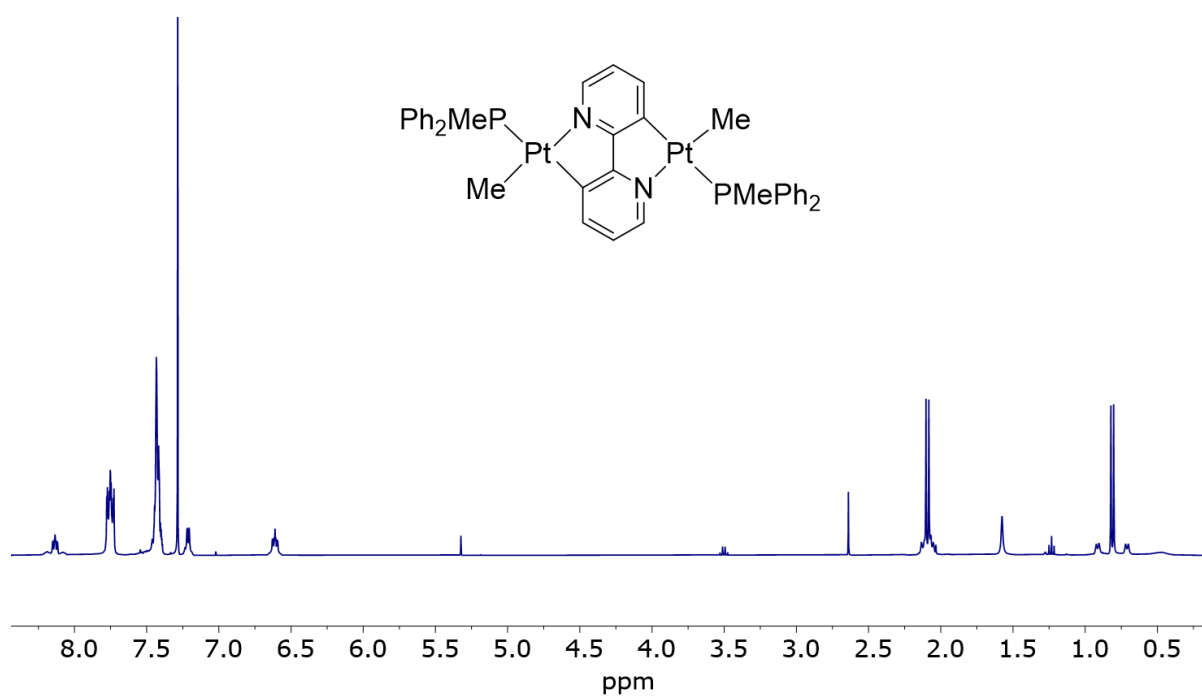


Figure S2. ^1H NMR spectrum (400 MHz) of complex **2** in CDCl_3 .

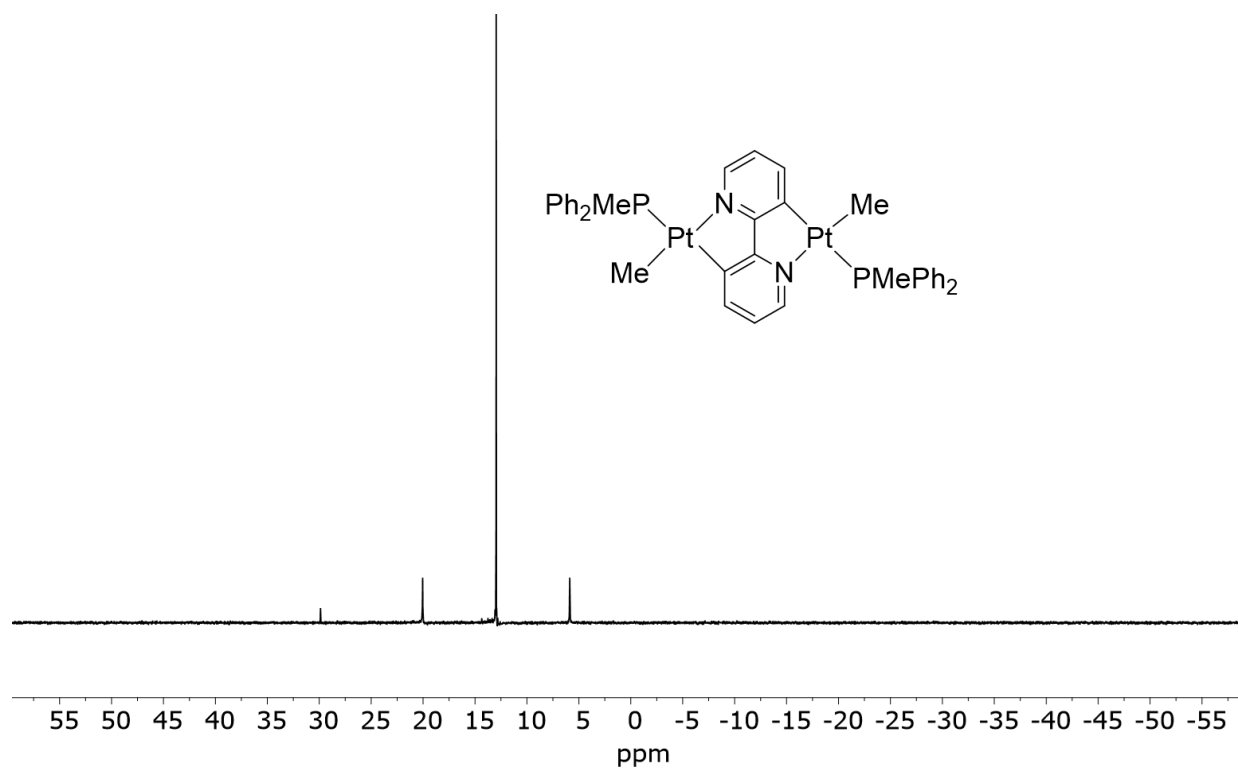


Figure S3. ^{31}P NMR spectrum of complex **2** in CDCl_3 .

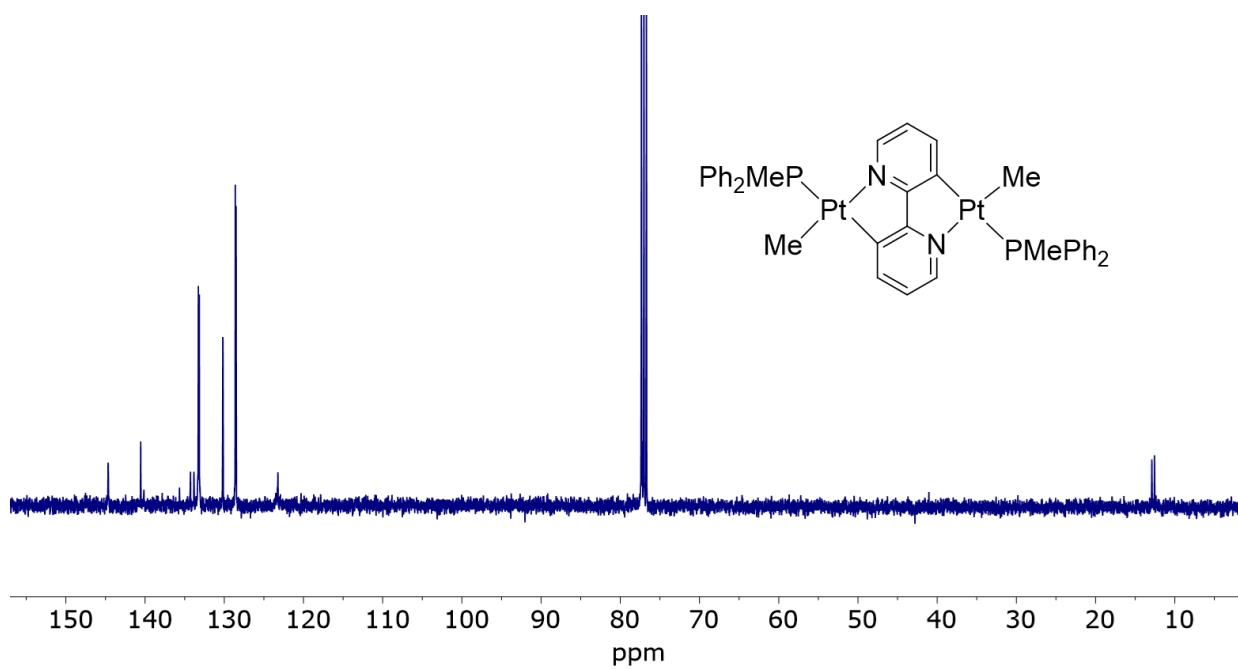


Figure S4. ^{13}C NMR spectrum of complex **2** in CDCl_3 .

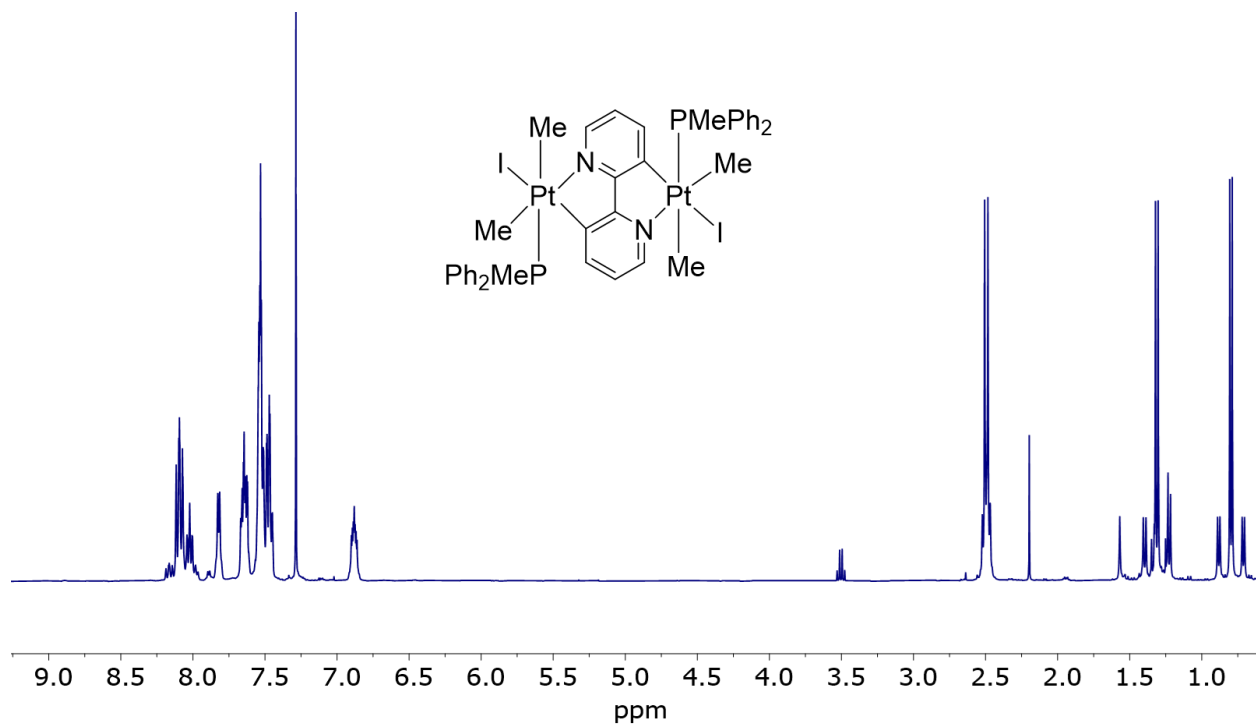


Figure S5. ^1H NMR spectrum (400 MHz) of complex **3** in CDCl_3 .

