

Electronic Supplementary Information

Mechanistic insights into the tropo-inversion of the biphenyl moiety in chiral bis-amido phosphites and in their palladium(II) complexes

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1. Configurations of the biphenyl moiety

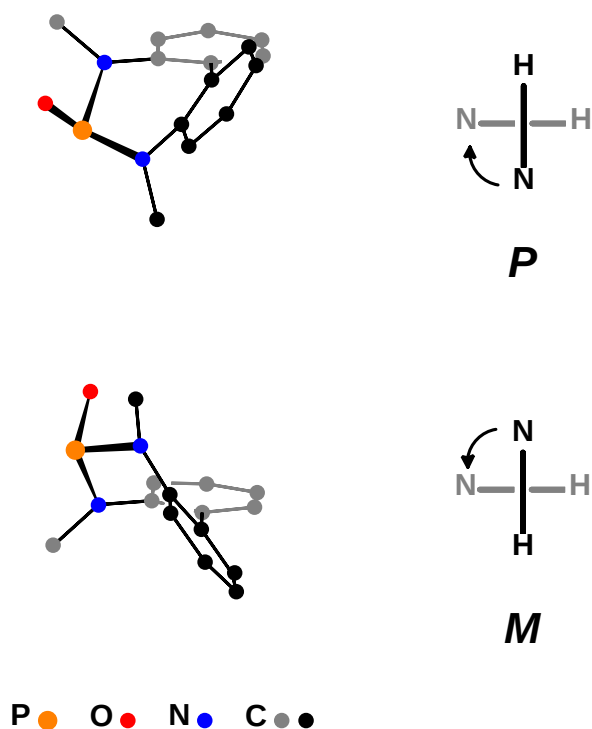
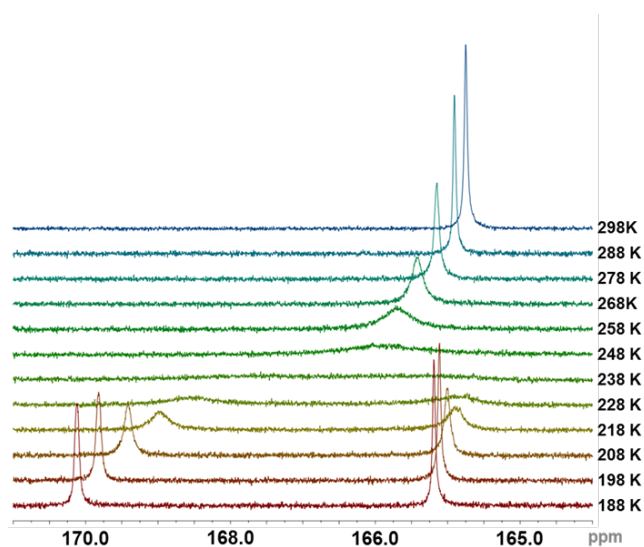
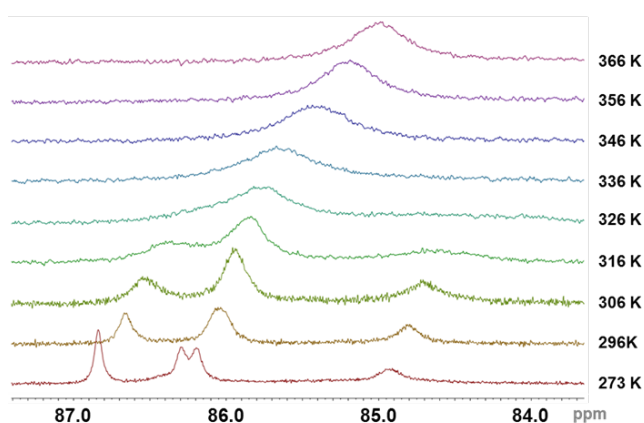


Figure S1. Configurations of the biphenyl moiety of **L1** or **L2** and assignment of descriptors *M* and *P*. For clarity the alkoxy substituents has been omitted. (see G. Bringmann, A. J. Price Mortimer, P. A. Keller, M. J. Gresser, J. Garner, M. Breuning, *Angew. Chem. Int. Ed.* 2005, **44**, 5384).

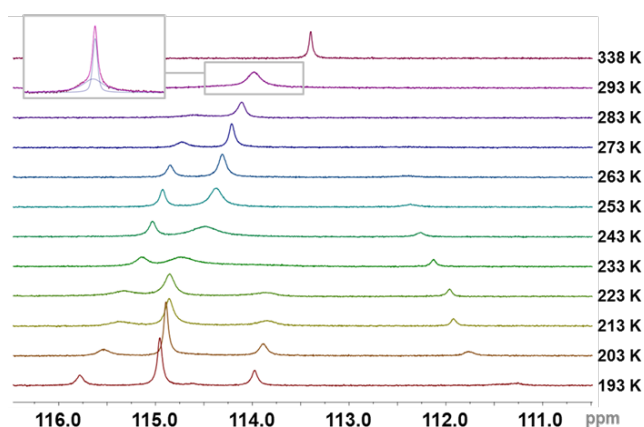
2. Variable temperature $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **L2**, **1b** and **2b**



(A)



(B)



(C)

Figure S2. Vertically stacked $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **L2** (A), **1b** (B) and **2b** (C) at different temperatures. Inset in (C) shows the deconvolution analysis of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2b** at 293 K (δ_{P} 113.98 ppm, $\Delta\nu_{1/2}$ 25 Hz, 64 %; δ_{P} 114.03, $\Delta\nu_{1/2}$ 120 Hz, 36 %).

3. Kinetic constants and activation parameters of L1 and L2

Table S1. Kinetic constants at different temperatures for the equilibrium $(M)-L \rightleftharpoons (P)-L$ ($L = L1, L2$; toluene).

$(M)-L1 \rightleftharpoons (P)-L1$		$(M)-L2 \rightleftharpoons (P)-L2$	
T (K)	$k (s^{-1})$	T (K)	$k (s^{-1})$
244	9.5	198	18
254	38	208	47
264	$1.2 \cdot 10^2$	218	$1.3 \cdot 10^2$
274	$3.0 \cdot 10^2$	228	$3.2 \cdot 10^2$
284	$9.0 \cdot 10^2$	238	$7.3 \cdot 10^2$
294	$2.0 \cdot 10^3$	248	$1.5 \cdot 10^3$
		258	$3.0 \cdot 10^3$
		268	$5.5 \cdot 10^3$
		278	$1.0 \cdot 10^4$

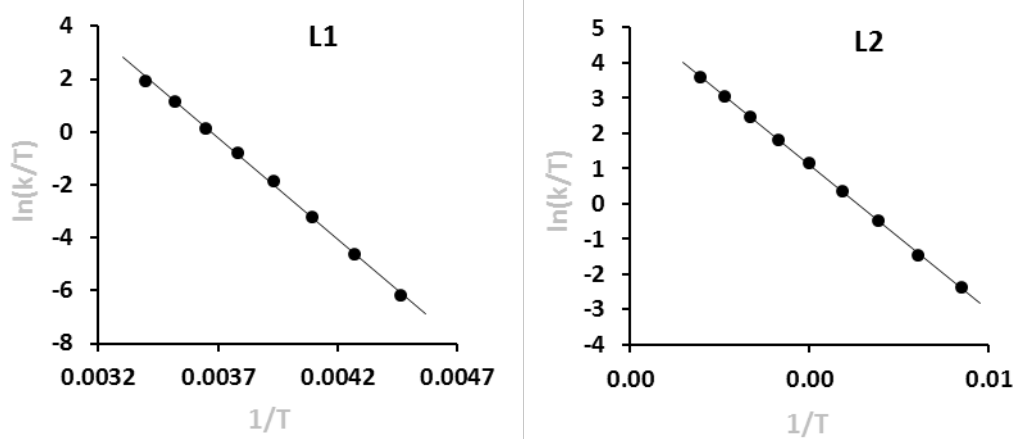


Figure S3. Eyring plots for the equilibrium $(M)-L \rightleftharpoons (P)-L$ ($L = L1, L2$; toluene). Least square regression results: L1: slope= -7371.1 ± 147.5 , intercept= 27.051 ± 0.552 ; L2: slope= -4146.8 ± 22.7 , intercept= 18.513 ± 0.097 .

4. Gibbs free energy profile for $(M)\text{-L2} \rightleftharpoons (P)\text{-L2}$

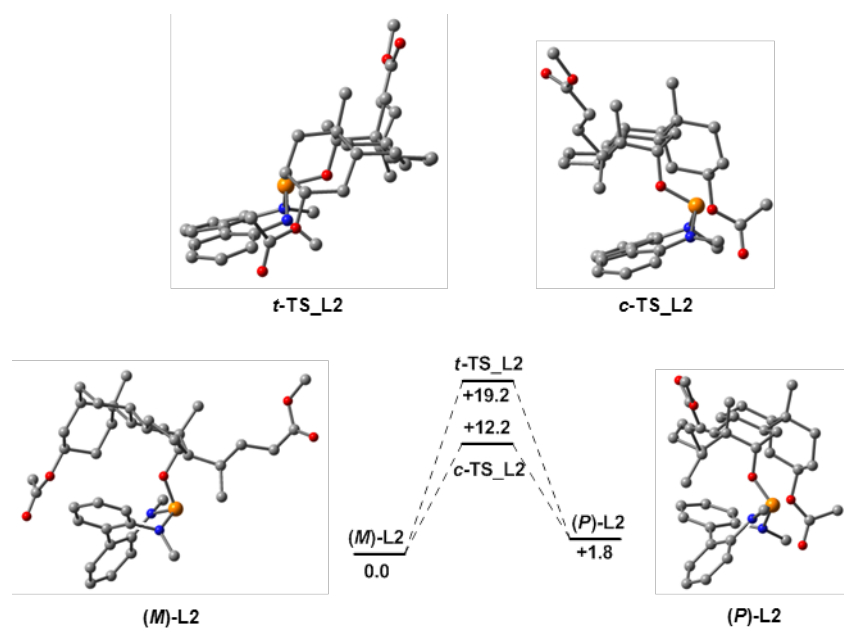


Figure S4. Gibbs free energy profile for the tropo-inversion $(M)\text{-L2} \rightleftharpoons (P)\text{-L2}$ along with the calculated structures. Energies are given in kcal mol⁻¹ and hydrogen atoms are omitted for clarity.

5. Kinetic constants and activation parameters of 1a

Table S2. Kinetic constants at different temperatures for the equilibria^a $(M,M)\text{-1a} \rightleftharpoons (M,P)\text{-1a} \rightleftharpoons (P,P)\text{-1a}$ (toluene).

T (K)	k_1^b (s ⁻¹)	k_2^c (s ⁻¹)
303	14	44
313	25	70
323	42	$1.05 \cdot 10^2$
333	70	$1.6 \cdot 10^2$
343	$1.15 \cdot 10^2$	$2.4 \cdot 10^2$
353	$1.75 \cdot 10^2$	$3.5 \cdot 10^2$
363	$2.7 \cdot 10^2$	$5.0 \cdot 10^2$
373	$40 \cdot 10^2$	$7.0 \cdot 10^2$
383	$6.0 \cdot 10^2$	$9.5 \cdot 10^2$

^a δ_P 86.0 (M,M or P,P: **1a_1**); 86.4 and 88.6 (M,P: **1a_2**); 88.9 (P,P or M,M: **1a_3**) (toluene, 233 K).