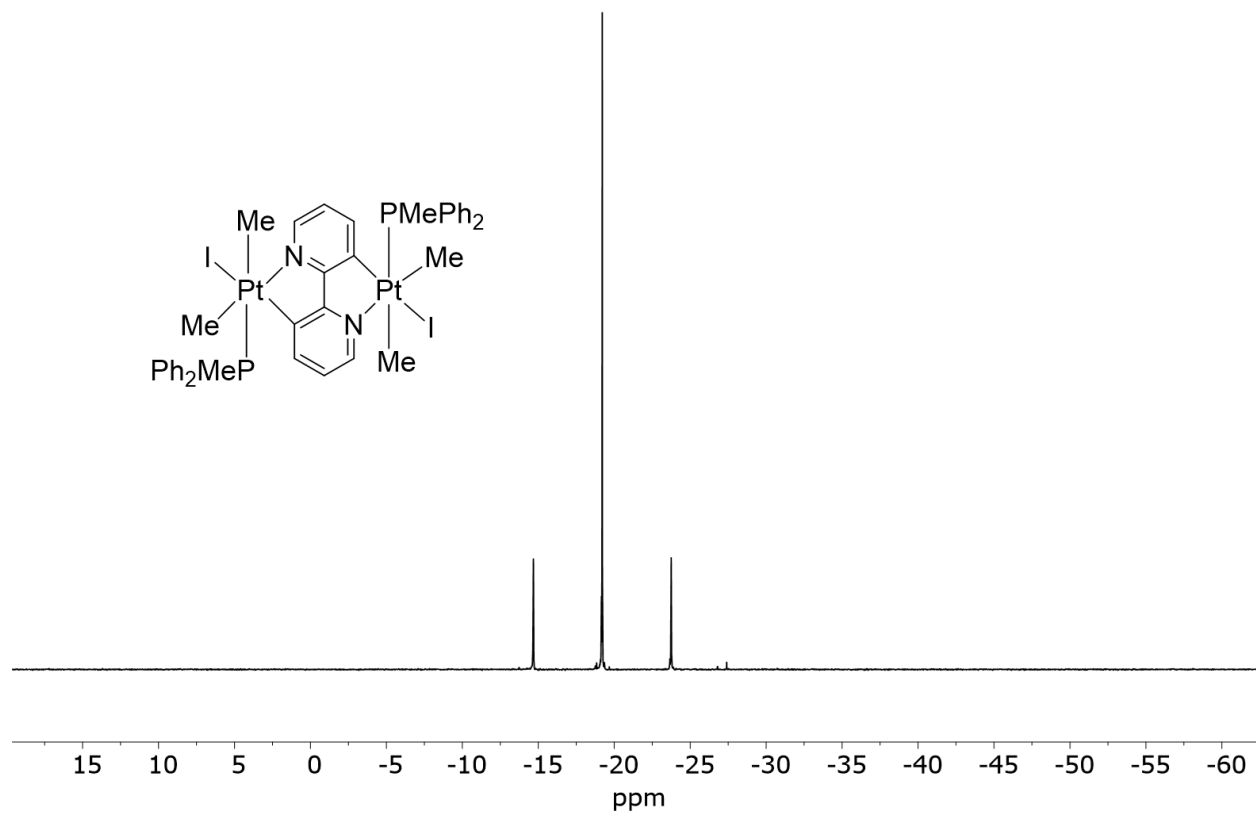


Figure S6. ^{31}P NMR spectrum of complex **3** in CDCl_3 .

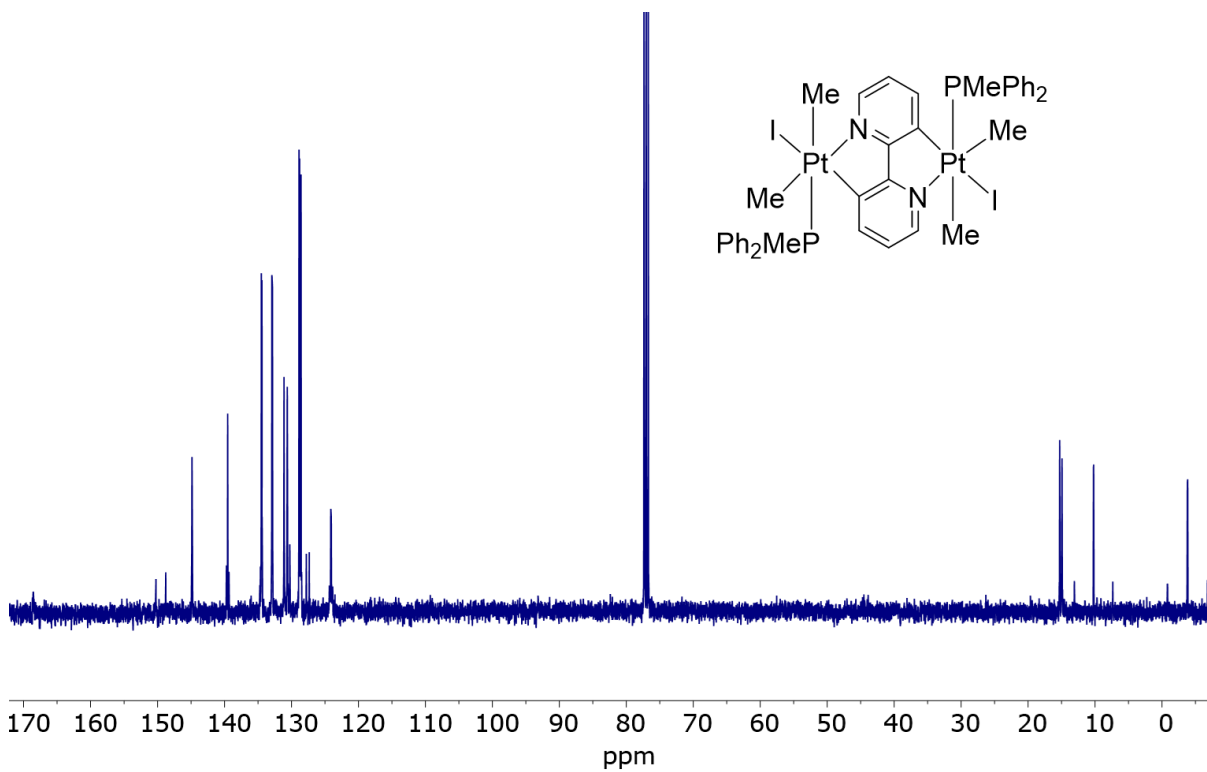


Figure S7. ¹³C NMR spectrum of complex **3** in CDCl₃.

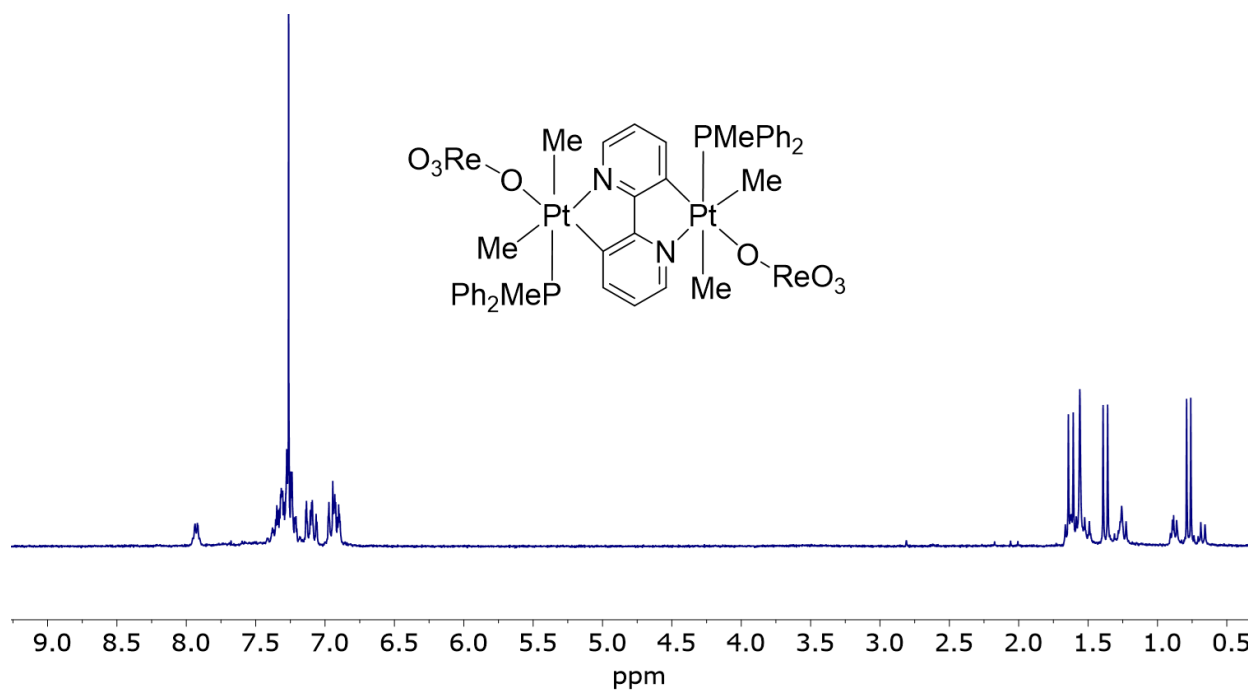


Figure S8. ¹H NMR spectrum (400 MHz) of complex **4** in CDCl₃.

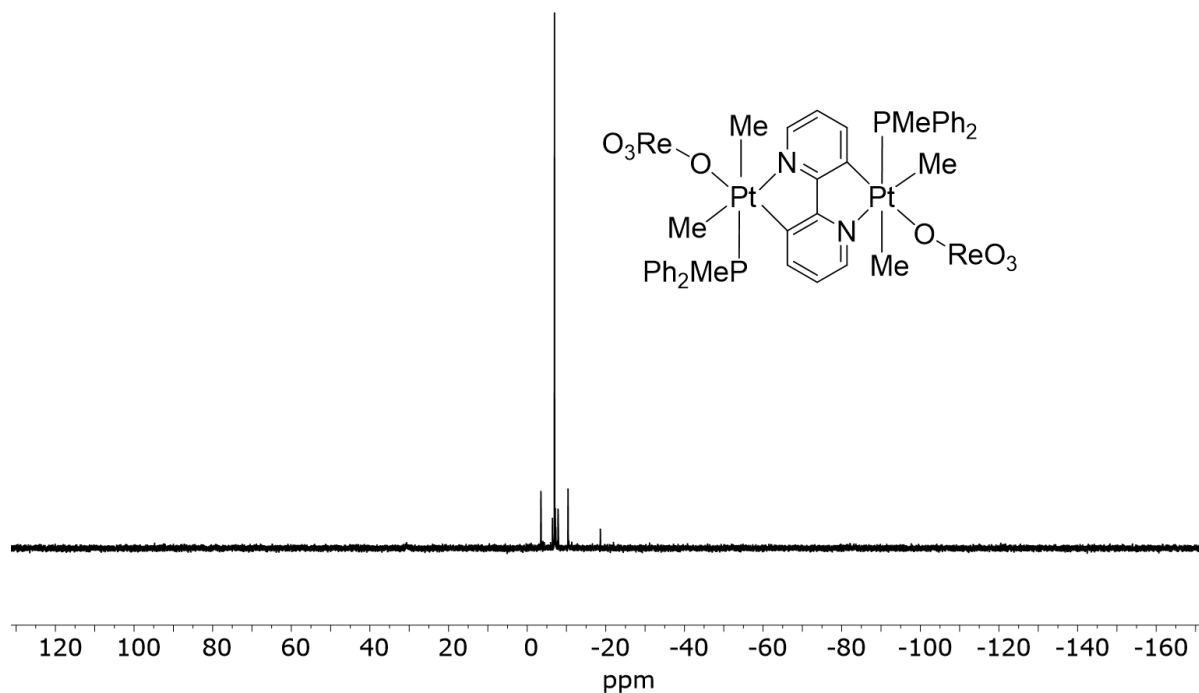
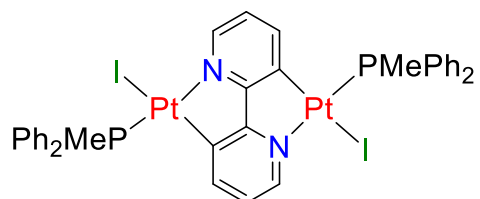


Figure S9. ^{31}P NMR spectrum of complex **4** in CDCl_3 .

Table S1. Crystal Data and Structure Refinement for **5.Hexane**

Empirical formula	C ₄₂ H ₄₆ I ₂ N ₂ P ₂ Pt ₂
Formula weight	1284.73
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.721(3) Å α = 71.461(11)° b = 13.229(4) Å β = 84.633(8)° c = 14.256(4) Å γ = 76.338(6)°
Volume	2036.1(10) Å ³
Z	2
Density (calculated)	2.096 Mg/m ³
Absorption coefficient	8.490 mm ⁻¹
F(000)	1208
Theta range for data collection	1.507 to 27.219°
Reflections collected	12953
Independent reflections	8645 [R(int) = 0.0476]
Max. and min. transmission	0.7455 and 0.4740
Data / restraints / parameters	8645 / 0 / 455
Goodness-of-fit on F ²	0.992
Final R indices [I > 2σ(I)]	R1 = 0.0475, wR2 = 0.1048

Espenson's Approach for Determination of Higher and Lower Rate Constants

As explained in the main text, a double oxidative addition was observed during the reaction of dimeric Pt(II)-Pt(II) complex **2** with MeI and found that the rates were slower in the second step as compared to the first step.

To confirm that the higher rate constant, k_2 , belongs to the first step and the second step is proceeded with the slower rate constant, k'_2 , we used the biphasic equation (equation S1) in evaluating the two rate constants:

$$Abs_t = Abs_\infty + \alpha [\exp(-k_f t) + \beta [\exp(-k_s t)]] \quad (S1)$$

In this equation, k_f and k_s are the rate constants for the fast and slow steps, respectively, but do not identify a particular reaction step. Therefore, there are two cases pertaining to a sequence of reactions:

Case I: $k_2 = k_f > k'_2 = k_s$ and Case II: $k_2 = k_s < k'_2 = k_f$

By using the molar absorptivities of Pt(II)-Pt(II) dimer **2** (ϵ_2) and the final Pt(IV)-Pt(IV) product **3** (ϵ_3), the molar absorptivity of the Pt(II)-Pt(IV) intermediate **A** (ϵ_A) can be calculated from the following equations (S2 and S3), depending upon which case is applicable:

$$\text{Case I: } \epsilon_A = (\epsilon_2 - \alpha)(1 - k_s/k_f) + \epsilon_3 k_s/k_f \quad (S2)$$

$$\text{Case II: } \epsilon_A = (\epsilon_2 - \beta)(1 - k_f/k_s) + \epsilon_3 k_f/k_s \quad (S3)$$

The calculated ϵ_A values from the experimental data for different supposed cases are listed in Table S1. As an example, at 25 °C and 375 nm, the end results are as follows:

Before the MeI addition: $\epsilon_2 = Abs/[2] = 0.999/(3.0 \times 10^{-4} \text{ M}) = 3330 \text{ M}^{-1} \text{ cm}^{-1}$

End of reaction: $\epsilon_3 = Abs/[3] = 0.455/(3.0 \times 10^{-4} \text{ M}) = 1516 \text{ M}^{-1} \text{ cm}^{-1}$

The data for case I are preferable for two reasons. First, in case I, the value of ϵ_A for 4 experiments at 375 nm is almost constant; $\epsilon_A = 2.36 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$, whereas large scatter and in some cases negative values are obtained for ϵ_A when case II was assumed. Second, the value of ϵ_A at 375 nm in case I lies close to ϵ_2 ($3330 \text{ M}^{-1} \text{ cm}^{-1}$), in which both of the related complexes have MLCT bands, and higher than ϵ_3 , as one would expect for the final product **3** with no MLCT band in the visible region.

Table S2. Rate Constants (k_2 and k'_2) and Calculated ϵ_A Values at 375 nm for Cases I and II

[MeI] / M	$10^3 k_s / \text{L mol}^{-1} \text{s}^{-1}$	$10^3 k_f / \text{L mol}^{-1} \text{s}^{-1}$	$\epsilon_A / \text{M}^{-1} \text{cm}^{-1}$	
			Case I	Case II
0.42	2.1	4.7	2508.8	-674.3
0.76	3.7	6.9	2366.4	-82.6
1.00	5.0	8.4	2249.3	287.1
1.23	6.6	11.9	2323.1	64.7

XYZ Cartesian coordinates of optimized structures

2				C	-0.29631300	0.46952900	-0.47580300
Pt	2.54011800	0.84841400	-1.05331300	C	-2.24941700	1.36946000	-1.32715000
P	4.85127800	0.32180100	-0.70220300	C	-1.51992600	2.14206700	-2.22692100
C	0.29657900	-0.46928100	0.47568000	C	-0.12495500	2.06882300	-2.22218000
C	2.24969600	-1.36875700	1.32748200	H	-3.33059200	1.41878000	-1.29345700
C	1.52019100	-2.14128300	2.22730900	H	-2.04722900	2.79489200	-2.91637800
C	0.12520700	-2.06826400	2.22233800	H	0.43678300	2.67883200	-2.92373300
C	5.16293100	-1.50063900	-0.64533800	Pt	-2.53986800	-0.84831500	1.05302800
C	4.47708800	-2.29864000	-1.57783300	P	-4.85109500	-0.32138100	0.70263500
C	4.68845700	-3.67707000	-1.62418600	C	-5.16234300	1.50106100	0.64393400
C	5.57626600	-4.28003600	-0.72880100	C	-4.47547900	2.30004400	1.57482900
C	6.25329500	-3.49748900	0.20849200	C	-4.68656000	3.67856800	1.61972500
C	6.05153400	-2.11500100	0.24957800	C	-5.57510600	4.28061500	0.72445300
C	5.59826300	1.01546300	0.83299700	C	-6.25316700	3.49706800	-0.21126200
C	4.74073000	1.45660400	1.85458300	C	-6.05168600	2.11449800	-0.25088300
C	5.25738600	2.00011900	3.03284900	C	-5.59928400	-1.01647900	-0.83130400
C	6.63821800	2.11788200	3.20286500	C	-4.74249800	-1.45791600	-1.85339000
C	7.50158700	1.69164900	2.19014300	C	-5.26000000	-2.00244100	-3.03081100
C	6.98662200	1.14526400	1.01327200	C	-6.64094100	-2.12096600	-3.19944700
H	3.33088300	-1.41790600	1.29397200	C	-7.50355700	-1.69447400	-2.18619500
H	2.04749100	-2.79385800	2.91700500	C	-6.98774700	-1.14705400	-1.01017000
H	-0.43652600	-2.67818800	2.92396900	H	-3.76449000	1.83863700	2.25607500
H	3.76665100	-1.83655300	-2.25919500	H	-4.15002800	4.28258700	2.34624300
H	4.15271500	-4.28031000	-2.35193400	H	-5.73338500	5.35514900	0.75296500
H	5.73476600	-5.35450600	-0.75845400	H	-6.94053500	3.95956800	-0.91441400
H	6.94007800	-3.96070400	0.91174500	H	-6.58477000	1.51978600	-0.98583400
H	6.58380800	-1.52110300	0.98576800	H	-3.66718200	-1.38357400	-1.71780300
H	3.66550800	1.38279300	1.71798200	H	-4.58328700	-2.33974900	-3.81091600
H	4.58009500	2.33721100	3.81254500	H	-7.04436300	-2.54898800	-4.11296600
H	7.04098500	2.54509800	4.11705100	H	-8.57887600	-1.79030200	-2.30849300
H	8.57683600	1.78687700	2.31352000	H	-7.67559300	-0.82611600	-0.23389200
H	7.67505200	0.82452700	0.23742500	C	3.01884700	2.31985000	-2.43135000

H	2.46460900	3.23578900	-2.19130300	H	-6.38464600	-2.08060200	-4.11489600
H	4.07982100	2.58102900	-2.47486100	H	-4.34303700	-2.01752400	-5.53652500
H	2.71368200	1.99556900	-3.43656700	H	-2.12755600	-1.57549700	-4.48869400
C	-3.01892500	-2.31886400	2.43190700	H	-1.95916800	-1.18881200	-2.06678500
H	-4.07960100	-2.58164700	2.47341200	C	0.06605000	-0.36098500	0.63037900
H	-2.46282600	-3.23424500	2.19415400	C	1.41457900	-1.72080400	1.93939900
H	-2.71643900	-1.99291800	3.43740900	C	0.43679700	-1.75953600	2.93259500
N	1.65124500	-0.53936100	0.45731100	C	-0.75976400	-1.05789900	2.75631000
N	-1.65096400	0.53985000	-0.45718600	H	2.36176900	-2.24044800	2.03319400
C	0.54209400	1.21996100	-1.32690900	H	0.61788700	-2.33046400	3.83764500
C	-0.54185100	-1.21975800	1.32673300	H	-1.51172800	-1.08332800	3.53749600
C	6.04005500	0.83415100	-2.02896300	Pt	2.55888500	-0.79613000	-1.00897700
H	6.13812900	1.92255800	-2.05013600	P	3.91465700	1.17575700	-0.12968700
H	7.02481800	0.38591600	-1.87263400	C	3.34432900	2.80841100	-0.78113100
H	5.64918100	0.49756300	-2.99318700	C	3.83085200	3.29022700	-2.00856700
C	-6.03897900	-0.83190600	2.03090900	C	3.34855600	4.48659400	-2.54553300
H	-7.02358000	-0.38310500	1.87518000	C	2.37359500	5.21973300	-1.86758600
H	-6.13777400	-1.92022400	2.05309300	C	1.88401100	4.75016900	-0.64627500
H	-5.64691500	-0.49480600	2.99446900	C	2.36226300	3.55430400	-0.10886000
3				C	4.07466800	1.43458200	1.68774300
Pt	-2.55884200	0.79635100	1.00878900	C	5.31874800	1.68672900	2.28991200
P	-3.91457800	-1.17578500	0.12987300	C	5.41207800	1.89151400	3.66806400
C	-0.06593200	0.36135300	-0.63049600	C	4.26675800	1.85457000	4.46541800
C	-1.41438200	1.72133800	-1.93943100	C	3.02465500	1.60587900	3.87818600
C	-0.43654200	1.76018800	-2.93256300	C	2.93045200	1.38950300	2.50251500
C	0.75997900	1.05846600	-2.75632300	H	4.59648000	2.74692000	-2.55268300
C	-3.34409400	-2.80834100	0.78139700	H	3.74265900	4.84495800	-3.49248500
C	-3.82995400	-3.28978000	2.00924600	H	2.00088200	6.15113600	-2.28419800
C	-3.34749700	-4.48607800	2.54621700	H	1.13117700	5.31657300	-0.10509300
C	-2.37303300	-5.21951300	1.86787100	H	1.97473300	3.21561100	0.84621700
C	-1.88410500	-4.75031300	0.64615800	H	6.22388600	1.72677100	1.69481500
C	-2.36252200	-3.55451900	0.10872900	H	6.38351800	2.08185700	4.11556500
C	-4.07491000	-1.43498700	-1.68747000	H	4.34195600	2.01540700	5.53710900
C	-5.31930500	-1.68596200	-2.28946900	H	2.12710600	1.57082400	4.48903800
C	-5.41294900	-1.89128200	-3.66752000	H	1.95927600	1.18501200	2.06695200
C	-4.26760500	-1.85621800	-4.46492100	C	-3.50031800	0.58654800	2.85838300
C	-3.02515500	-1.60894300	-3.87782400	H	-2.86938200	1.03083300	3.63217900
C	-2.93063700	-1.39197600	-2.50226600	H	-4.46103100	1.10410800	2.83017600
H	-2.36157100	2.24098400	-2.03322800	H	-3.65384500	-0.47074300	3.09207800
H	-0.61756500	2.33125100	-3.83754200	C	3.50047900	-0.58616300	-2.85850100
H	1.51198200	1.08397400	-3.53746800	H	4.46115000	-1.10380100	-2.83030400
H	-4.59517800	-2.74623600	2.55369100	H	2.86955100	-1.03031200	-3.63238100
H	-3.74108200	-4.84415300	3.49349400	H	3.65409200	0.47113900	-3.09208400
H	-2.00019500	-6.15086100	2.28449200	N	-1.23037700	1.02480500	-0.81117200
H	-1.13166200	-5.31694500	0.10467100	N	1.23048500	-1.02444900	0.81104600
H	-1.97552000	-3.21608800	-0.84666200	C	-0.97190200	-0.33873000	1.57773400
H	-6.22446800	-1.72460100	-1.69430600	C	0.97204700	0.33914900	-1.57782300
				C	-1.57492700	2.45788700	1.85973000