^b kinetic constant for the exchange **1a_2** $\rightleftharpoons$ **1a_3**.

^c kinetic constant for the exchange of **1a_2** $\rightleftharpoons$ **1a_1**.

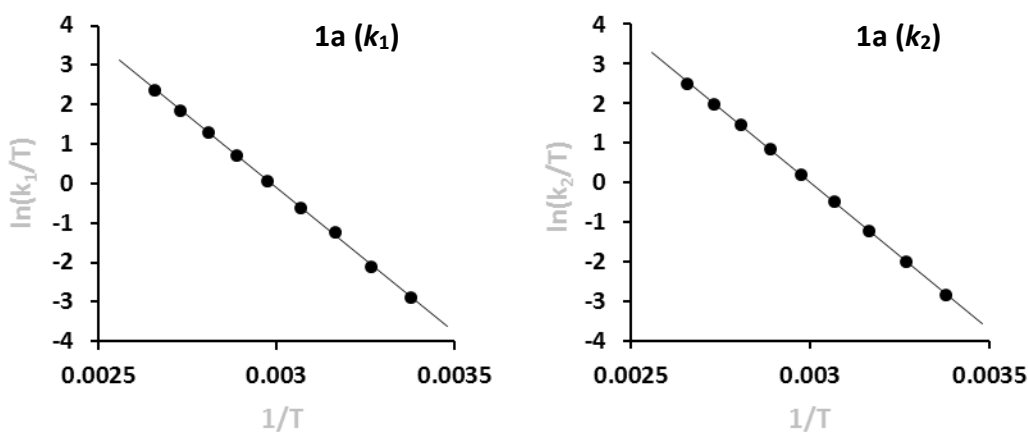


Figure S5. Eyring plots for the equilibria $(M,M)\text{-1a} \rightleftharpoons (M,P)\text{-1a} \rightleftharpoons (P,P)\text{-1a}$ (toluene). Least square regression results: k_1 , slope= -5091.8 ± 16.8 , intercept= 13.733 ± 0.049 ; k_2 , slope= -4141.2 ± 22.0 , intercept= 11.721 ± 0.065 .

6. Kinetic constants and activation parameters of 2a

Table S3. Kinetic constants at different temperatures for the equilibria^a (M,M)-**2a** ⇌ (M,P)-**2a** ⇌ (P,P)-**2a** (toluene).

T (K)	k_1 (s ⁻¹)	k_2 (s ⁻¹)
296	16	17
306	37	40
316	90	90
326	$1.7 \cdot 10^2$	$2.0 \cdot 10^2$
336	$3.5 \cdot 10^2$	$4.0 \cdot 10^2$
346	$7.0 \cdot 10^2$	$8.0 \cdot 10^2$
356	$1.3 \cdot 10^3$	$1.5 \cdot 10^3$
366	$2.3 \cdot 10^3$	$2.6 \cdot 10^3$
376	$4.0 \cdot 10^3$	$4.5 \cdot 10^3$

^a δ_p 119.1 (M,M or P,P: **2a_1**); 116.7 and 115.9 (M,P: **2a_2**); 117.2 (P,P or M,M: **2a_3**) (toluene, 266 K).

^b Kinetic constant for the exchange **2a_2** ⇌ **2a_3**;

^c Kinetic constant for the exchange **2a_2** ⇌ **2a_1**.

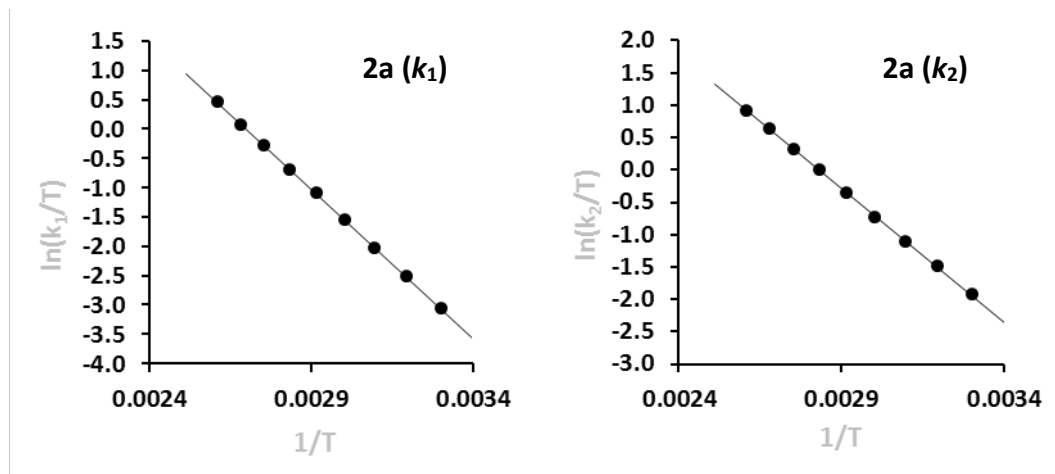
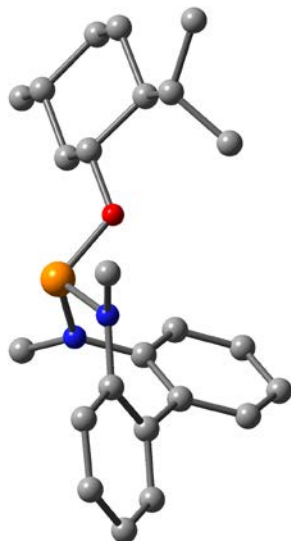


Figure S6. Eyring plots for the equilibria (M,M)-**2a** ⇌ (M,P)-**2a** ⇌ (P,P)-**2a** (toluene). Least square regression results: k_1 , slope= -7345.6 ± 50.0 , intercept= 21.915 ± 0.150 ; k_2 , slope= -7464.8 ± 42.8 , intercept= 22.378 ± 0.129 .

8. Atomic coordinates and relative Gibbs free energies of calculated structure

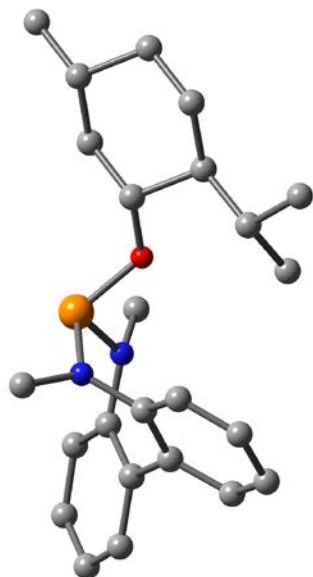
8.1 Ligand L1



I (+0.6 vs. II)

C	-2.81384800	-1.29634200	2.26620000
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C	-1.35855900	-1.57230200	0.35079200
C	-0.58149100	-2.47546700	1.09095000
C	-0.91889700	-2.79085700	2.40832900
C	-2.03753900	-2.19507700	3.00031600
H	-3.68567900	-0.82683000	2.72823700
H	0.29713400	-2.92731800	0.62700500
H	-0.30147400	-3.49203900	2.97551800
H	-2.30367300	-2.42740900	4.03442900
C	-3.36847600	-0.06713200	0.14608900
C	-2.84470800	1.03784000	-0.57863500
C	-4.75688800	-0.27773700	0.15456400
C	-3.74309400	1.89168100	-1.24750400
C	-5.63641300	0.57504500	-0.51651500
H	-5.15033100	-1.13515800	0.70635500
C	-5.12121200	1.66812600	-1.21590100
H	-3.35762900	2.74602000	-1.80489700
H	-6.71225900	0.38650200	-0.49006200
H	-5.79022900	2.34942100	-1.74824800
N	-1.02269500	-1.24792900	-0.99555600
N	-1.45545600	1.31919800	-0.55851700
C	-0.87666400	-2.34382400	-1.94892000
H	-0.66568300	-1.92934700	-2.94598200
H	-0.05527400	-3.03762200	-1.69227400

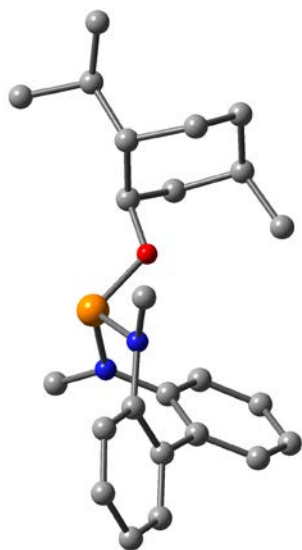
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H	-1.16614600	3.18385800	-1.62234100
H	-1.66231400	3.31001700	0.09137500
P	-0.31248200	0.26019200	-1.36982900
C	4.60960700	0.74201800	0.18760500
C	3.12714300	0.90790700	0.57709400
C	2.26608800	0.32493500	-0.56010900
C	2.62481700	-1.13294300	-0.86175300
C	4.10361200	-1.31703300	-1.22208100
C	4.97717100	-0.71434700	-0.11507800
H	2.95342100	0.27054900	1.46494900
H	4.82865400	1.36692100	-0.69782100
H	5.25396400	1.11500100	0.99669400
H	1.98858100	-1.50343300	-1.68350000
H	2.37715500	-1.73701900	0.02935000
H	4.29566600	-0.74150300	-2.14832300
H	4.85291100	-1.31903300	0.80300800
H	6.04234600	-0.78528700	-0.39433000
H	2.45626600	0.93089400	-1.47024100
O	0.88490200	0.43881100	-0.20635300
C	4.43989200	-2.78434600	-1.49363000
H	3.81968600	-3.19480900	-2.30724800
H	5.49758200	-2.90702600	-1.77824300
H	4.26124900	-3.39833500	-0.59417700
C	2.70027400	2.36230400	0.94920600
H	2.29516200	2.82433600	0.02906900
C	3.84963700	3.26219400	1.42708400
H	4.62755500	3.40468300	0.66231000
H	3.46111200	4.25930400	1.69087400
H	4.33293400	2.85093800	2.32957700
C	1.58721600	2.35777000	2.01018600
H	0.74990300	1.71455100	1.71311100
H	1.98221100	1.98222900	2.97043400
H	1.20376800	3.37670000	2.18556800



II (0.0)

C	3.05706100	2.31146900	-0.46394900
C	2.60101600	1.10878800	0.10568400
C	1.45566900	1.14754400	0.92954600
C	0.82630900	2.37111700	1.19797500
C	1.30042400	3.55658800	0.63526400
C	2.41512400	3.52473000	-0.20904900
H	3.93194800	2.28653500	-1.11812300
H	-0.04773800	2.38372300	1.85178300
H	0.79079000	4.50056500	0.84365300
H	2.78597100	4.44452800	-0.66793900
C	3.35697600	-0.15510000	-0.10033700
C	2.72021700	-1.35508600	-0.51587700
C	4.75025200	-0.15383600	0.07943700
C	3.51171400	-2.49541000	-0.75079300
C	5.52388800	-1.29312500	-0.15447300
H	5.23320800	0.76929100	0.40948600
C	4.89704900	-2.46719900	-0.57732300
H	3.03405800	-3.42132600	-1.07388300
H	6.60623600	-1.26092500	-0.00871300
H	5.48360500	-3.37014800	-0.76635800
N	0.96694000	-0.05728200	1.51169000