H	-1.03672700	2.97725300	1.06300000	H	-8.31044155	-1.12712777	-2.94872549
H	-2.33263500	3.11445900	2.28997100	H	-7.44994055	-0.71274877	-0.68419649
H	-0.87710000	2.13203000	2.63509800	C	0.20445400	0.68084400	0.12256800
I	-4.60298800	2.58374400	0.00948900	C	1.98006800	2.13970500	0.36920300
C	1.57486800	-2.45760300	-1.85990700	C	1.09008400	3.17227900	0.64885700
H	1.03732600	-2.97737000	-1.06299700	C	-0.28720600	2.93743000	0.64059600
H	0.87646200	-2.13165600	-2.63471600	H	3.04612000	2.30991000	0.35492800
H	2.33246300	-3.11383500	-2.29087000	H	1.48667300	4.15903900	0.86602200
I	4.60283100	-2.58377100	-0.00977100	H	-0.96717400	3.75556400	0.85014100
C	-5.65480200	-1.06641100	0.73004800	Pt	2.67552100	-0.84695100	-0.32340300
H	-5.65506900	-0.84378900	1.79886500	P	4.78301968	0.15914423	-0.35376883
H	-6.14594100	-0.23458000	0.22061900	C	4.77516068	1.77243723	-1.25559083
H	-6.20385800	-1.99595700	0.55808600	C	4.06870768	1.83053123	-2.46962083
C	5.65495200	1.06633200	-0.72965900	C	4.05755768	3.00258223	-3.22639683
H	6.14599300	0.23446600	-0.22019500	C	4.74006168	4.13521523	-2.77364383
H	5.65534600	0.84372300	-1.79847700	C	5.43749568	4.08831723	-1.56509383
H	6.20403100	1.99584600	-0.55760500	C	5.45912368	2.91289923	-0.80937783
5				C	5.48335268	0.49149023	1.31500817
Pt	-2.67554100	0.84714900	0.32229800	C	4.62506568	0.46697223	2.42681817
P	-4.68954955	-0.11464577	0.35305751	C	5.11772968	0.70427623	3.71164417
C	-0.20449000	-0.68063000	-0.12375800	C	6.47642868	0.96113723	3.90399217
C	-1.98009700	-2.13950000	-0.37039100	C	7.34214768	0.97783823	2.80741317
C	-1.09010700	-3.17207100	-0.65002900	C	6.85126668	0.74312623	1.52204317
C	0.28718300	-2.93722000	-0.64174300	H	3.51915668	0.95860223	-2.81639383
C	-4.68074155	-1.72767577	1.25533751	H	3.50927868	3.03347523	-4.16374083
C	-3.97326655	-1.78532577	2.46879151	H	4.72448068	5.05053523	-3.35855883
C	-3.96132555	-2.95715877	3.22589551	H	5.96629968	4.96682023	-1.20579183
C	-4.64405655	-4.09001277	2.77403851	H	6.00366368	2.89224923	0.12933417
C	-5.34250855	-4.04355477	1.56605951	H	3.57103268	0.24511123	2.28843017
C	-5.36492455	-2.86835677	0.81002251	H	4.44040368	0.67896023	4.56048517
C	-5.39104655	-0.44758177	-1.31511549	H	6.86136668	1.14057223	4.90391017
C	-4.53364055	-0.42295277	-2.42760249	H	8.40172168	1.16963323	2.95102917
C	-5.02722255	-0.66067977	-3.71199949	H	7.54283668	0.75600123	0.68574717
C	-6.38597455	-0.91808677	-3.90323649	N	-1.54516000	-0.89670200	-0.09640000
C	-7.25082755	-0.93490477	-2.80597649	N	1.54512300	0.89691400	0.09518900
C	-6.75902955	-0.69976677	-1.52103549	C	-0.77804800	1.65237300	0.36978200
H	-3.04614800	-2.30971300	-0.35612800	C	0.77802100	-1.65216400	-0.37091400
H	-1.48668900	-4.15883400	-0.86719400	C	-6.04924455	0.75952123	1.25214951
H	0.96715600	-3.75535700	-0.85125800	H	-6.31521455	1.68027123	0.72992951
H	-3.42353755	-0.91322477	2.81485251	H	-6.92502355	0.11142723	1.34417151
H	-3.41225755	-2.98770977	4.16278751	H	-5.69332255	1.01783323	2.25260351
H	-4.62786555	-5.00516177	3.35920351	C	6.14320868	-0.71497677	-1.25216283
H	-5.87149455	-4.92223077	1.20745151	H	7.01912968	-0.06696877	-1.34344283
H	-5.91024755	-2.84805277	-0.12824149	H	6.40871468	-1.63589077	-0.72999683
H	-3.47958155	-0.20067977	-2.29008049	H	5.78791768	-0.97299277	-2.25291783
H	-4.35057155	-0.63526877	-4.56137549	I	3.82327257	-3.27553511	-0.58074323
H	-6.77162755	-1.09785377	-4.90281849	I	-3.82491480	3.27903440	0.58046464

A				C	4.33716600	2.28827500	-0.50037400
Pt	-2.60619300	-1.04720100	-0.84035900	C	4.64927300	3.53192200	-1.04606600
P	-3.18936400	1.45059900	-0.77345100	C	5.97531600	3.95617900	-1.10521900
C	-0.25072700	-0.75764500	1.00913500	C	6.98846900	3.13266500	-0.61606600
C	-2.08695300	-1.06576300	2.38031400	C	6.67867700	1.88615600	-0.07594700
C	-1.26793100	-0.99365100	3.50242500	H	4.16812600	-2.95640600	0.47360300
C	0.09901400	-0.76754200	3.34639400	H	4.74604200	-4.76862300	-1.10360300
C	-2.02764500	2.68327700	-1.52516600	H	6.16094200	-4.28741900	-3.08855000
C	-1.36118500	2.34496300	-2.71028900	H	7.00756700	-1.98555800	-3.46938700
C	-0.53889100	3.26687100	-3.35427100	H	6.46255100	-0.18248400	-1.88113500
C	-0.36539700	4.54234000	-2.82026300	H	3.30125400	1.97407900	-0.43293400
C	-1.02597500	4.89137400	-1.64397500	H	3.85421900	4.17134100	-1.41488700
C	-1.85402400	3.97199500	-1.00218200	H	6.21866700	4.92705800	-1.52394500
C	-3.51696300	2.12650400	0.90409800	H	8.02217100	3.46033800	-0.65206300
C	-4.81172800	2.44625000	1.33059900	H	7.48262200	1.26469400	0.30144600
C	-5.03202300	2.93415000	2.61826200	C	-3.33042800	-1.20859700	-2.79188000
C	-3.96427300	3.10989100	3.49472600	H	-2.99599000	-2.14855000	-3.23143400
C	-2.67180200	2.78844900	3.08097400	H	-4.41850200	-1.19234700	-2.76963100
C	-2.45000400	2.29347000	1.79917200	H	-2.97423900	-0.38289400	-3.41009400
H	-3.15564000	-1.22330800	2.45250300	C	3.20735800	-0.02531800	3.40571600
H	-1.70722200	-1.10880700	4.48729100	H	4.14991200	0.51720600	3.49970000
H	0.72254400	-0.70520800	4.23172900	H	2.44821900	0.55453200	3.93614300
H	-1.48029400	1.35824800	-3.13837800	H	3.32133900	-0.98534500	3.92354800
H	-0.03067300	2.98426200	-4.27025400	N	-1.58152900	-0.94648000	1.14862200
H	0.27789700	5.25998400	-3.31860900	N	1.57656300	-0.63456900	-0.51650100
H	-0.90149500	5.88368300	-1.22293100	C	-0.66383200	-0.87188200	-1.43400600
H	-2.36218700	4.26493000	-0.09180200	C	0.66295900	-0.63176100	2.07060300
H	-5.65844600	2.31631700	0.66828000	C	-2.27215500	-3.12631300	-0.90821800
H	-6.04172900	3.17704900	2.93236500	H	-1.89020700	-3.43803200	0.06409900
H	-4.13700500	3.49262500	4.49512600	H	-3.22298500	-3.61434600	-1.10965600
H	-1.83362000	2.91759600	3.75744200	H	-1.55134400	-3.37498900	-1.68650800
H	-1.43754500	2.04926900	1.49597300	I	-5.23772100	-1.56342300	0.23608900
C	0.23537000	-0.73719700	-0.36507900	C	6.16677300	-0.51873500	1.96391300
C	2.07439300	-0.67369900	-1.75933800	H	7.14690100	-0.63926300	1.50215300
C	1.26250500	-0.83580200	-2.87565800	H	6.20940100	0.28761800	2.69559700
C	-0.11808400	-0.94491200	-2.71272100	H	5.90986400	-1.44380200	2.48099400
H	3.14818700	-0.59406100	-1.85821200	C	-4.72529600	1.79749700	-1.73225000
H	1.71250300	-0.88326600	-3.86071700	H	-4.52654100	1.58552100	-2.78290900
H	-0.74784900	-1.08983600	-3.58254200	H	-5.53139000	1.14485400	-1.39842500
Pt	2.60362100	-0.35245400	1.45292800	H	-5.01945600	2.84360900	-1.63668100
P	4.86436000	-0.18065400	0.69805600				
C	5.29238300	-1.44676500	-0.57912000	IMA			
C	4.80820900	-2.74760800	-0.37821800	Pt	-2.15262100	-0.68201900	1.39541600
C	5.12590800	-3.76642500	-1.27244900	P	-4.50619800	-1.20292400	0.89381800
C	5.91925700	-3.49560500	-2.38727300	C	0.11723700	-0.89150900	-0.57557200
C	6.39458400	-2.20338800	-2.60085800	C	-1.77142600	-1.53046600	-1.75101100
C	6.08658600	-1.18306200	-1.70076000	C	-1.01486800	-1.69143900	-2.90887900
C	5.34829400	1.44652200	-0.01697400	C	0.35931200	-1.44999900	-2.86798600