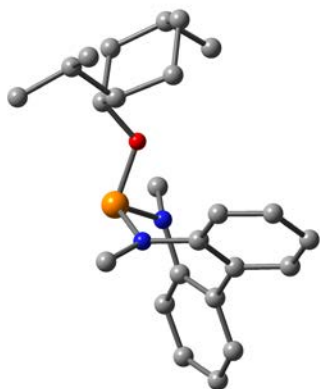
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H	0.58079200	-1.14186200	3.26524200
H	0.35135000	0.61614300	3.44830800
C	0.85159800	-2.21689400	-1.86147200
H	-0.15967300	-1.89813900	-2.14637900
H	0.81521600	-3.29722000	-1.61728000
H	1.51307600	-2.08661000	-2.73096900
P	0.21939300	-1.29106800	0.60192300
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C	-2.30685400	-0.39826500	0.17897200
C	-3.04653000	0.67937500	-0.64120400
C	-3.01533100	-1.75526700	0.12025300
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C	-4.50306000	0.74618100	-0.13700000
H	-3.07887500	0.31557500	-1.68634800
C	-2.30131900	2.04994300	-0.63624600
C	-4.46757100	-1.68763600	0.60612500
H	-2.98879100	-2.10880000	-0.92662100
H	-2.44590400	-2.48645700	0.71725400
C	-5.21529500	-0.60896500	-0.18594500
H	-4.51087200	1.12651400	0.90152900
H	-5.07250100	1.47148700	-0.73556600
H	-1.81191500	2.14334800	0.34920300
C	-3.22165700	3.27007500	-0.79546600
C	-1.20420300	2.10906100	-1.71096800
H	-4.45155700	-1.37169100	1.66743100
C	-5.15696200	-3.05074700	0.52509000
H	-5.29976100	-0.93793500	-1.23888000
H	-6.24669700	-0.50683000	0.19312100
H	-3.94856700	3.37125900	0.02412100
H	-2.61872800	4.19251100	-0.81454500
H	-3.78422400	3.22815500	-1.74401700
H	-0.49942500	1.27584200	-1.61346100
H	-1.65653600	2.06729100	-2.71780500
H	-0.63584900	3.04988200	-1.63595900
H	-4.62017700	-3.80867700	1.11869200
H	-6.19287100	-2.99828800	0.89805400
H	-5.19414100	-3.40783500	-0.51847000



III (+1.0 vs. II)

C	-3.27710600	2.11157900	-0.76248500
C	-2.75931900	1.01576900	-0.04925400
C	-1.70770700	1.24266900	0.86462600
C	-1.21926200	2.54267100	1.06126000
C	-1.75307000	3.62038400	0.35283000
C	-2.78204500	3.40269100	-0.56920100
H	-4.08108500	1.93973300	-1.48229100
H	-0.40791600	2.70374400	1.77359800
H	-1.35611500	4.62628700	0.51090100
H	-3.19848000	4.23734600	-1.13844800
C	-3.35099600	-0.33797800	-0.21310200
C	-2.54597500	-1.48050400	-0.46688100
C	-4.74656300	-0.48809500	-0.16390500
C	-3.17794800	-2.72057800	-0.67794300
C	-5.36130300	-1.72512000	-0.37201200
H	-5.35957800	0.39314200	0.04117500
C	-4.56839200	-2.84408000	-0.63569000
H	-2.57027500	-3.60429300	-0.87739700
H	-6.44969600	-1.81115900	-0.33003200
H	-5.02905400	-3.82146400	-0.80186000
N	-1.16750200	0.14405300	1.59224500
N	-1.13863600	-1.34961900	-0.58448700
C	-1.20031300	0.20890700	3.05091100
H	-0.77939400	-0.72063200	3.46256600

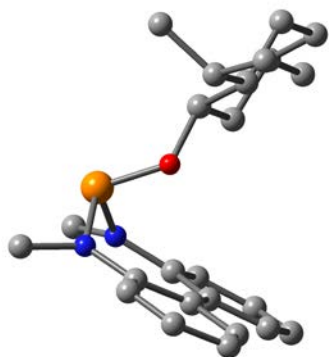
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C	-0.46932700	-2.20339100	-1.56682800
H	0.52064400	-1.78349200	-1.79003200
H	-0.32921800	-3.25148500	-1.23570900
H	-1.05483300	-2.21574400	-2.49816900
P	-0.17405200	-1.02928800	0.84708500
O	0.97950000	-0.15408600	0.00408700
C	2.28304800	0.02680500	0.58245500
C	3.29870300	-0.82720100	-0.20872300
C	2.62747600	1.52030000	0.56910300
H	2.25127200	-0.31256700	1.63220200
C	3.40025800	-0.24972700	-1.63548000
H	2.86225200	-1.84077200	-0.28025400
C	4.65964300	-0.98338500	0.52630300
C	2.85537700	2.11713800	-0.83744500
H	1.82659500	2.06709700	1.09162100
H	3.54382500	1.65612100	1.16866700
C	3.82846100	1.22368500	-1.63635500
H	2.41034900	-0.33918500	-2.10953100
H	4.08489500	-0.85106700	-2.25164800
H	5.05277500	0.02227400	0.75845500
C	5.70679800	-1.69264800	-0.34433900
C	4.50353600	-1.73809500	1.85641100
H	3.34632000	3.09635700	-0.69225700
C	1.54925600	2.38416300	-1.60156400
H	4.84081900	1.31106100	-1.20397100
H	3.90545600	1.59417100	-2.67278300
H	5.98603500	-1.10303900	-1.22982100
H	6.62847000	-1.87779600	0.23032600
H	5.32965200	-2.66920600	-0.69462300
H	4.09229300	-2.74787400	1.68471800
H	5.47859600	-1.85535400	2.35584100
H	3.83618100	-1.22326000	2.56348700
H	0.87870500	3.03467600	-1.01842200
H	1.75987800	2.88460900	-2.56147600
H	0.99349000	1.45837800	-1.80134300



IV (+0.9 vs. II)

C	-2.59729200	2.27048100	1.44091800
C	-2.31029800	1.35675000	0.41135500
C	-1.08068900	1.47492900	-0.27319700
C	-0.18658800	2.50057400	0.06939700
C	-0.49160900	3.40271100	1.09008200
C	-1.70053400	3.28430900	1.78314400
H	-3.54178200	2.17457400	1.98202500
H	0.75947200	2.58541800	-0.46740100
H	0.22038800	4.19006200	1.35011100
H	-1.94464600	3.97937000	2.59025900
C	-3.30664300	0.32542900	0.02244900
C	-2.94656200	-1.04199300	-0.10299200
C	-4.64642400	0.69597000	-0.17722400
C	-3.94776300	-1.98304700	-0.40646400
C	-5.63104900	-0.24715900	-0.48156800
H	-4.91609400	1.75133100	-0.08816600
C	-5.27640800	-1.59379000	-0.59038500
H	-3.68120100	-3.03680000	-0.50074100
H	-6.66630900	0.06910500	-0.63001900
H	-6.03245400	-2.34702900	-0.82721800
N	-0.77778700	0.56457200	-1.32651600
N	-1.61080400	-1.44869100	0.15294800
C	-0.45811800	1.12379200	-2.63747600
H	-0.31038700	0.30168200	-3.35373400
H	0.46285800	1.73511600	-2.63534100
H	-1.28802400	1.75291800	-2.99944400
C	-1.42362000	-2.73438300	0.82802800
H	-0.41766200	-2.76431700	1.26725500
H	-1.53708300	-3.61492400	0.16476500
H	-2.15775800	-2.82521400	1.64226700
P	-0.37011000	-1.07054600	-1.02800000
O	0.85635100	-1.02951800	0.11246800
C	2.22052800	-1.19251300	-0.30679600

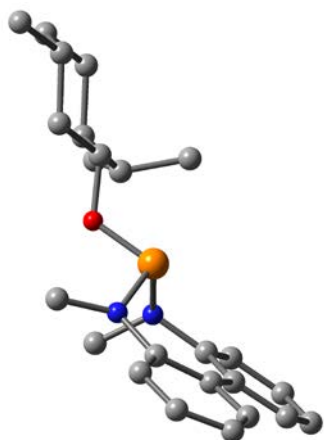
C	2.86792600	0.20174900	-0.47923800
C	2.94671500	-2.05498200	0.73047600
H	2.22410500	-1.72774300	-1.27222800
C	2.94066100	0.86918500	0.90833800
H	2.17387300	0.79295700	-1.10308000
C	4.21233200	0.15395800	-1.25679800
C	3.14836800	-1.37928800	2.10450000
H	2.39510000	-3.00284700	0.84462700
H	3.93336800	-2.31691000	0.31199400
C	3.74245500	0.03284000	1.91356200
H	1.91050300	0.99385800	1.27399600
H	3.35676700	1.88474300	0.83108700
H	4.88486900	-0.56719600	-0.75935900
C	4.92293200	1.51483800	-1.26055600
C	4.00890700	-0.32150500	-2.70452900
H	3.89416000	-1.98349000	2.65171600
C	1.87322100	-1.36332400	2.96193400
H	4.78715000	-0.05743200	1.56692400
H	3.78628000	0.55108400	2.88664900
H	5.24833400	1.82140800	-0.25571400
H	5.81898500	1.48382700	-1.90096100
H	4.25788000	2.30310100	-1.65460700
H	3.32600200	0.35826900	-3.24341900
H	4.96563100	-0.33492500	-3.25076200
H	3.58508700	-1.33486200	-2.76507300
H	1.48165000	-2.38528100	3.09606100
H	2.08475600	-0.95089100	3.96246400
H	1.07447600	-0.76900200	2.49853100



c-TS_I-II (+9.8 vs. II)

C	-3.11076600	-2.19596300	-0.16705600
C	-2.46265200	-0.97504000	0.14018500
C	-2.23988600	0.00403000	-0.89318000
C	-2.70165200	-0.40286000	-2.17453200
C	-3.34541000	-1.60123800	-2.46137100
C	-3.56400600	-2.51820100	-1.43702900
H	-3.24495000	-2.92692600	0.62810000
H	-2.57591400	0.25019800	-3.02959700
H	-3.67150100	-1.80469800	-3.48399500
H	-4.06410000	-3.47266500	-1.61928100
C	-1.61538300	1.39757500	-0.78946600
C	-1.55718700	2.15232500	-1.99343800
C	-1.08710200	2.09572200	0.35983300
C	-1.10179600	3.45909600	-2.11583900
H	-1.90040400	1.71231300	-2.92158700
C	-0.63810000	3.43409200	0.21990400
C	-0.64593700	4.12429600	-0.98111500
H	-1.11499900	3.94537800	-3.09393300
H	-0.23802400	3.94276300	1.09366800
H	-0.28618900	5.15525200	-1.02611800
P	-0.56994100	-0.11782700	1.93982900
C	-0.77204500	2.41756800	2.80353000
H	0.20262500	2.93996500	2.83744000
H	-1.56978500	3.17684800	2.83321700
H	-0.84874000	1.80909000	3.71611700
C	-2.75588600	-1.55351000	2.53856900
H	-3.84658100	-1.45443000	2.42204500
H	-2.50933500	-2.63140400	2.57452400
H	-2.47927100	-1.12095800	3.51149400
N	-0.93319400	1.54652900	1.64340400
N	-2.06796800	-0.82095900	1.48001400
O	0.28554600	-0.53213500	0.57976000
C	1.71305600	-0.40980300	0.53198000

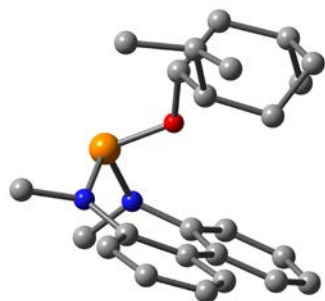
C	2.22882300	-1.43005600	-0.49371400
C	2.12138400	1.01968000	0.17081800
H	2.13217300	-0.65513100	1.52783700
C	3.75586200	-1.28512700	-0.62270400
H	1.78425900	-1.12858200	-1.46116500
C	1.72841900	-2.87057500	-0.21495700
C	3.63984300	1.17477600	0.01436300
H	1.74573400	1.71474500	0.93862200
H	1.61538000	1.29527700	-0.77052200
C	4.16803000	0.14401600	-0.99347400
H	4.23592800	-1.56277900	0.33257800
H	4.13651300	-1.99020800	-1.37770400
H	0.62969900	-2.79472800	-0.17075500
C	2.19922800	-3.44545000	1.12783500
C	2.07064400	-3.82510300	-1.36632500
H	4.10390400	0.94776400	0.99413400
C	4.01443000	2.60721600	-0.37079800
H	3.76936200	0.39104900	-1.99519900
H	5.26667000	0.21730700	-1.06618200
H	1.88502000	-2.82090100	1.97898300
H	1.77359700	-4.44973600	1.28579700
H	3.29660300	-3.54556400	1.16837000
H	1.74893200	-3.41494600	-2.33787200
H	3.15344100	-4.02451200	-1.42779300
H	1.56801600	-4.79628700	-1.22914000
H	3.64977000	3.33120200	0.37610100
H	5.10660100	2.72773300	-0.45745000
H	3.56698800	2.87827000	-1.34231000



t-TS_I-II (+13.8 vs. II)

C	-2.89529100	-3.07780100	0.37257500
C	-2.40187900	-1.74890700	0.26485200
C	-3.27775500	-0.72283100	-0.28107200
C	-4.49478100	-1.22186000	-0.81873700
C	-4.93661600	-2.53611800	-0.74376700
C	-4.13542800	-3.47618500	-0.09906800
H	-2.25399700	-3.83687100	0.81322200
H	-5.17059800	-0.54250300	-1.32572000
H	-5.90179800	-2.80979300	-1.17553300
H	-4.45169100	-4.51693300	0.00855100
C	-3.12853300	0.80432200	-0.30049000
C	-4.21139500	1.58316600	-0.80314700
C	-2.03562500	1.59088900	0.17827800
C	-4.23846800	2.97285600	-0.82479700
H	-5.10635800	1.10336200	-1.18393400
C	-2.06519100	2.99880600	0.14264900
C	-3.15362900	3.70789800	-0.34150200
H	-5.12163300	3.47937800	-1.22216100
H	-1.17656800	3.51865900	0.50766300
H	-3.15306500	4.80026300	-0.35510800
P	-0.21380700	-0.27393400	-0.18751200
C	-0.72823100	1.04115500	2.17427600
H	-0.91992200	2.05320700	2.56126800
H	-1.44500800	0.34200900	2.64458600
H	0.29059200	0.74765800	2.46244800
C	-0.38488900	-2.56392800	1.45663800
H	-0.99185300	-2.84303600	2.33303200
H	-0.15827600	-3.48541000	0.88689500
H	0.56319000	-2.15022200	1.81440600
N	-0.84010100	1.04113500	0.71465700

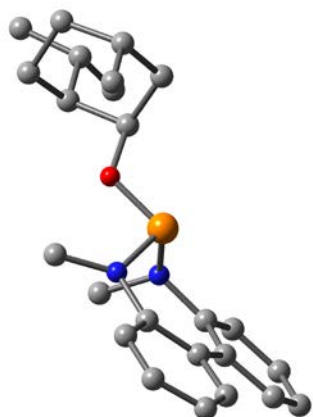
N	-1.07528000	-1.55253500	0.66753000
O	1.26004800	-0.44875100	0.54595500
C	2.46586600	-0.37847100	-0.23944300
C	3.33177900	0.79516700	0.24412700
C	3.19033100	-1.71756700	-0.12665100
H	2.19473500	-0.21318000	-1.29870400
C	4.65787500	0.78816900	-0.53978200
H	3.57006000	0.57547300	1.30246600
C	2.58277900	2.15280900	0.23523000
C	4.52281200	-1.72810400	-0.88939300
H	2.52433500	-2.51638700	-0.49388500
H	3.37491400	-1.92145200	0.94371800
C	5.39307100	-0.55142900	-0.42417200
H	4.45540900	0.99609300	-1.60529100
H	5.30724000	1.60248000	-0.18304000
H	1.66033200	1.99198200	0.81447500
C	2.15256100	2.62586600	-1.15994500
C	3.38083300	3.24686600	0.95677600
H	4.29578100	-1.56938900	-1.96149800
C	5.24166000	-3.07093600	-0.74819600
H	5.68508600	-0.72025800	0.62931900
H	6.32895400	-0.52309000	-1.00781400
H	1.51785800	1.88794100	-1.67508900
H	1.56457900	3.55456800	-1.08196600
H	3.01952600	2.83804300	-1.80711000
H	3.69689500	2.91949400	1.96114600
H	4.28637500	3.53357200	0.39689500
H	2.77106400	4.15702600	1.07675700
H	4.61524100	-3.90230700	-1.11041500
H	6.18392600	-3.08182700	-1.31968800
H	5.48792200	-3.27272400	0.30841100



c-TS_III-IV (+13.4 vs. II)

C	-0.81330500	-3.09129100	0.65478700
C	0.12627300	-2.12866600	0.19458100
C	0.80619000	-1.29910300	1.16959200
C	0.32866100	-1.45553200	2.49888500
C	-0.62323900	-2.37323400	2.92134300
C	-1.18403800	-3.23442100	1.98188100
H	-1.30222400	-3.73340500	-0.07222300
H	0.71632700	-0.81448400	3.28151900
H	-0.91020000	-2.41184500	3.97444300
H	-1.91959700	-3.99117800	2.26591000
C	1.94158200	-0.29624900	0.99291900
C	2.46245100	0.33974400	2.15690400
C	2.58492400	0.11107600	-0.21546400
C	3.48377800	1.28210800	2.15691700
H	2.07721400	0.08945700	3.13890100
C	3.60239200	1.08751800	-0.20953500
C	4.07145000	1.67631700	0.95368700
H	3.81484900	1.70760800	3.10746800
H	4.01001100	1.37783600	-1.18014800
H	4.86461700	2.42699700	0.92349200
P	0.68656000	-0.57978200	-2.06079500
C	3.25113300	-1.31267400	-2.09906700
H	4.26365100	-0.88031200	-2.09070800
H	3.28376400	-2.28358300	-1.56670200
H	2.97724900	-1.50869800	-3.14884600
C	-0.32178000	-3.07366700	-2.05692600
H	0.06261400	-4.07046900	-1.78726100
H	-1.42666400	-3.10716900	-2.02538200
H	-0.02841500	-2.86766300	-3.09602000
N	2.28885800	-0.38842100	-1.50913200
N	0.25698700	-2.04031700	-1.20196400
O	0.04678600	0.62460800	-1.12267400
C	-1.33886900	0.99656800	-1.26573600
C	-2.09456600	0.57220800	0.01313800
C	-1.41666500	2.50222800	-1.53643400

H	-1.75299800	0.46512800	-2.13990200
C	-1.58855700	1.43793700	1.18383700
H	-1.80195300	-0.46804600	0.22287700
C	-3.63567400	0.55200700	-0.18413100
C	-1.01717700	3.39739100	-0.34342400
H	-0.79384800	2.73069000	-2.41718800
H	-2.45785600	2.73167100	-1.82086000
C	-1.76700300	2.93825300	0.92474200
H	-0.52086400	1.21453400	1.32443800
H	-2.07939700	1.14198700	2.12234300
H	-3.95869900	1.52068400	-0.60624000
C	-4.38233300	0.35555000	1.14270100
C	-4.05150800	-0.55254700	-1.17025000
H	-1.36022700	4.41948000	-0.58522500
C	0.50132000	3.47713900	-0.12233700
H	-2.84174800	3.16900100	0.81504900
H	-1.41454800	3.51851400	1.79461200
H	-4.25828100	1.20997500	1.82409000
H	-5.46268400	0.22927100	0.96622900
H	-4.01908200	-0.54696500	1.66418200
H	-3.75102800	-1.54309300	-0.78652400
H	-5.14427200	-0.56495400	-1.31061000
H	-3.59697300	-0.43003300	-2.16491700
H	1.01415600	3.80315200	-1.04212500
H	0.73689600	4.20659100	0.67035200
H	0.93395400	2.50840300	0.16030000

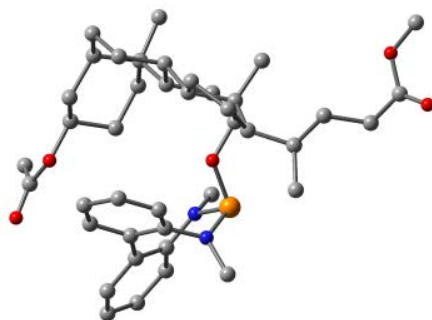


t-TS_III-IV (+19.1 vs. II)

C	-2.95096000	-2.80130700	0.69877200
C	-2.44889200	-1.49915700	0.43775700
C	-3.35529400	-0.48076900	-0.06410200
C	-4.65206100	-0.96702000	-0.38406100
C	-5.11398500	-2.25601600	-0.15158200
C	-4.25513400	-3.18498300	0.43267600
H	-2.26741800	-3.55104300	1.09131600
H	-5.37851000	-0.29918000	-0.83253300
H	-6.13995600	-2.51934900	-0.41819500
H	-4.58132700	-4.20525400	0.65007800
C	-3.15350600	1.03398100	-0.23134600
C	-4.26711000	1.81192500	-0.66341400
C	-1.98433600	1.81498500	0.03853600
C	-4.26304400	3.19600300	-0.79014100
H	-5.21186200	1.33663000	-0.90250400
C	-1.98693600	3.21714800	-0.10159400
C	-3.10945400	3.92675400	-0.49826500
H	-5.17482700	3.70095400	-1.11889000
H	-1.04625200	3.73238500	0.10514700
H	-3.08284700	5.01463400	-0.59471400
P	-0.30557900	-0.16124500	-0.39967700
C	-0.41724200	1.39646200	1.87173000
H	-0.51855400	2.44560800	2.18772900
H	-1.08215600	0.77517600	2.50145600
H	0.62084200	1.08098900	2.04439100
C	-0.35036700	-2.20888100	1.55871200
H	-0.91736800	-2.35193200	2.49259200
H	-0.15355800	-3.20370400	1.11749400
H	0.61583300	-1.75865300	1.80770500
N	-0.73600100	1.27008900	0.44869100