C	-4.75022200	-2.63461200	-0.23238700	H	4.78104300	5.21750600	2.00423000
C	-3.99696800	-3.79583200	0.02463200	H	6.39651100	3.51654300	2.84149300
C	-4.17315600	-4.93436300	-0.76111600	H	6.58928700	1.32291500	1.72704600
C	-5.09185400	-4.92229300	-1.81593000	H	4.42341400	-2.20717800	0.80522100
C	-5.83673700	-3.77053500	-2.07902800	H	5.70213700	-3.83495200	2.16589500
C	-5.67109700	-2.62955000	-1.29022700	H	8.16743800	-3.59098000	2.41050200
C	-5.23123700	0.33337600	0.20573900	H	9.33935300	-1.70663500	1.28701800
C	-4.44844100	0.95177700	-0.79762500	H	8.07341800	-0.07778500	-0.05171700
C	-4.81100900	2.16877300	-1.35702700	C	-2.78492500	-0.12279300	3.29002700
C	-5.98720400	2.78872700	-0.93219600	H	-2.10694900	0.62390200	3.70687000
C	-6.78460800	2.18708600	0.05718600	H	-3.78862700	0.30978400	3.26735000
C	-6.40836700	0.96290400	0.63453600	H	-2.78642900	-1.01680400	3.92804000
H	-2.83478300	-1.73224200	-1.73923700	C	3.48454100	-1.05012800	-3.19946900
H	-1.50582300	-2.00463800	-3.82579100	H	4.56335500	-1.06368100	-3.37469500
H	0.94265300	-1.57852300	-3.77509800	H	3.09669000	-2.04588400	-3.44912700
H	-3.26784000	-3.80994100	0.83502700	H	3.03862300	-0.32677800	-3.89710100
H	-3.58866800	-5.82676700	-0.55543100	N	-1.21090600	-1.13798300	-0.59854100
H	-5.22333300	-5.80750400	-2.43231500	N	1.98594000	-0.20838500	0.73626900
H	-6.55024800	-3.75681400	-2.89903900	C	-0.19442200	-0.25099100	1.81297000
H	-6.25611800	-1.73988600	-1.50121000	C	0.98122100	-1.03724100	-1.67823600
H	-3.51708800	0.49776100	-1.12052900	C	-2.43514300	1.22394600	0.80364400
H	-4.17171600	2.63136400	-2.10075700	H	-2.02385000	1.13393700	-0.19406200
H	-6.27322900	3.74507100	-1.35872400	H	-3.51186000	1.37933600	0.84767300
H	-7.69323900	2.67861600	0.39345000	H	-1.87619200	1.87660800	1.47049400
H	-7.02790200	0.52757500	1.41134500	C	-5.55696100	-1.79662200	2.29092900
C	0.65361200	-0.43478300	0.70761600	H	-5.08485200	-2.68960300	2.71237600
C	2.53839000	0.18190800	1.89652300	H	-5.63392200	-1.04079300	3.07635000
C	1.78555900	0.35811400	3.05316500	H	-6.55624000	-2.06165900	1.93487400
C	0.40457000	0.15112700	3.00790700	C	6.26873400	0.59722900	-2.10728500
H	3.60559600	0.36528500	1.89177300	H	7.16924600	1.09932000	-1.74347200
H	2.27617100	0.66868900	3.97063500	H	6.55535800	-0.30281600	-2.65776600
H	-0.18016700	0.30710500	3.90835100	H	5.73951300	1.27240000	-2.78590400
Pt	2.92994200	-0.56894800	-1.26630500	I	-2.75117600	4.20000700	-0.94619900
P	5.13798100	0.16131200	-0.70551800				
C	5.08016600	1.75263500	0.23577000	IMB			
C	4.16261000	2.71994800	-0.22268700	Pt	2.45909700	-0.60967200	0.86696400
C	4.06036000	3.96224600	0.40414900	P	3.05989400	1.43453200	-0.53595800
C	4.86557300	4.25359700	1.50916800	C	-0.00017000	-1.13848000	-0.76482500
C	5.77269400	3.29767500	1.97877100	C	1.74397000	-2.11386700	-1.94533800
C	5.88287400	2.05381000	1.34633000	C	0.84523200	-2.52868500	-2.92753900
C	6.14588100	-1.01296700	0.29387200	C	-0.51097000	-2.20864000	-2.80806200
C	5.49667600	-2.08762200	0.92459600	C	1.64016600	2.56450700	-0.81170800
C	6.21963900	-3.00871000	1.68603600	C	1.02967600	3.17974900	0.29655900
C	7.60302900	-2.87266300	1.82148200	C	-0.07066400	4.01930400	0.12658900
C	8.26179700	-1.81405200	1.19089500	C	-0.58928100	4.24503300	-1.15209200
C	7.54059000	-0.89135100	0.43162600	C	0.00046700	3.62988400	-2.25735400
H	3.51529100	2.49117100	-1.06654800	C	1.11049400	2.79695100	-2.09064900
H	3.34475800	4.69469600	0.03637000	C	4.42940700	2.48764800	0.10122500

C	4.33745600	3.88308000	0.21306700	H	-7.66486500	1.11461700	-0.02330500
C	5.42675900	4.62527700	0.67654800	C	3.37096100	0.14174400	2.57958100
C	6.61712800	3.98518600	1.02598300	H	2.97458500	-0.34648200	3.47307000
C	6.71729200	2.59597700	0.91088600	H	4.43843100	-0.08305700	2.48491500
C	5.63008200	1.84852500	0.45736500	H	3.23856100	1.22409000	2.65592600
H	2.80690600	-2.33132800	-1.98842000	C	-3.70583200	-1.48722400	-2.94561500
H	1.21238300	-3.09774500	-3.77620300	H	-4.48686700	-0.79237000	-3.27735400
H	-1.19154100	-2.54105000	-3.58621300	H	-2.94797300	-1.52603800	-3.73332000
H	1.41902300	3.01118500	1.29615900	H	-4.15860600	-2.48456800	-2.85508100
H	-0.52340600	4.49447900	0.99217300	N	1.31691500	-1.42183700	-0.87977000
H	-1.44486400	4.90106100	-1.28573700	N	-1.69100400	-0.20954100	0.64456900
H	-0.39560900	3.80103400	-3.25424100	C	0.60604000	-0.09142100	1.40738900
H	1.55745800	2.33747300	-2.96547600	C	-0.99216300	-1.48280700	-1.70494700
H	3.42237900	4.39642900	-0.06212500	C	2.11466200	-2.38379500	1.93982800
H	5.34228800	5.70534300	0.75977000	H	1.41536600	-3.01103100	1.38138300
H	7.46274000	4.56498000	1.38548300	H	3.09533200	-2.86566100	1.99716000
H	7.64084400	2.09000400	1.17803400	H	1.72737500	-2.18481000	2.94112600
H	5.71963600	0.76787200	0.37158200	C	-6.47958800	-1.18785000	-1.20277900
C	-0.37225500	-0.44929400	0.46462000	H	-7.42486500	-1.01871800	-0.68054700
C	-2.07819900	0.40106000	1.77501200	H	-6.55409600	-0.80338100	-2.22301500
C	-1.17057100	0.78507000	2.75940800	H	-6.28955800	-2.26372200	-1.24702000
C	0.19309000	0.53177500	2.58238300	C	3.65111200	0.96008400	-2.21636100
H	-3.14049600	0.57029200	1.89962200	H	4.52988300	0.32229400	-2.08370900
H	-1.53060400	1.26974800	3.66100000	H	2.88482700	0.38019400	-2.73764000
H	0.90130800	0.81891700	3.35051800	H	3.91889800	1.84100600	-2.80673800
Pt	-2.88008700	-0.89737800	-1.14601100	I	5.70801500	-2.27416300	-0.43124900
P	-5.06637100	-0.37866900	-0.32241800				
C	-5.29528400	-1.00984500	1.39986900	IMC			
C	-4.78564200	-2.28945500	1.68423100	Pt	-3.17944000	-0.96954500	-1.14603700
C	-4.94279700	-2.85086500	2.95165300	P	-4.06361500	1.21325900	-0.11308000
C	-5.59715800	-2.13525200	3.95832200	C	-0.65276400	-0.98146200	0.50266400
C	-6.09586900	-0.85945700	3.68919100	C	-2.24496400	-2.05160700	1.79642500
C	-5.94935900	-0.29877300	2.41695500	C	-1.30273500	-2.28270500	2.79172100
C	-5.53150300	1.40226900	-0.28698300	C	0.00360500	-1.82309000	2.62286500
C	-4.51986900	2.36497600	-0.43976600	C	-3.17310000	2.81085500	-0.40735000
C	-4.82752500	3.72728200	-0.42225500	C	-2.53357400	3.01742600	-1.63633500
C	-6.14952400	4.14566400	-0.26050100	C	-1.92578700	4.23715600	-1.92812300
C	-7.16587500	3.19707900	-0.11865900	C	-1.94486100	5.26936300	-0.99218100
C	-6.86033500	1.83533900	-0.13278600	C	-2.58195700	5.07673700	0.23293100
H	-4.25410600	-2.84000300	0.91166200	C	-3.19543200	3.85950800	0.52322100
H	-4.54654800	-3.84189500	3.15476800	C	-4.26545100	1.16385700	1.71317600
H	-5.71289200	-2.56866700	4.94780700	C	-5.52360900	1.03001700	2.31275400
H	-6.60066800	-0.29553700	4.46880800	C	-5.64146700	0.96367400	3.70086400
H	-6.34165700	0.69481800	2.22521700	C	-4.50755100	1.03012600	4.50642200
H	-3.49141800	2.04524300	-0.58582100	C	-3.24949300	1.15920600	3.91808700
H	-4.03401500	4.45957900	-0.54132100	C	-3.12847100	1.21908100	2.53287200
H	-6.38921700	5.20528600	-0.25046900	H	-3.27383500	-2.37795100	1.88349700
H	-8.19756400	3.51586600	0.00074100	H	-1.59322200	-2.81534200	3.68966400