N	-1.07869900	-1.31566100	0.66609800
O	1.23968000	-0.39286700	0.16132500
C	2.32472200	0.30083200	-0.49863300
C	3.48519400	0.34634300	0.51547500
C	2.71698600	-0.38761000	-1.81184200
H	1.98142200	1.32469700	-0.71661900
C	3.99849100	-1.09327100	0.72705600
H	3.05220400	0.69839100	1.46910400
C	4.58231700	1.37559200	0.12335600
C	3.34498000	-1.78785800	-1.64581500
H	1.83461500	-0.43829900	-2.47092200
H	3.43831100	0.27398400	-2.32072700
C	4.46303000	-1.74528300	-0.58212700
H	3.17697000	-1.68520500	1.16031300
H	4.80643800	-1.11097300	1.47302000
H	4.95230700	1.13190900	-0.88817800
C	5.78531500	1.31711300	1.07565600
C	4.02933700	2.80926300	0.08105400
H	3.81273900	-2.04231700	-2.61345300
C	2.30883400	-2.88438900	-1.35427200
H	5.32489500	-1.18460400	-0.98424300
H	4.82813600	-2.76781200	-0.38623700
H	6.32322800	0.35970500	1.01541100
H	6.50750000	2.11408600	0.83704700
H	5.46481700	1.45888100	2.12241300
H	3.60942500	3.09399700	1.06134500
H	4.82824900	3.52809000	-0.16103700
H	3.23747100	2.93921300	-0.67147600
H	1.50470900	-2.87689000	-2.10819800
H	2.78261300	-3.87951600	-1.37684700
H	1.83574300	-2.75312600	-0.37226500

8.2 Ligand L2

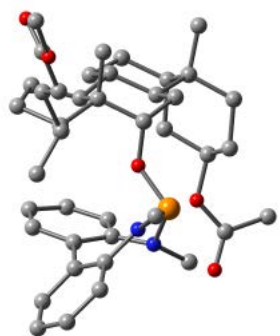


(M) -L2 (0.0)

C	-1.49467000	2.90395100	-1.15764100
C	-0.43633600	1.93048200	-0.54020200
C	0.50089900	2.61683200	0.49461700
C	-0.29750500	3.34836900	1.58071100
C	-1.31908500	4.32063100	0.98357300
C	-2.27092200	3.62874300	-0.00769200
H	-0.98823200	1.16568200	0.02933500
H	-0.80478800	2.60046000	2.21531300
H	0.39260800	3.89281600	2.24585600
H	-1.90772400	4.79758700	1.78574300
H	-0.78375900	5.13651800	0.47039000
H	-2.88760800	4.40952400	-0.49054400
H	1.11872100	3.37026500	-0.02626100
C	1.41691100	1.54126500	1.08190100
C	0.37667100	1.15718100	-1.59854400
H	0.94344600	1.85286200	-2.23461900
H	-0.30113700	0.61043900	-2.26653800
C	2.29308100	0.81583900	0.02987800
C	1.35582500	0.13794000	-0.99034900
H	1.95366100	-0.32027600	-1.80282500
C	-2.53363500	2.14316500	-2.02354000
C	-0.82289700	3.95165900	-2.06859500
H	-0.41846900	3.48458300	-2.97955600
H	-1.55575200	4.70981000	-2.38946100
H	0.00454700	4.47943700	-1.57391600
C	-3.23899300	2.69721800	0.74530400
H	-3.82195500	3.28334100	1.47430100
H	-2.68407000	1.94408500	1.32209200
C	-4.19627900	1.94802100	-0.17223100
H	-4.88054200	2.66702900	-0.65406900
C	-3.42440500	1.17860300	-1.23778000
H	-2.82484200	0.40228500	-0.74387200
H	-4.10997900	0.64904600	-1.91681700
H	-2.02881500	1.60248800	-2.83858600
H	-3.17450700	2.89496600	-2.51941700

C	2.40449700	1.89250300	2.20466300
H	1.89974200	1.98427100	3.17799600
H	2.89172300	2.86218400	2.00792700
C	3.06255500	-0.15777300	0.96441600
C	3.44478200	0.73138200	2.18146000
H	2.28612300	-0.84910500	1.31827200
H	3.42914500	0.14668500	3.11411800
H	4.46306200	1.13516300	2.08691400
O	-4.95195400	1.06409600	0.68613600
O	0.61686500	-0.88117700	-0.31593100
C	3.24587700	1.76339100	-0.72355900
H	3.94702700	2.26490600	-0.04212100
H	3.84268100	1.20668500	-1.46305900
H	2.71066900	2.55309400	-1.26749100
C	4.16247700	-1.05031800	0.33810700
H	3.85907500	-1.23592800	-0.70938500
C	4.19313400	-2.41460000	1.04574800
H	4.40620100	-2.28903400	2.12089600
H	3.22159600	-2.92432900	0.95376900
H	4.95974700	-3.08636900	0.62910100
C	5.56807300	-0.41989700	0.29785100
H	5.51054900	0.64650700	0.04811300
H	6.02458100	-0.47643100	1.30148600
C	6.50622800	-1.08824700	-0.72012000
H	6.64616700	-2.15710900	-0.51108000
H	6.07055400	-0.99433400	-1.73013500
C	7.88124700	-0.46256500	-0.75009400
O	7.81633600	0.85184500	-1.04199200
O	8.92412900	-1.03693500	-0.53951200
C	9.05833300	1.55859300	-1.08251800
H	9.56994200	1.50633300	-0.10911600
H	9.72505900	1.13465500	-1.84920900
H	8.81256700	2.59942400	-1.32666700
C	-6.18325900	0.58247800	0.41977300
C	-6.87146700	1.03332100	-0.84938000
H	-7.01299100	2.12497200	-0.85668900
H	-6.27565200	0.76662800	-1.73396900
H	-7.84833600	0.53970100	-0.90387200
O	-6.68516000	-0.17872200	1.21116400
P	0.26222000	-2.36832000	-0.98792000
N	-1.27169600	-2.06732400	-1.77084200
N	-0.25472800	-3.13086900	0.46165100
C	-2.57260500	-2.28033200	-1.27183100
C	-1.11098500	-1.83690500	-3.20592800
C	-0.79835300	-2.27316100	1.45730100
C	0.43119900	-4.35215100	0.87462400
C	-2.94935100	-2.11164300	0.09839400
C	-3.58949500	-2.61394600	-2.19848500
H	-1.75136600	-1.00670400	-3.54567100
H	-1.33764800	-2.72577700	-3.82217600
H	-0.06710800	-1.55971700	-3.41273100
C	-2.05745100	-1.68329600	1.21826400

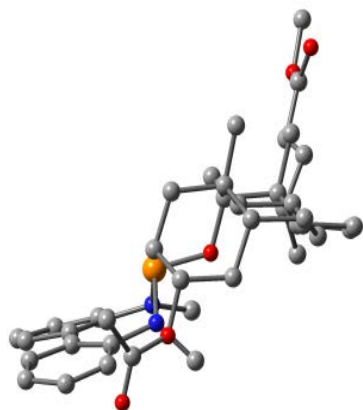
C	-0.06704700	-1.94335000	2.60851000
H	1.36312200	-4.17539700	1.44330600
H	0.69045500	-4.94513100	-0.01469100
H	-0.24236000	-4.95708900	1.50148900
C	-4.30432400	-2.29396900	0.43832500
C	-4.92197100	-2.77522700	-1.82383600
H	-3.33671300	-2.75187300	-3.24768900
C	-2.51677100	-0.71683100	2.13590700
C	-0.55214800	-1.00180200	3.51631000
H	0.90614800	-2.40758000	2.77532500
C	-5.29228400	-2.61418500	-0.48999000
H	-4.59903400	-2.15507000	1.47899000
H	-5.66515600	-3.03072100	-2.58405100
C	-1.77481500	-0.37101700	3.26683900
H	-3.47480600	-0.22699100	1.95301500
H	0.03575100	-0.74489000	4.40119500
H	-6.32996900	-2.71595100	-0.16816700
H	-2.15742700	0.38741300	3.95435100
H	0.74760000	0.76384600	1.48840700



(P) -L2 [+1.8 vs. (M) -L2]

C	2.84694400	-3.10768800	-0.70284900
C	1.61689000	-2.23630700	-0.29783200
C	0.92128600	-2.73523300	1.00116300
C	1.92780500	-2.86079500	2.15699700
C	3.18627700	-3.65101900	1.78053300
C	3.84951000	-3.12265800	0.49581700
H	1.99860400	-1.23816900	-0.03845200
H	2.20646600	-1.84504900	2.48629700
H	1.43777600	-3.33290800	3.02412600
H	3.91290400	-3.61994300	2.61058600
H	2.92574700	-4.71313800	1.64446500
H	4.66818300	-3.81385900	0.22181000
H	0.48285800	-3.73260900	0.82004600
C	-0.19531900	-1.74759600	1.35008300
C	0.61581700	-1.98471500	-1.44152300
H	0.17445700	-2.92526000	-1.80270200
H	1.13032200	-1.53322500	-2.30324700
C	-1.24226700	-1.54390200	0.22610200
C	-0.49981800	-1.01472300	-1.01911000
H	-1.21459400	-0.88272800	-1.85291200
C	3.59127800	-2.51756800	-1.92619100
C	2.42968200	-4.54316700	-1.07460300
H	1.81806000	-4.54973900	-1.99024300
H	3.31927300	-5.16443200	-1.26993100
H	1.84635900	-5.03892800	-0.28708800
C	4.47872100	-1.73615300	0.74536600
H	5.25875100	-1.81721100	1.51973800
H	3.72583700	-1.04142700	1.14050200
C	5.08125200	-1.09050200	-0.49861500
H	6.00990500	-1.62078400	-0.76680800
C	4.12387200	-1.10670400	-1.68743500
H	3.29619300	-0.41242400	-1.47781700
H	4.63271800	-0.72466700	-2.58717400
H	2.94259100	-2.52822200	-2.81521500
H	4.43719300	-3.18722200	-2.16564500
C	-1.04171700	-1.95809000	2.61232500

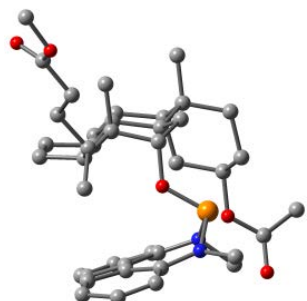
H	-0.49190000	-1.67619500	3.52279000	H	2.62430100	2.99330100	-2.44277600
H	-1.32167800	-3.01921300	2.72413400	H	3.24880400	3.48900100	-0.84988800
C	-2.18042000	-0.52056600	0.93021800	C	-1.06416300	4.69210000	1.49135100
C	-2.29926400	-1.06917600	2.38088500	C	-2.55601500	5.59212200	-0.15254200
H	-1.57293000	0.39334600	0.98739100	H	-2.72123900	4.48562800	-1.96789100
H	-2.35098400	-0.24129100	3.10438200	C	0.04950000	2.20771900	2.61892800
H	-3.21740400	-1.65963500	2.51632800	C	2.22053200	1.15267100	2.63641700
O	5.37708000	0.27758100	-0.13603800	H	3.31189000	1.22158700	0.77817700
O	0.10253500	0.24110300	-0.68457800	C	-1.96101200	5.68629200	1.10521100
C	-1.97385400	-2.84650300	-0.15047100	H	-0.57981200	4.76834600	2.46710800
H	-2.56444400	-3.23715100	0.68916700	H	-3.26179500	6.35366200	-0.49473800
H	-2.66402400	-2.67758000	-0.99200600	C	1.02804800	1.47332800	3.29222300
H	-1.28341400	-3.64506800	-0.45210400	H	-0.86825600	2.48775800	3.14112500
C	-3.49399500	-0.09825900	0.23019400	H	3.01183600	0.60929700	3.15926100
H	-3.26338500	-0.03555000	-0.84999000	H	-2.18270600	6.52048800	1.77455600
C	-3.89860100	1.31082900	0.69507600	H	0.86576900	1.16931000	4.32904700
H	-4.09334800	1.31471200	1.78070300	H	0.29718700	-0.76830100	1.46839000
H	-3.10474900	2.04270900	0.49756900				
H	-4.81268700	1.66706100	0.19380000				
C	-4.68320100	-1.06718200	0.39450700				
H	-4.36006700	-2.11391000	0.37753000				
H	-5.14567500	-0.91923200	1.38512400				
C	-5.75368600	-0.89435800	-0.68169600				
H	-6.18822800	0.11722600	-0.69122900				
H	-5.31797300	-1.03545200	-1.68824100				
C	-6.88507900	-1.89029300	-0.55988300				
O	-7.93861400	-1.53021100	-1.31619000				
O	-6.86636000	-2.90010800	0.10567000				
C	-9.05707700	-2.42146500	-1.31535500				
H	-8.76523800	-3.41723200	-1.68359400				
H	-9.46775300	-2.53289200	-0.29998400				
H	-9.80665800	-1.97553700	-1.98064800				
C	6.31655000	1.04547400	-0.72983100				
C	7.34831700	0.36353200	-1.60247200				
H	7.90369600	-0.39376800	-1.02772800				
H	6.87951300	-0.14486700	-2.45791900				
H	8.04391800	1.12625600	-1.97071700				
O	6.30815900	2.23235400	-0.51363000				
P	0.32378000	1.50641200	-1.75417200				
N	-1.13026400	2.43790000	-1.51023100				
N	1.45434200	2.39507400	-0.79903900				
C	-1.33676300	3.50479800	-0.61570600				
C	-2.12686700	2.20564000	-2.55522400				
C	1.38148700	2.18205600	0.60234900				
C	2.76094900	2.67105800	-1.40027300				
C	-0.73535400	3.58868100	0.67749200				
C	-2.24373500	4.52443000	-0.99069800				
H	-3.13578300	2.12482200	-2.12068200				
H	-2.14161000	2.99287600	-3.33079300				
H	-1.90435000	1.25553600	-3.06182800				
C	0.21992000	2.61240400	1.28162900				
C	2.39230000	1.49794500	1.29468500				
H	3.45154200	1.81042000	-1.39201000				



t-TS_L2 [+19.2 vs. (M)-L2]

C	-0.98511500	5.07206200	0.18722100
C	0.00531500	4.05771400	0.16407400
C	1.33929100	4.36840400	-0.29929000
C	1.48821100	5.69374000	-0.78947000
C	0.50010300	6.67138200	-0.77942900
C	-0.75621400	6.36367600	-0.26009300
H	-1.98153400	4.81583900	0.54330000
H	2.44479000	6.01997300	-1.18119900
H	0.72564400	7.66925300	-1.16243100
H	-1.55498200	7.10876200	-0.22198500
C	2.61382800	3.51207900	-0.23561800
C	3.81866000	4.11108800	-0.70821800
C	2.80306000	2.19736300	0.31057900
C	5.08720900	3.56867400	-0.55448300
H	3.78945000	5.07030500	-1.21306900
C	4.10038300	1.66764100	0.48231600
C	5.24654400	2.33945100	0.08902400
H	5.95208900	4.11944700	-0.93291200
H	4.18998900	0.67317700	0.91994400
H	6.22734900	1.89065000	0.25386200
P	0.34469000	1.46022800	-0.29808400
C	1.62098600	0.96143900	2.08964700
H	2.60109500	0.70096300	2.51280600
H	1.20266000	1.80480600	2.67183800
H	0.95737600	0.09335100	2.19925400
C	-1.52859500	2.62428800	1.47921200
H	-1.47098800	3.36196900	2.29535600
H	-2.50930700	2.74033200	0.98102200
H	-1.49988000	1.62341400	1.92012600
N	1.75687900	1.29801800	0.67098100
N	-0.39520600	2.78486400	0.58286400
O	-0.55290000	0.20888300	0.32243500

C	-1.24555700	-0.69176700	-0.57251900	H	2.95861400	-2.58277300	1.17398300
C	-0.23677500	-1.51030600	-1.39423200	C	4.38820400	-2.32111900	-0.38576200
C	-2.14168300	-1.62617400	0.26120200	H	2.94531800	-0.74658000	-0.66668100
H	-1.87260500	-0.08941400	-1.25528800	H	4.18172300	-0.80539500	-1.92386000
C	0.62805100	-2.45283300	-0.53474500	H	-6.90106200	0.98241800	0.77082800
H	-0.78818400	-2.07213100	-2.16156300	H	-5.92525500	1.28493900	-0.65775900
H	0.40288000	-0.80202900	-1.94147700	C	-7.48803200	-0.10232300	-0.96257000
C	-1.23323400	-2.51766100	1.14990500	H	5.04617000	-2.95257700	-1.00488600
C	-2.99562100	-0.95575400	1.37820100	O	5.18557500	-1.52591700	0.51662200
C	-2.99319900	-2.47070100	-0.71373000	O	-8.54471700	0.72501700	-1.05151100
C	1.69120700	-3.25335000	-1.35802200	O	-7.42722500	-1.15937700	-1.54772400
C	-0.23752200	-3.37593600	0.36999600	C	6.42472400	-1.07307600	0.23793400
H	1.17896700	-1.79545300	0.15721000	C	-9.61260900	0.30617100	-1.90621800
C	-2.22361400	-3.19594000	2.11112500	C	7.09271700	-1.53314400	-1.03985600
H	-0.62622600	-1.81667700	1.74966800	O	6.95264800	-0.32396400	1.02504100
C	-3.35794900	-2.14671500	2.30709200	H	-9.25851300	0.17650500	-2.94061100
H	-2.26273800	-0.35150900	1.93264900	H	-10.03767100	-0.64893000	-1.56122500
C	-4.12748900	0.04006200	1.03221300	H	-10.37107700	1.09729100	-1.86097900
H	-3.79662700	-3.00822900	-0.19374600	H	7.22103500	-2.62651400	-1.04687300
H	-3.46308600	-1.83657400	-1.47984000	H	6.49505100	-1.26039000	-1.92220800
H	-2.39663200	-3.22343100	-1.24466600	H	8.07573300	-1.05267500	-1.10175800
C	2.56556100	-4.09582000	-0.37034300				
C	2.63607200	-2.31674600	-2.15649600				
C	1.01704000	-4.18538800	-2.38610900				
C	0.64273600	-4.21994400	1.30128700				
H	-0.80210100	-4.07509800	-0.27011600				
H	-1.74685000	-3.48105800	3.06056600				
H	-2.61652100	-4.12348200	1.66276600				
H	-3.43944700	-1.81661100	3.35338900				
H	-4.33556300	-2.57715200	2.04199100				
H	-3.69127500	0.76235600	0.31644700				
C	-4.52156400	0.82394300	2.29817400				
C	-5.37702100	-0.56135400	0.36226800				
C	1.70960100	-5.00245300	0.53056500				
H	3.20545800	-4.74710100	-0.99438300				
C	3.51607000	-3.22385900	0.47383300				
C	3.53769000	-1.43536100	-1.28957200				
H	2.05704700	-1.69171200	-2.85271000				
H	3.27534300	-2.95393500	-2.79423500				
H	0.51432200	-3.60607600	-3.17579100				
H	1.77114700	-4.82053400	-2.87849300				
H	0.26710300	-4.85161200	-1.93860000				
H	1.11972800	-3.55414200	2.04258600				
H	0.01374200	-4.91660000	1.87910800				
H	-5.06738700	0.17526600	3.00364600				
H	-3.63792600	1.21342500	2.82552000				
H	-5.16922100	1.68298000	2.06722500				
H	-5.10271500	-1.13593800	-0.52772700				
H	-5.86184200	-1.27855500	1.04637800				
C	-6.40893300	0.47906400	-0.07449500				
H	2.36430300	-5.54745400	1.23169200				
H	1.21679600	-5.77124200	-0.08690700				
H	4.16195700	-3.87165000	1.08867400				



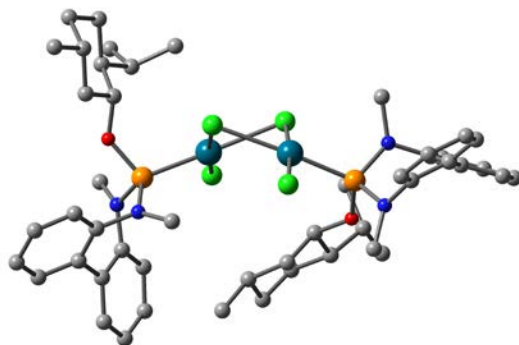
c-TS_L2 [+12.2 vs. (*M*)-L2]

C	2.98066200	1.27376200	1.45907000
C	1.91332600	1.82506600	0.71748600
C	0.79038400	2.40928000	1.38518600
C	0.86356100	2.34072800	2.80713800
C	1.90705600	1.77229100	3.52561800
C	2.99946200	1.23441000	2.84320800
H	3.81973200	0.86266200	0.90080200
H	0.08209400	2.78842100	3.41096800
H	1.86943700	1.77481500	4.61766100
H	3.84601600	0.79107900	3.37303300
C	-0.40674900	3.13614400	0.78988900
C	-1.41135600	3.54645200	1.70575100
C	-0.64600800	3.54155700	-0.57605100
C	-2.44971600	4.42434700	1.42115000
H	-1.39281200	3.16459400	2.72099200
C	-1.68698900	4.46933300	-0.84116500
C	-2.55793600	4.93815000	0.13215000
H	-3.16054100	4.69638600	2.20439400
H	-1.83419700	4.81829500	-1.85997900
H	-3.33790200	5.65624100	-0.13279500
P	0.78697800	1.48045300	-1.77551000
C	-0.10485000	3.70854000	-2.99098000
H	-1.12270200	3.60983900	-3.41246000
H	0.13849800	4.78119900	-2.92538500
H	0.59392200	3.24703900	-3.70293300
C	3.23000200	2.42357300	-1.27751600
H	3.11187300	3.52253900	-1.21678700
H	4.17760300	2.14565800	-0.79343600
H	3.31046200	2.14688800	-2.34132300
N	0.05647700	3.05981200	-1.69277400
N	2.08988200	1.71922100	-0.68666000
O	-0.20085600	0.61347400	-0.77062700
C	-0.75696700	-0.67534600	-1.09922300
C	0.34571900	-1.69028100	-1.43836000
C	-1.56659800	-1.15017700	0.12391500
H	-1.42311000	-0.55608400	-1.97429700
C	1.26026600	-2.04803600	-0.24871100