H	0.72391500	-2.00879800	3.41029000	H	2.90994100	0.41638200	3.33259600
H	-2.50646400	2.22622400	-2.37381900	H	2.54515100	-1.32495300	3.30319500
H	-1.43646900	4.37754900	-2.88623400	N	-1.92095000	-1.41303100	0.66846200
H	-1.47065900	6.21889500	-1.21720100	N	0.91249700	0.02524900	-0.98869800
H	-2.60857700	5.87708700	0.96511800	C	-1.36393400	-0.29042800	-1.77144700
H	-3.69006300	3.73225000	1.47844500	C	0.36058000	-1.13928500	1.46039000
H	-6.41983900	0.97490900	1.70780400	C	-2.60579100	-2.81365700	-1.99352900
H	-6.62394300	0.86079600	4.14936000	H	-2.10414800	-3.39784800	-1.22193300
H	-4.60179400	0.98145500	5.58611000	H	-3.50575400	-3.32723100	-2.32287600
H	-2.36011900	1.21110200	4.53725400	H	-1.93386200	-2.65736400	-2.83651300
H	-2.14248600	1.32530100	2.09315000	I	-5.55059300	-2.25050000	-0.14839100
C	-0.36377600	-0.37249200	-0.79241400	C	5.67482600	0.82514200	1.21151200
C	1.26650400	0.47232900	-2.19886300	H	6.48913000	1.43911600	0.82571700
C	0.35504500	0.53484500	-3.24762600	H	5.54959300	1.01489300	2.27712000
C	-0.96797600	0.15511300	-3.03244300	H	5.94258700	-0.22492300	1.06724000
H	2.29750100	0.76907200	-2.33055500	C	-5.73725300	1.61770100	-0.76753700
H	0.68550700	0.87833900	-4.22088700	H	-5.64335500	1.83792200	-1.83132100
H	-1.67486700	0.20135600	-3.85270500	H	-6.39910200	0.76023200	-0.65186500
Pt	2.12837700	-0.20861000	0.92043300	H	-6.15517500	2.49048700	-0.26373500
P	4.11973800	1.19536800	0.31008200	C	2.88817800	-2.05204200	0.33103100
C	4.65859500	1.18780700	-1.44846900	H	3.95986800	-2.04898800	0.51349100
C	5.23466100	0.01628100	-1.96375500	H	2.65179100	-2.12570300	-0.72828300
C	5.64588200	-0.03184000	-3.29310700	H	2.39365600	-2.83022100	0.90479500
C	5.48392500	1.07861700	-4.12143300	I	6.79347200	-3.14258600	0.45050300
C	4.91692400	2.24512200	-3.61261800				
C	4.50583600	2.30334000	-2.28126100	IMD			
C	3.70733700	2.93815300	0.71566300	Pt	-2.76621400	-1.23707500	-0.89906300
C	2.39524600	3.39278600	0.51893700	P	-4.59958800	0.38386400	-0.10853300
C	2.04781900	4.70753200	0.82146800	C	-0.53068300	0.14101500	0.57207700
C	3.00551300	5.58197500	1.33160200	C	-1.45843300	-1.27999500	2.14135000
C	4.31137600	5.13856000	1.53464600	C	-0.52820800	-0.87276900	3.09317300
C	4.66330000	3.82580500	1.22812700	C	0.42555500	0.09404500	2.76871200
H	5.38965200	-0.85633700	-1.33556600	C	-4.61280800	2.14449500	-0.68157800
H	6.09804400	-0.94001000	-3.67715600	C	-4.13064900	2.45364200	-1.95923800
H	5.80444500	1.03604100	-5.15695700	C	-4.20646700	3.75449100	-2.45419300
H	4.79723600	3.11616900	-4.24823100	C	-4.76276200	4.76726500	-1.67602500
H	4.07129500	3.21916800	-1.89777100	C	-5.25124200	4.47010200	-0.40466100
H	1.63848800	2.72517500	0.12163100	C	-5.18169600	3.16901600	0.08883500
H	1.02869400	5.04310500	0.66227200	C	-4.72726300	0.52359400	1.71960100
H	2.73540300	6.60465100	1.57222400	C	-5.72488900	-0.14262400	2.44161600
H	5.06070600	5.81443400	1.93251100	C	-5.77400400	-0.04555900	3.83206600
H	5.68440100	3.50365100	1.39258400	C	-4.83044000	0.71587000	4.51719600
C	-4.11141100	-0.54588000	-2.96384700	C	-3.83087900	1.38008500	3.80632100
H	-3.72817500	-1.21347300	-3.73547200	C	-3.77579200	1.28003800	2.41927900
H	-5.18368300	-0.69921900	-2.85921800	H	-2.22176600	-2.01599800	2.36010400
H	-3.92377400	0.48701900	-3.26097500	H	-0.55558500	-1.30361800	4.08678800
C	3.02437000	-0.51211000	2.76390200	H	1.14115400	0.42013600	3.51167100
H	4.08102700	-0.74881200	2.66133100	H	-3.69442700	1.68024000	-2.57739500

H	-3.82764700	3.97400800	-3.44687200	C	7.50674600	1.83621000	-0.04262000
H	-4.81799700	5.78114400	-2.05812300	H	6.51579600	0.00221500	0.43451200
H	-5.69158400	5.25120100	0.20631300	C	7.37687700	3.15638400	-0.47012500
H	-5.57069700	2.95743300	1.07756800	H	6.00471200	4.70343100	-1.07742600
H	-6.46739600	-0.74278400	1.93074500	H	8.48680500	1.42267400	0.16976100
H	-6.55405700	-0.56664700	4.37700900	H	8.25753800	3.77856800	-0.58994900
H	-4.87259800	0.79218800	5.59857600	C	3.42445600	-0.39099800	-1.56307000
H	-3.09199600	1.97613100	4.33149800	C	3.98829700	0.10048800	-2.74712100
H	-2.99668500	1.80895600	1.88067000	C	2.67983000	-1.57797100	-1.60357700
C	-0.53646800	0.60806900	-0.80397200	C	3.81729200	-0.58795600	-3.94674500
C	0.54125000	1.91843600	-2.37644300	H	4.57850700	1.00957200	-2.73547400
C	-0.32954100	1.46711200	-3.36346500	C	2.51718400	-2.26557800	-2.80379100
C	-1.33662000	0.55821700	-3.03545200	H	2.23180500	-1.98122600	-0.70230400
H	1.33899800	2.61907900	-2.59057000	C	3.08413300	-1.77221300	-3.97819800
H	-0.21171400	1.82038600	-4.38111300	H	4.26863600	-0.20162800	-4.85453600
H	-1.99730800	0.19893200	-3.81579300	H	1.95066100	-3.19032000	-2.81789800
Pt	1.64334500	1.98647000	0.69729300	H	2.95918900	-2.31168000	-4.91097100
C	-3.75456000	-1.56418200	-2.70306800	C	3.99202800	-0.77079900	1.26525100
H	-3.07251400	-2.03100300	-3.41307000	H	3.10527200	-1.37708600	1.45286800
H	-4.59864400	-2.22767900	-2.52629400	H	4.80621800	-1.42097300	0.93753900
H	-4.11468800	-0.62184300	-3.11693600	H	4.28191600	-0.29380500	2.20190900
C	2.63563500	2.47268500	2.45837900	I	7.62776100	-2.82132600	0.98428500
H	3.31244100	3.29238500	2.19618500				
H	1.93792100	2.81557700	3.22073100	IME			
H	3.22273400	1.64250800	2.84796000	Pt	-2.89155300	-0.62003900	-1.08704100
N	-1.45657700	-0.77910500	0.90274500	P	-3.41255800	0.55571500	1.12430800
N	0.43855700	1.48540500	-1.11740800	C	0.03041300	-0.68553800	-0.35512400
C	-1.47736900	0.11813300	-1.71880800	C	-0.85778700	-2.61546800	0.55848500
C	0.42692600	0.61111900	1.47919300	C	0.40155900	-2.98406100	1.01499100
C	-1.38161400	-2.70212400	-1.52636500	C	1.49510100	-2.14860100	0.78430600
H	-0.70730100	-2.90314100	-0.69388200	C	-2.26130500	1.94244800	1.49341000
H	-1.93550000	-3.60218000	-1.78196500	C	-2.37256000	3.13733300	0.76594500
H	-0.81466000	-2.35205700	-2.38757500	C	-1.48932600	4.18874900	0.98917600
I	-4.22445800	-3.32744200	0.40354200	C	-0.47068500	4.06059100	1.93425200
C	0.18718200	3.39181800	1.25349600	C	-0.34433800	2.87517400	2.65304000
H	-0.70508800	3.28024700	0.63833500	C	-1.23328100	1.82170000	2.43588800
H	-0.07356700	3.32709100	2.30823600	C	-5.08662700	1.29241100	1.38216900
H	0.65948700	4.35882000	1.05020800	C	-5.28240200	2.36780000	2.26094600
C	-6.26555000	-0.17484000	-0.66209400	C	-6.56255500	2.86481400	2.49345100
H	-6.30694400	-0.10225300	-1.74935500	C	-7.66346300	2.29308400	1.85671300
H	-6.42782600	-1.21478200	-0.38199500	C	-7.47842700	1.21990500	0.98800400
H	-7.04681600	0.45781100	-0.23823600	C	-6.19812800	0.72254400	0.74871200
P	3.59835300	0.52069600	0.02384500	H	-1.73788700	-3.22622400	0.71763400
C	5.10630400	1.54793900	-0.15654400	H	0.52432900	-3.91943500	1.54911200
C	4.98235900	2.87842300	-0.58397900	H	2.46068200	-2.46142400	1.15703000
C	6.38044800	1.03034600	0.11281500	H	-3.15922400	3.25445300	0.02839500
C	6.11270700	3.67679400	-0.74385200	H	-1.59467400	5.10811800	0.42290300
H	4.00496200	3.30002200	-0.80157400	H	0.22001400	4.87924200	2.10608600

H	0.44400000	2.76636200	3.39051500	C	4.04173700	-2.19785400	4.44258100
H	-1.11518500	0.91200100	3.01191400	H	5.00068600	-2.67603500	2.58576900
H	-4.43726000	2.82402900	2.76328700	C	3.25177400	-1.28706900	5.14004600
H	-6.69852300	3.69882900	3.17419000	H	2.18263300	0.58117100	5.03903500
H	-8.65992400	2.68237400	2.03803200	H	4.38829000	-3.10363200	4.92888200
H	-8.32989400	0.76741000	0.49051700	H	2.98249300	-1.47922500	6.17325200
H	-6.06809100	-0.11865300	0.07969100	C	5.85467400	0.77408800	1.08843800
C	-0.22182700	0.48762300	-1.17131900	H	6.52970800	0.29892300	1.80142000
C	0.71660700	2.31452800	-2.23402000	H	5.48485600	1.70349700	1.51886300
C	-0.52084800	2.65551300	-2.76696000	H	6.38272400	1.00294600	0.16549200
C	-1.64171600	1.87865300	-2.47780700	I	4.23233400	2.65055800	-1.46180000
H	1.60732200	2.89333400	-2.43202800	I	-4.60197100	-2.82424300	-0.36616900
H	-0.59834300	3.52799000	-3.40531600				
H	-2.60267600	2.15080500	-2.89733700	TS_{conc}			
Pt	2.65514900	0.52065600	-0.45613800	Pt	-2.51969800	-1.15618100	-0.51696900
C	-4.40412300	0.30191800	-2.18655300	P	-3.01016500	1.12431000	-1.23236900
H	-4.07883700	0.41629500	-3.22041100	C	-0.12912700	-0.14957400	1.03578600
H	-5.29307100	-0.32548900	-2.16446300	C	-1.96685300	0.27140600	2.37748400
H	-4.63831400	1.28050800	-1.76700900	C	-1.14067200	0.78938000	3.37162800
N	-1.03548200	-1.47714900	-0.12008300	C	0.23836100	0.84448500	3.15907700
N	0.86727900	1.24260300	-1.44433700	C	-1.69774800	2.33825200	-0.77837300
C	-1.50627700	0.76329200	-1.65542700	C	-0.35734300	1.93975200	-0.92118900
C	1.34026300	-0.94253200	0.09195800	C	0.67874100	2.83039300	-0.63939500
C	-2.43736100	-1.63542700	-2.87704500	C	0.38866800	4.12525700	-0.19980700
H	-1.69531600	-2.40124600	-2.65044000	C	-0.94009100	4.52713800	-0.05040300
H	-3.34850300	-2.10036300	-3.24693600	C	-1.98059500	3.64071400	-0.34132700
H	-2.04285400	-0.94441100	-3.62143600	C	-4.58746100	1.86428100	-0.64667500
C	-3.25663400	-0.56621000	2.57739800	C	-4.90198500	1.78739900	0.72225300
H	-4.01875000	-1.33892700	2.48202800	C	-6.09435300	2.32232900	1.20928900
H	-2.28210900	-1.05460700	2.58602400	C	-6.99768600	2.93078600	0.33370500
H	-3.40549200	-0.02247800	3.51155100	C	-6.70041600	3.00486300	-1.02790400
P	4.42889900	-0.33735700	0.74766700	C	-5.50241800	2.47775900	-1.51697600
C	5.19422800	-1.81640900	-0.03247500	H	-3.04171100	0.23901900	2.50165800
C	6.44475800	-2.29713300	0.38594200	H	-1.58315800	1.14848800	4.29596200
C	4.54332300	-2.45699900	-1.09501500	H	0.87466500	1.25528700	3.93765800
C	7.01969900	-3.40288200	-0.23498200	H	-0.12396600	0.92815100	-1.24541800
H	6.98343400	-1.81341500	1.19211400	H	1.71060700	2.51061100	-0.75408300
C	5.12175900	-3.56366000	-1.71377500	H	1.19552500	4.81620700	0.02780500
H	3.58927500	-2.08102200	-1.44540900	H	-1.17115600	5.53196900	0.29210600
C	6.35822500	-4.03988800	-1.28411300	H	-3.00967400	3.96562600	-0.22487800
H	7.98713000	-3.76238200	0.09903000	H	-4.21665800	1.30291400	1.41221900
H	4.60681600	-4.04730000	-2.53690800	H	-6.32207400	2.25198300	2.26880300
H	6.80926900	-4.89921000	-1.76891800	H	-7.93089400	3.33886900	0.71109500
C	3.94382200	-0.79433700	2.47035400	H	-7.39966600	3.47277400	-1.71508700
C	3.14081100	0.11292400	3.17502100	H	-5.29208300	2.54966500	-2.57863900
C	4.39101200	-1.95281700	3.11451500	C	0.34954800	-0.69316700	-0.23450200
C	2.80276300	-0.13003600	4.50355600	C	2.18058600	-1.06981400	-1.59637000
H	2.76671200	1.00176500	2.67739900	C	1.35596700	-1.57751100	-2.59598200