H	-0.13299300	-2.58882300	-1.85313100
H	0.94808100	-1.27160800	-2.25902900
C	-0.57730800	-1.32743000	1.30359300
C	-2.54278800	-0.09594300	0.71728300
C	-2.30269900	-2.45532600	-0.23872900
C	2.33687000	-3.12935300	-0.60144000
C	0.47715000	-2.40494400	1.04707500
H	1.79546200	-1.11680800	-0.00463000
C	-1.48538100	-1.43542200	2.53605500
H	-0.03774400	-0.36924600	1.38785700
C	-2.71015600	-0.53285000	2.20272700
H	-1.96469800	0.83697200	0.72983600
C	-3.82954000	0.20744800	-0.09619700
H	-2.90022500	-2.82417500	0.60605800
H	-2.98819800	-2.29504100	-1.08525000
H	-1.62081000	-3.26636700	-0.52384400
C	3.30844100	-3.28942300	0.61356700
C	3.18062800	-2.71951200	-1.83402800
C	1.68838000	-4.48838600	-0.93448800
C	1.44865400	-2.57351800	2.22326300
H	-0.04036900	-3.36923000	0.90663000
H	-0.96778600	-1.11885300	3.45396800
H	-1.80028000	-2.48084000	2.69406800
H	-2.75487500	0.34974800	2.85948400
H	-3.64481600	-1.08712200	2.36690600
H	-3.57640000	0.02874600	-1.15853200
C	-4.19694600	1.69252600	0.02867700
C	-5.04377500	-0.68156000	0.23830000
C	2.54946600	-3.59820000	1.91871400
H	3.96237300	-4.15141800	0.38505100
C	4.21700100	-2.06105800	0.81071000
C	3.98053000	-1.43481800	-1.62847600
H	2.54106000	-2.62874700	-2.72495200
H	3.88147100	-3.54519400	-2.05470400
H	1.07875600	-4.42525900	-1.84907400
H	2.46641600	-5.24805600	-1.11414200
H	1.04017400	-4.86502700	-0.13208000
H	1.89050100	-1.59027900	2.46269400
H	0.89391100	-2.88494200	3.12343700
H	-4.38193700	1.96034200	1.08197600
H	-3.38218000	2.33442200	-0.33224400
H	-5.10305500	1.94638100	-0.54477300
H	-4.74295800	-1.71884900	0.43003400
H	-5.50900000	-0.33207100	1.17587000
C	-6.10246200	-0.70344600	-0.86275800
H	3.26632400	-3.64597700	2.75625800
H	2.09691600	-4.60090500	1.84829600
H	4.96393000	-2.27597000	1.59218700
C	3.62409400	-1.21506000	1.17743500
C	4.93714800	-1.60117200	-0.45199100
H	3.31691600	-0.58139000	-1.41793300
H	4.54318700	-1.18093200	-2.54154800
H	-6.51867800	0.29366600	-1.07354200

H	-5.66181400	-1.04482000	-1.81784100
C	-7.25247300	-1.63825200	-0.56219300
H	5.72318900	-2.33084600	-0.71037000
O	5.53521800	-0.32484800	-0.12908000
O	-8.29550700	-1.41136800	-1.38224700
O	-7.25611200	-2.50225100	0.28430600
C	6.56130700	0.23145700	-0.80515500
C	-9.42958700	-2.26758200	-1.22165500
C	7.42612400	-0.67168900	-1.65759400
O	6.76405600	1.41424700	-0.67089600
H	-9.15425500	-3.31957200	-1.39456300
H	-9.84577000	-2.17959600	-0.20623200
H	-10.16878400	-1.94210200	-1.96395400
H	7.83805100	-1.49620000	-1.05552300
H	6.84886300	-1.11735600	-2.48121600
H	8.24489500	-0.07326000	-2.07324100

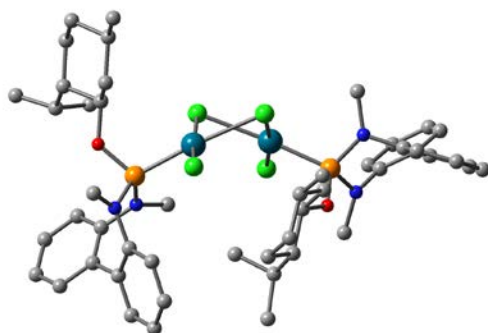
8.3 Dinuclear complex 1a



Va (°.°)

C	5.78961700	-0.30332200	1.02322800
C	6.00621900	0.50035200	2.14714200
H	5.16994600	0.69578300	2.81956500
C	7.27297800	1.03286100	2.39598800
H	7.43586100	1.66618800	3.27117400
C	8.32521500	0.75509700	1.51661200
H	9.31749900	1.17477800	1.69916300
C	8.11148100	-0.05579000	0.39978900
H	8.93424300	-0.26242100	-0.28860200
C	6.84339600	-0.60066800	0.13195100
C	6.61985300	-1.49634300	-1.03058400
C	7.52427500	-2.53969900	-1.29757200
H	8.37529100	-2.68251300	-0.62748100
C	7.34640200	-3.39565800	-2.38546500
H	8.06289600	-4.20013400	-2.56788900
C	6.24333500	-3.22683800	-3.22828700
H	6.08596400	-3.90057300	-4.07402100
C	5.32919500	-2.20183100	-2.98037500
H	4.44898700	-2.07581600	-3.61156500
C	5.50958800	-1.33077400	-1.89587300
C	4.25965700	-2.16522500	1.49729800
H	5.07664100	-2.86871600	1.26709400
H	3.31459700	-2.61173700	1.16534700
C	4.20711600	-2.01318600	2.58637300
C	4.36990800	0.64137100	-2.86951100
H	5.32124400	0.79409100	-3.39890700
H	4.00957800	1.61505600	-2.51551900
H	3.62714400	0.21616200	-3.56149800
C	2.15596700	2.08670900	0.08454700
H	1.51546800	1.49230000	0.74984500
C	2.54987200	3.38553600	0.79560900
H	3.14952700	3.96906100	0.07067500
C	1.25407000	4.17399800	1.06929700

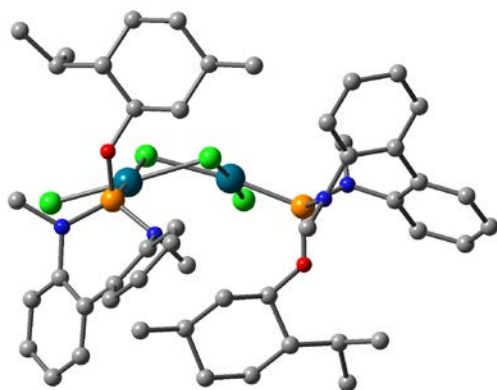
H	0.61104700	3.59758000	1.75405500	C	-4.10950300	-2.32836300	0.83569200
H	1.49565100	5.12189500	1.57430200	H	-3.04151500	-2.58072500	0.79246200
C	0.47785300	4.46052000	-0.21997000	C	-4.62910500	-2.57403800	2.25757100
H	1.07853700	5.12654300	-0.86829900	H	-5.66492800	-2.18588700	2.27044100
H	-0.45422300	5.00155400	0.00902300	C	-4.69265000	-4.09003500	2.52341000
C	0.14632600	3.18264000	-1.00477400	H	-5.11570400	-4.26909400	3.52463400
H	-0.53970900	2.57738400	-0.38474100	H	-3.66895100	-4.50060100	2.54130400
C	1.42281700	2.35813000	-1.22518100	C	-5.49614800	-4.84317200	1.46027700
H	1.18052000	1.40271500	-1.71971200	H	-6.54739500	-4.49909000	1.46951000
H	2.10257300	2.90624200	-1.90216600	H	-5.51534400	-5.92133300	1.69306500
C	3.45548600	3.16446900	2.03158900	C	-4.91131700	-4.61959800	0.05868900
H	4.34189200	2.63247700	1.65088700	H	-3.87147400	-4.99922800	0.06664500
C	3.94998400	4.49263300	2.61920400	C	-4.85651500	-3.11538400	-0.23596200
H	4.37318400	5.14837500	1.84008600	H	-4.37295100	-2.92928300	-1.20833000
H	4.73627500	4.31326000	3.37052200	H	-5.88329200	-2.71416500	-0.30420400
H	3.13987400	5.04645200	3.12147100	C	-3.82021500	-1.79016700	3.32600300
C	2.82469200	2.28497900	3.11843800	H	-3.63027600	-0.79045900	2.90715700
H	1.89338100	2.72402500	3.51074100	C	-4.63512900	-1.58030800	4.60787200
H	3.51713300	2.17219600	3.96934100	H	-4.88345300	-2.53954300	5.09228600
H	2.58309200	1.27795700	2.74986900	H	-5.58139800	-1.05383400	4.40066700
C	-0.54750300	3.50083100	-2.32948700	H	-4.06835300	-0.98003700	5.33774400
H	-1.51019700	4.00415600	-2.15992400	C	-2.44930900	-2.40467800	3.64486100
H	-0.73957900	2.58879700	-2.91282100	H	-1.83954000	-1.69242000	4.22223300
H	0.08107600	4.16370600	-2.94893500	H	-1.88030200	-2.65298100	2.73547000
C	-3.91097600	2.80801000	-0.13214500	H	-2.54544000	-3.32472400	4.24371300
C	-3.33843800	3.88672000	0.55749400	C	-5.68686500	-5.37070100	-1.02464800
H	-2.92712400	3.71177800	1.55172000	H	-5.70113000	-6.45460400	-0.82641000
C	-3.28073100	5.15260600	-0.02616500	H	-5.24021500	-5.21348900	-2.01994000
H	-2.83304000	5.98321500	0.52443600	H	-6.73337000	-5.02314400	-1.06789800
C	-3.78207100	5.34869200	-1.31683400	N	4.49634200	-0.89029400	0.81113900
H	-3.73097600	6.33424900	-1.78538800	N	4.61819300	-0.22674900	-1.71258200
C	-4.33152800	4.27363500	-2.01615800	N	-4.09958400	1.55791200	0.53713800
H	-4.70112200	4.42108500	-3.03343700	N	-3.17536100	0.38377700	-1.58804000
C	-4.41134600	2.99097300	-1.44432400	O	3.37546700	1.33282900	-0.18537000
C	-5.03520400	1.87736700	-2.19891300	O	-4.28932400	-0.92243700	0.51608500
C	-6.23698500	2.06955400	-2.90506400	P	3.54241300	-0.26031200	-0.41130800
H	-6.72829700	3.04401500	-2.85782300	P	-3.20810500	0.20259400	0.07777500
C	-6.81463700	1.03754300	-3.64568700	Cl	1.14496800	-0.90636600	1.82108100
H	-7.75137800	1.21170100	-4.18054000	Cl	-0.87076500	-2.20394100	-0.43889100
C	-6.19833500	-0.21764200	-3.69604300	Cl	1.74050400	-1.66073300	-2.82678600
H	-6.64590100	-1.03129100	-4.27161800	Cl	-1.29891600	1.59395800	2.41053600
C	-5.00938500	-0.43097300	-2.99744100	Pd	1.55459900	-1.29213800	-0.52853800
H	-4.51609600	-1.40407500	-3.02519200	Pd	-1.19471300	-0.24130600	0.95961800
C	-4.42851200	0.60327500	-2.25283300				
C	-4.76559000	1.59629300	1.84776800				
H	-4.05306600	1.74868100	2.67283700				
H	-5.30933800	0.65724700	2.00869100				
H	-5.49106200	2.42105900	1.83908000				
C	-2.01615100	0.11496800	-2.44972900				
H	-1.99858300	-0.91968800	-2.82255800				
H	-1.08352200	0.29215800	-1.90208600				
H	-2.05633100	0.80844800	-3.30090800				



Vb (+1.1 vs. Va)