C	-0.02079600	-1.66156000	-2.37380400	H	-2.09327200	0.94641700	-3.46351600
H	3.25388800	-1.01849200	-1.72836300	C	-3.45797312	-3.12794194	0.75568612
H	1.79486600	-1.91019700	-3.53161500	H	-3.47276989	-3.24307755	1.84049224
H	-0.65203100	-2.06851400	-3.15748500	H	-3.99757387	-3.96795660	0.32583034
Pt	2.74564900	0.27213800	1.33098700	H	-2.50530157	-3.64931422	0.67501637
P	5.00140300	-0.00597000	0.58011800				
C	5.29354300	-1.66054600	-0.19057000	TS1			
C	4.70494700	-2.77494300	0.43254900	Pt	-2.27192800	-0.23945400	1.30257700
C	4.90823400	-4.05982600	-0.07203300	P	-4.53822800	-1.05765300	0.90790100
C	5.69041300	-4.24771700	-1.21505900	C	0.08605100	-0.88440000	-0.46446500
C	6.27062800	-3.14602700	-1.84670900	C	-1.76220700	-1.74363200	-1.54854600
C	6.07685600	-1.85888000	-1.33739500	C	-0.96199600	-2.17756300	-2.59802400
C	5.58046400	1.23812500	-0.64833800	C	0.41391100	-1.96004700	-2.54761900
C	4.61633100	1.98241800	-1.34823300	C	-4.55992600	-2.78670600	0.26163800
C	5.00159600	2.94353700	-2.28518700	C	-3.63915000	-3.69790700	0.79834200
C	6.35612200	3.17950600	-2.52902900	C	-3.64024200	-5.02766200	0.38573500
C	7.32478900	2.45197600	-1.83262400	C	-4.55282000	-5.46044500	-0.57631200
C	6.94104900	1.48821400	-0.89834800	C	-5.46650700	-4.55933800	-1.11910500
H	4.07484600	-2.63163800	1.30717200	C	-5.47432800	-3.22866100	-0.70119400
H	4.44748700	-4.91130600	0.42095500	C	-5.61023800	-0.09588600	-0.23601900
H	5.84162100	-5.24703300	-1.61366400	C	-5.05519900	0.39517400	-1.42704500
H	6.87496800	-3.28450700	-2.73911200	C	-5.82918200	1.12825900	-2.32214800
H	6.53304100	-1.01267600	-1.84157000	C	-7.16780000	1.39197700	-2.03531000
H	3.56235400	1.81302100	-1.14520600	C	-7.72715100	0.91840900	-0.85071700
H	4.24366900	3.51184100	-2.81704700	C	-6.95567700	0.17790300	0.04388000
H	6.65691300	3.93083500	-3.25391600	H	-2.82790000	-1.92501100	-1.54746100
H	8.38022500	2.63550700	-2.01354400	H	-1.41996100	-2.68591400	-3.43947900
H	7.70973900	0.93581900	-0.36665000	H	1.02745200	-2.30574900	-3.37229100
C	-3.21921400	-2.12965900	-2.21248300	H	-2.91082400	-3.36471700	1.53155300
H	-2.45131800	-2.79134100	-2.62089900	H	-2.92245800	-5.72265300	0.80859800
H	-4.10013200	-2.74512400	-1.99933200	H	-4.54844700	-6.49476300	-0.90372100
H	-3.48872700	-1.39276400	-2.98080300	H	-6.17682400	-4.88951300	-1.86991000
C	3.37342400	1.20939800	3.06683700	H	-6.19129000	-2.53877300	-1.13172000
H	4.42864700	1.49576400	3.08051300	H	-4.01102500	0.21544700	-1.65708400
H	2.78292100	2.12235400	3.21459200	H	-5.38105200	1.50580400	-3.23473200
H	3.19472200	0.54804200	3.92624300	H	-7.76888600	1.97108100	-2.72815000
N	-1.47218300	-0.19354500	1.21911000	H	-8.76633300	1.12511300	-0.61753000
N	1.69046700	-0.63110500	-0.42607700	H	-7.41476800	-0.17853200	0.95773600
C	-0.56988100	-1.22376200	-1.16194900	C	0.58434100	-0.17081300	0.70757000
C	0.79759300	0.37528400	1.96064100	C	2.44426300	0.61339800	1.82564100
I	-5.17583504	-1.43468725	0.53956884	C	1.65458200	1.00608800	2.89898600
C	6.31994400	0.01127900	1.88180400	C	0.27354700	0.82324600	2.83881800
H	7.28181400	-0.31028900	1.47386900	H	3.51428400	0.76641600	1.83321700
H	6.42413700	1.01339200	2.30520000	H	2.12202300	1.45949100	3.76600700
H	6.02720300	-0.67827400	2.67853600	H	-0.33296600	1.14532900	3.67753900
C	-3.04122400	1.32409000	-3.07041500	Pt	2.94298500	-0.76772400	-1.06790300
H	-3.85463000	0.74618700	-3.51425700	P	5.15742700	0.06982700	-0.74096400
H	-3.14195400	2.37690600	-3.34755100	C	5.24323600	1.69727600	0.12842900

C	4.39925000	2.71588300	-0.33917300	Pt	3.02332500	-1.34837100	0.36977900
C	4.41280700	3.97447000	0.25472900	P	3.50701900	1.03484000	1.14566500
C	5.26001100	4.22940000	1.33383500	C	0.51700300	-0.81159000	-1.20951200
C	6.09255000	3.22043400	1.81224700	C	2.26349800	-0.55827300	-2.70615100
C	6.08753800	1.96009800	1.21242000	C	1.35904500	-0.31372000	-3.73351100
C	6.32395100	-1.03965000	0.14988400	C	-0.00905800	-0.30388500	-3.46078000
C	5.78948800	-2.07164000	0.93237300	C	2.38419700	1.63532300	2.48753500
C	6.62817000	-2.94540900	1.62249300	C	2.65835500	1.31219500	3.82484100
C	8.01124000	-2.80273400	1.53194900	C	1.79284000	1.70634900	4.84413600
C	8.55419300	-1.78291500	0.75045900	C	0.63856400	2.42671200	4.54577900
C	7.71736700	-0.90596200	0.06412300	C	0.35564400	2.75144400	3.22014300
H	3.71537800	2.51690700	-1.15874600	C	1.21831200	2.35750000	2.19935600
H	3.75491000	4.75246700	-0.11813700	C	3.51610700	2.40186100	-0.09003200
H	5.26568400	5.20831500	1.80163800	C	4.55276200	3.34496400	-0.13723800
H	6.74955100	3.41014200	2.65484400	C	4.53240800	4.37300300	-1.07770300
H	6.74009500	1.18515200	1.59753500	C	3.47664900	4.47972400	-1.98023700
H	4.71278500	-2.19493400	0.98616500	C	2.44130600	3.54834900	-1.94248400
H	6.20005900	-3.74107600	2.22311200	C	2.46414600	2.51335600	-1.01025600
H	8.66514400	-3.48585200	2.06396800	H	3.33487300	-0.56563200	-2.86282400
H	9.63056100	-1.66998900	0.67333500	H	1.72919300	-0.12919300	-4.73571300
H	8.16034000	-0.11906300	-0.53595300	H	-0.69904300	-0.10874000	-4.27364500
C	-2.95297200	0.67500500	3.03825600	H	3.55479800	0.76459800	4.09006100
H	-2.30227800	1.50311100	3.31998400	H	2.02885100	1.45341500	5.87266300
H	-3.96157500	1.07940700	2.93093400	H	-0.03201300	2.73792700	5.33986000
H	-2.96025700	-0.05103400	3.85868200	H	-0.53342000	3.32125800	2.97121800
C	3.62767600	-1.74789200	-2.76223500	H	0.97852700	2.63915300	1.18106000
H	4.66593800	-2.08194800	-2.67906100	H	5.38496700	3.29080300	0.55318000
H	3.02489400	-2.63830700	-2.95476500	H	5.34462100	5.09201100	-1.10053400
H	3.55654300	-1.09598800	-3.64123000	H	3.46139400	5.28257300	-2.70968900
N	-1.25059700	-1.09954900	-0.49047900	H	1.61507300	3.62231800	-2.64107100
N	1.92212000	0.03548000	0.73544100	H	1.65621700	1.79246300	-1.00553500
C	-0.30971500	0.22756900	1.71710000	C	0.14218100	-1.13632900	0.16223500
C	0.99476000	-1.30640800	-1.45378600	C	-1.57887000	-1.46649500	1.66554900
C	-2.42345000	2.02719600	0.26518400	C	-0.66998100	-1.73694800	2.68141800
H	-1.89534100	1.67433600	-0.60206800	C	0.69650400	-1.71650600	2.40624500
H	-3.49663200	1.99237600	0.29465100	H	-2.64366000	-1.50483100	1.84727100
H	-1.88079000	2.49049500	1.06679300	H	-1.03492800	-1.97208700	3.67453600
I	-2.60569100	4.45474800	-0.92615400	H	1.40229600	-1.94580000	3.19470400
C	6.03102700	0.48131900	-2.31577500	Pt	-2.39057700	-0.68170100	-1.41354600
H	6.97553500	0.99294600	-2.12907700	P	-4.64114900	-1.15387300	-0.57809900
H	6.21713500	-0.42334100	-2.89291200	C	-4.69485200	-2.62373000	0.53704000
H	5.38903500	1.13962600	-2.90223500	C	-3.88779100	-3.72318300	0.21175000
C	-5.53663200	-1.25108200	2.44582600	C	-3.92872300	-4.88119800	0.98370600
H	-5.77352900	-0.28304000	2.88544900	C	-4.76754400	-4.94991100	2.09593000
H	-6.45844400	-1.79915100	2.24882600	C	-5.56844800	-3.85921400	2.42868300
H	-4.94386900	-1.81864100	3.16377700	C	-5.53744800	-2.70144800	1.65183500
				C	-5.52229600	0.17777000	0.33350800
				C	-4.84642900	0.85752200	1.35777600

TS2

C	-5.47762000	1.87061300	2.07338400	C	0.39731100	-0.03310500	0.01181700
C	-6.78993100	2.22943600	1.76735300	C	-0.52988900	-0.97755000	1.95089100
C	-7.46661200	1.56926900	0.74467000	C	0.57121700	-0.61439900	2.71210400
C	-6.83931300	0.54789300	0.03218700	C	1.59293800	0.10126000	2.10018600
H	-3.21750900	-3.67000700	-0.64073300	C	-3.32763700	2.54999300	-0.87969400
H	-3.29981500	-5.72530300	0.72130900	C	-3.00517700	2.52420600	-2.24197900
H	-4.79417800	-5.84930500	2.70201500	C	-2.88609200	3.70823900	-2.96818000
H	-6.22163600	-3.90703600	3.29368800	C	-3.08344000	4.93628200	-2.34063600
H	-6.16835500	-1.86157600	1.91932000	C	-3.40898200	4.97366500	-0.98542300
H	-3.81994900	0.60301400	1.59762300	C	-3.53533900	3.79083000	-0.25997100
H	-4.93947700	2.38753700	2.86039800	C	-3.40651400	1.42011100	1.78464700
H	-7.27894400	3.02495000	2.31929700	C	-4.41553400	1.19005000	2.72766300
H	-8.48581800	1.84646200	0.49723300	C	-4.22618800	1.53718000	4.06502500
H	-7.38799500	0.04761600	-0.75621600	C	-3.02924100	2.11673100	4.47843100
C	3.86703200	-2.06581800	2.14038400	C	-2.01555200	2.34378400	3.54782900
H	3.49675100	-3.07256500	2.33422500	C	-2.20082500	1.99265200	2.21383500
H	4.95015300	-2.09845000	2.03459100	H	-1.37522900	-1.50757800	2.37061600
H	3.60109800	-1.42796500	2.98432500	H	0.61978400	-0.87403900	3.76261000
C	-3.23327400	-0.14664300	-3.23104100	H	2.45379500	0.40178900	2.68489600
H	-4.18527100	0.37433500	-3.11092000	H	-2.84488500	1.57932500	-2.74375600
H	-2.56903700	0.51869800	-3.78267400	H	-2.63649500	3.66787200	-4.02330500
H	-3.40455100	-1.04381100	-3.83521600	H	-2.98828800	5.85856200	-2.90404700
N	1.84440200	-0.80170000	-1.46058500	H	-3.57199100	5.92538100	-0.49036600
N	-1.18522100	-1.17243700	0.41990900	H	-3.79861400	3.83912400	0.78985500
C	1.13138400	-1.40708400	1.11999400	H	-5.35373400	0.73839800	2.43176500
C	-0.47892700	-0.54877500	-2.16571600	H	-5.01940400	1.35374400	4.78196700
C	2.76408700	-3.37566800	-0.15776500	H	-2.88602800	2.38997800	5.51851000
H	2.40670200	-3.41910000	-1.18675900	H	-1.07924400	2.79417500	3.86047700
H	3.72960400	-3.87063600	-0.07992500	H	-1.40482600	2.17967600	1.50119300
H	2.04435000	-3.85470000	0.50574200	C	0.19070200	0.09351800	-1.44770300
I	5.56825200	-1.36342800	-0.98268900	C	1.03394200	0.65929900	-3.51593300
C	-2.26619600	1.75594500	-0.93193000	C	-0.11060800	0.19979000	-4.16184900
H	-1.63276000	1.55836700	-0.08684600	C	-1.14108000	-0.32926000	-3.39015600
H	-1.82591800	1.99171400	-1.88250600	H	1.86166700	1.08118500	-4.07947200
H	-3.33201200	1.80302600	-0.80987200	H	-0.18942700	0.24887100	-5.24238100
I	-2.17247200	4.38230100	-0.27705000	H	-2.03103000	-0.70657400	-3.87890800
C	5.16685400	1.12221000	1.93245700	Pt	2.92245800	1.59599100	-0.04396200
H	5.27774300	0.30071900	2.63798500	P	4.32366100	-0.24710900	-0.54522400
H	5.92675900	0.99399900	1.16311900	C	5.75941600	-0.40876100	0.58768000
H	5.31597700	2.06476700	2.45980300	C	5.97033700	0.50731500	1.62289800
C	-5.80572100	-1.67833200	-1.90644100	C	7.09170500	0.39491600	2.44423300
H	-6.74405800	-2.04027200	-1.48509900	C	8.00838200	-0.63243600	2.23750000
H	-6.00508000	-0.86297100	-2.60050400	C	7.80352000	-1.55153000	1.20744700
H	-5.33660500	-2.49207500	-2.46032300	C	6.68593300	-1.44333000	0.38604300
TS3				C	3.59753700	-1.92285100	-0.63819600
Pt	-2.34473700	-1.17372100	-0.68498800	C	3.18251700	-2.46425100	-1.86105600
P	-3.60428200	0.95233200	0.01654100	C	2.61790900	-3.73754500	-1.90680700
				C	2.45559100	-4.47538300	-0.73631200

C	2.86134400	-3.93855600	0.48523600	C	1.02032600	-3.21777100	-1.20113600
C	3.42975700	-2.66928000	0.53665400	C	1.90863200	-2.23347100	-0.77211500
H	5.25953500	1.30742400	1.79241000	C	-5.66560300	-0.46457400	1.27430800
H	7.24439600	1.10957400	3.24567600	C	-4.74614300	-0.49854300	2.33211300
H	8.87966300	-0.72060500	2.87741500	C	-5.19073200	-0.59535600	3.64839800
H	8.51343600	-2.35517400	1.04487600	C	-6.55466200	-0.66684700	3.92371400
H	6.53439800	-2.17201500	-0.40295100	C	-7.47576000	-0.64397300	2.87787800
H	3.29746100	-1.90691600	-2.78262900	C	-7.03748600	-0.54378300	1.55991100
H	2.30618900	-4.15109800	-2.85962700	C	-5.29066700	1.41512000	-1.00198200
H	2.01594900	-5.46601600	-0.77492600	C	-6.13817600	2.29983000	-0.32501200
H	2.73940600	-4.50940800	1.39925300	C	-6.33705100	3.58935100	-0.81634500
H	3.75269900	-2.26937000	1.49117900	C	-5.69788900	4.00177700	-1.98338800
C	-3.79323200	-1.57986100	-2.13369200	C	-4.85247300	3.12348100	-2.66087800
H	-3.44662700	-2.38221600	-2.78451900	C	-4.64496600	1.83697200	-2.17205900
H	-4.71483700	-1.89121800	-1.64616000	H	-1.05193800	-3.73179900	-1.48527400
H	-3.98784000	-0.69174000	-2.73656700	H	1.38182900	-4.17826700	-1.54895900
C	2.76257700	3.32620300	1.45515600	H	2.96668900	-2.45400000	-0.80082200
H	3.70457600	3.79870100	1.18247300	H	-3.68273900	-0.46240600	2.12878400
H	2.05859100	4.07501300	1.79623800	H	-4.46849700	-0.62152500	4.45695000
H	2.88395500	2.59041700	2.24575000	H	-6.89927600	-0.74601200	4.94902700
N	-0.60549200	-0.69180500	0.65081600	H	-8.53846100	-0.70643300	3.08471400
N	1.18569300	0.59765900	-2.19415500	H	-7.77450200	-0.53241500	0.76609800
C	-1.02124800	-0.37412700	-2.00140700	H	-6.63674400	1.99585400	0.58794000
C	1.51136700	0.42483300	0.74437600	H	-6.99084000	4.27041100	-0.28251700
C	-1.47096000	-3.02032900	-1.20317300	H	-5.85301500	5.00628800	-2.36177800
H	-1.16144700	-3.01850300	-2.24736700	H	-4.34652700	3.44199900	-3.56569900
H	-0.60381400	-3.17931600	-0.56224000	H	-3.96461400	1.17142600	-2.69216700
H	-2.21029900	-3.79909700	-1.03240200	C	-0.56138900	0.40235700	0.05507300
I	-3.91319100	-2.57155300	1.30638000	C	-0.16515900	2.51521300	0.89965500
C	1.51424000	3.37706900	-0.18168900	C	-1.53200400	2.74594400	0.97465300
H	1.35383500	2.89153900	-1.15018300	C	-2.42786700	1.76597800	0.54965700
H	0.59544300	3.35148700	0.39068100	H	0.56249700	3.25601100	1.19998800
H	1.86359400	4.38841000	-0.35944000	H	-1.88882100	3.69356700	1.36048100
C	-5.41943100	0.73999900	-0.21178800	H	-3.48591100	1.97935500	0.61400700
H	-5.62056100	0.63826000	-1.27856500	Pt	2.37887500	0.68597100	0.34979200
H	-5.75704300	-0.16620500	0.28904000	C	-3.49217600	-2.58591800	-2.35590700
H	-5.96365300	1.60641600	0.16670800	H	-2.64201600	-3.16279800	-2.69627600
C	5.07352700	0.08148500	-2.18999200	H	-4.41553800	-3.12934700	-2.51332500
H	4.29492900	0.19826700	-2.94296000	H	-3.54210700	-1.64734000	-2.91619100
H	5.63915900	1.01238700	-2.12941400	N	-0.83148700	-1.79179400	-0.77929200
H	5.74886400	-0.72411600	-2.48196100	N	0.31771700	1.35047200	0.44643700
I	7.37231719	4.19469091	2.82740722	C	-1.95773200	0.54740200	0.05253800
TS4				C	1.43614500	-1.00109600	-0.30386400
Pt	-2.88956200	-1.15124000	-0.68043300	C	-6.31171600	-1.19772500	-1.47809900
P	-5.06277200	-0.32277700	-0.45048800	H	-6.01425900	-1.14762700	-2.52498500
C	0.03980100	-0.84557900	-0.36315500	H	-6.41969700	-2.24008000	-1.18074900
C	-0.34533600	-2.97473300	-1.17932800	H	-7.27735600	-0.70145300	-1.38322700
				P	4.50714200	-0.20370700	0.44098300

C	5.38156000	-0.19667700	-1.17096000
C	6.78132300	-0.24504100	-1.24514800
C	4.63859400	-0.12906500	-2.35695800
C	7.42081000	-0.23602900	-2.48245300
H	7.38331900	-0.28416800	-0.34513700
C	5.28201400	-0.12448400	-3.59256500
H	3.55746700	-0.06371000	-2.31207400
C	6.67287900	-0.17877200	-3.65746900
H	8.50407200	-0.26937900	-2.52612900
H	4.69534100	-0.06784700	-4.50313800
H	7.17352200	-0.16864100	-4.61974500
C	4.54648600	-1.93482600	1.07807900
C	3.75926900	-2.23980100	2.19695600
C	5.37931200	-2.92068700	0.53806600
C	3.81016300	-3.50839700	2.76759100
H	3.09417500	-1.48939700	2.61211200
C	5.42155600	-4.19309800	1.10842100
H	5.99152400	-2.70742100	-0.33041500
C	4.64062200	-4.48838100	2.22336800
H	3.19734000	-3.73300600	3.63417200
H	6.06690300	-4.95160600	0.67819700
H	4.67625200	-5.47818600	2.66592400
C	5.65823800	0.60450300	1.62616200
H	6.54611400	-0.01470400	1.76027700
H	5.15389600	0.70490100	2.58682800
H	5.93498100	1.59498800	1.27368000
I	3.38285300	3.27352600	0.87122200
C	-3.61657700	-3.30117000	-0.41582100
H	-3.16960800	-3.13986600	0.56963200
H	-3.19581400	-4.20732300	-0.83642700
H	-4.69146600	-3.39023200	-0.32740700
I	-2.61547816	-2.08945787	3.43098374