C	4.12112300	0.86306900	-2.33716600
C	4.84626000	-0.04313000	-3.12079300
H	4.57056100	-1.09771800	-3.09989200
C	5.89710500	0.40137900	-3.92460400
H	6.46023600	-0.31419900	-4.52833600
C	6.22488800	1.76140300	-3.94755200
H	7.05052000	2.11763300	-4.56827700
C	5.49868500	2.66665000	-3.17219200
H	5.76216300	3.72680000	-3.18311100
C	4.43552000	2.23815500	-2.35693900
C	3.65750300	3.20890800	-1.55157100
C	3.21143100	4.41296300	-2.12408900
H	3.40740100	4.59745700	-3.18285400
C	2.52015100	5.36161400	-1.36943200
H	2.17538700	6.28559100	-1.83937400
C	2.26600500	5.11961900	-0.01600400
H	1.71716100	5.85007800	0.58257900
C	2.69038600	3.92694200	0.56995200
H	2.46805500	3.71437300	1.61467200
C	3.37566000	2.96497600	-0.18624200
C	1.87168900	-0.10570300	-2.39885500
H	1.70968600	0.59210400	-3.23251600
H	0.95054500	-0.15584600	-1.81712200
H	2.07492400	-1.11023300	-2.79941900
C	4.66224400	1.93805400	1.65844900
H	5.35784200	2.77542500	1.50420100
H	5.24680100	1.02772200	1.83601300
H	4.03656500	2.13842600	2.54113300
C	4.28468800	-1.98360700	1.12688300
H	3.36516500	-2.48872400	0.79766600
C	5.49357700	-2.81578500	0.68696800
H	6.39021400	-2.29359300	1.07174300
C	5.41299400	-4.18071500	1.39808000

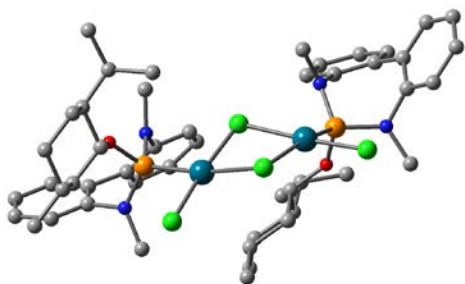
H	4.52599700	-4.73052700	1.03750100	H	-1.45731500	1.35921900	0.85115800
H	6.28870700	-4.79123300	1.13009800	C	-2.08113600	3.31675300	0.19904700
C	5.32972200	-4.03680900	2.92265400	H	-3.04251800	3.86390500	0.15579100
H	6.26890300	-3.58986700	3.29918400	C	-1.16389800	4.05672200	1.19280100
H	5.24579700	-5.03142400	3.39244900	H	-0.93701100	5.06240700	0.80793800
C	4.15427500	-3.15045900	3.36071200	H	-0.20370700	3.52181800	1.27071800
H	3.21978900	-3.64505500	3.03289700	C	-1.78848300	4.16209400	2.58817000
C	4.23247200	-1.79754600	2.63914800	H	-2.70719200	4.77740400	2.53657000
H	3.36502000	-1.17144100	2.90515600	H	-1.09755400	4.68539200	3.27124100
H	5.13715400	-1.25280500	2.96401600	C	-2.14023700	2.78353900	3.16381000
C	5.65348100	-2.88697900	-0.85226600	H	-1.19750300	2.22086500	3.27164700
H	5.75008100	-1.84000100	-1.18103100	C	-3.01980300	2.01280300	2.17148400
C	6.94524700	-3.60653700	-1.26030300	H	-3.18682100	0.98875300	2.53850500
H	7.81881800	-3.20677700	-0.71917100	H	-4.00621000	2.50118500	2.07862800
H	7.13276700	-3.48209400	-2.33916000	C	-1.53658000	3.25529200	-1.25058900
H	6.89302500	-4.68958800	-1.06124400	H	-2.32171500	2.76064800	-1.84353500
C	4.44114000	-3.48381900	-1.57987800	C	-1.33616100	4.65475200	-1.84692800
H	4.25458500	-4.52675500	-1.27593400	H	-0.47718600	5.17085200	-1.39000100
H	4.61370500	-3.49263900	-2.66875000	H	-2.22865200	5.28729100	-1.70721800
C	3.51743200	-2.91457100	-1.39732200	H	-1.13526400	4.58846000	-2.92853800
C	4.09234100	-2.97330100	4.87838100	C	-0.26481400	2.41375300	-1.40051400
H	4.00915800	-3.94554500	5.39051200	H	0.05380700	2.38275200	-2.45390700
H	3.22698500	-2.35806500	5.17335600	H	-0.42465900	1.37423400	-1.08266900
H	5.00282000	-2.47367700	5.25153500	H	0.57298400	2.81976700	-0.81562000
C	-5.25740300	-1.38293700	-2.05078200	C	-2.80736900	2.87883800	4.53629900
C	-4.96735700	-2.19847600	-3.15532700	H	-2.16090700	3.40360200	5.25851600
H	-4.04432600	-2.01939800	-3.70684000	H	-3.02617200	1.87833000	4.94445300
C	-5.82800500	-3.2353200	-3.52189300	H	-3.76070200	3.43251500	4.47502100
H	-5.58361700	-3.86203400	-4.38167000	N	2.98554200	0.40338400	-1.58576000
C	-6.98778100	-3.47242800	-2.77778200	N	3.86558300	1.77208400	0.43564900
H	-7.66179200	-4.28776400	-3.05114800	N	-4.40983100	-0.27310700	-1.74135300
C	-7.27861100	-2.66965600	-1.67432000	N	-4.51627300	-1.00364000	0.77482800
H	-8.17791100	-2.86231400	-1.08463800	O	4.36510900	-0.69101000	0.46878100
C	-6.43129400	-1.61397900	-1.29162900	O	-3.30435600	1.24953200	-0.11539600
C	-6.79143100	-0.76041600	-0.13263500	P	3.13121200	0.29281200	0.08106500
C	-8.09749500	-0.26111800	0.01766500	P	-3.46179600	-0.34378800	-0.34696600
H	-8.83901400	-0.47590900	-0.75523600	Cl	0.95493200	-2.33761800	-0.18621400
C	-8.45047300	0.51344300	1.12417900	Cl	-1.12094700	-1.03063900	2.01606200
H	-9.46987000	0.89629300	1.21524700	Cl	1.35638300	1.44834700	2.63884300
C	-7.50060900	0.80185700	2.10986200	Cl	-1.50298500	-1.70887400	-2.66069000
H	-7.77119300	1.40642100	2.97871800	Pd	1.22784200	-0.32313500	1.11696200
C	-6.19799400	0.31699900	1.97738400	Pd	-1.46976600	-1.38495300	-0.34884700
H	-5.44491800	0.52608600	2.73747500				
C	-5.84106100	-0.45354200	0.86515100				
C	-4.05992000	0.66551400	-2.81818200				
H	-3.04296700	0.49323600	-3.20296400				
H	-4.14235800	1.69648700	-2.44843200				
H	-4.77496000	0.52997700	-3.63951100				
C	-4.29498900	-2.24812600	1.51908800				
H	-4.34760800	-2.06521000	2.60362300				
H	-3.30747400	-2.66481800	1.28744700				
H	-5.06090500	-2.98961100	1.23912900				
C	-2.38904200	1.93629100	0.78688800				



Via (+7.9 vs. **Va**)

C	-5.62089500	-1.15577200	0.32607900
C	-6.75488300	-0.34153000	0.25778400
H	-6.80274000	0.42477100	-0.51798400
C	-7.79835200	-0.51079000	1.16982000
H	-8.67991800	0.13207700	1.11541400
C	-7.70132000	-1.49614100	2.15760700
H	-8.50827000	-1.62747500	2.88254500
C	-6.57039300	-2.31300900	2.22469200
H	-6.49508700	-3.07537400	3.00356900
C	-5.51358400	-2.16293900	1.30997800
C	-4.33581100	-3.06576000	1.34223000
C	-4.52156200	-4.45472200	1.46714100
H	-5.54013200	-4.84579100	1.52142400
C	-3.43888800	-5.33394400	1.50724500
H	-3.61271900	-6.40841500	1.60144400
C	-2.13638200	-4.83397800	1.41510300
H	-1.27909600	-5.50995400	1.43648000
C	-1.92883600	-3.46040600	1.28502000
H	-0.91554300	-3.06737700	1.19989400
C	-3.01216900	-2.56863700	1.25064600
C	-4.80993700	-1.77791800	-1.90325200
H	-5.01252700	-2.83361500	-1.65735400
H	-3.92411000	-1.72819100	-2.54552800
H	-5.66447900	-1.36566300	-2.46104900
C	-1.89870600	-0.60057100	2.23443400
H	-2.28328200	-0.89032300	3.22466700
H	-1.90920100	0.49306700	2.16732900
H	-0.85946200	-0.94727800	2.13505000
C	-3.02786700	2.44089100	-0.12285400
H	-3.27021700	2.42197500	-1.19567900
C	-3.85243300	3.55207200	0.53929300

H	-3.54056500	3.60873300	1.59933300	H	1.35447600	2.31906600	1.99415000
C	-3.41954200	4.87773000	-0.12540800	C	3.39839700	-2.43128700	-0.12205600
H	-3.70764000	4.86162200	-1.19175800	H	2.60168700	-2.25078400	-0.85807200
H	-3.96394000	5.71646400	0.33186900	C	4.47494100	-3.29754200	-0.78039800
C	-1.91085700	5.13297400	-0.00998500	H	5.28457300	-3.40715900	-0.03427300
H	-1.64555700	5.26578000	1.05594400	C	3.88318100	-4.69553900	-1.04656300
H	-1.65007900	6.07719100	-0.51719900	H	4.65844700	-5.34843200	-1.47657200
C	-1.07445400	3.98066200	-0.58199200	H	3.08756700	-4.61477800	-1.80702500
H	-1.29038300	3.90673100	-1.66446600	C	3.29261100	-5.33774000	0.21278900
C	-1.53092100	2.66492400	0.05800300	H	4.09409000	-5.50410800	0.95677800
H	-0.97356500	1.82915300	-0.39321100	H	2.87660500	-6.33055500	-0.02860900
H	-1.29782100	2.67073500	1.13755700	C	2.20765500	-4.45391500	0.84438200
C	-5.38288300	3.25003700	0.50943700	H	1.39500700	-4.33554600	0.10207100
H	-5.56115500	2.56599200	-0.34035100	C	2.78401200	-3.06059900	1.12314800
C	-5.80959000	2.52841000	1.79638400	H	1.99758100	-2.39032100	1.50457000
H	-5.21607400	1.62033200	1.96423400	H	3.56482400	-3.12740200	1.90111100
H	-6.87019000	2.23589100	1.75802200	C	5.09216400	-2.62230200	-2.03394200
H	-5.67623000	3.19471500	2.66670900	H	5.35216400	-1.59776900	-1.72670900
C	-6.27560700	4.47934800	0.29063900	C	6.39691700	-3.30779800	-2.45923700
H	-6.14585100	5.22117400	1.09665400	H	6.21981700	-4.33577500	-2.81660900
H	-7.33565100	4.17770200	0.29153800	H	7.11556800	-1.62477600	-1.62477600
H	-6.07753200	4.98241400	-0.66726600	H	6.87696400	-2.75482400	-3.28261200
C	0.43086600	4.19800300	-0.41204500	C	4.12719000	-2.50291000	-3.22253300
H	0.75760900	5.12521300	-0.90911600	H	4.57394300	-1.88015300	-4.01338300
H	1.01161100	3.36639700	-0.84301000	H	3.17230600	-2.02960500	-2.94623500
H	0.70204900	4.28064500	0.65426700	C	3.90111400	-3.48646200	-3.66528900
C	4.37536200	2.61267200	0.75426300	H	1.61306700	-5.07315500	2.11008500
C	4.42787100	3.70451400	-0.12448300	H	1.17963100	-6.06527200	1.90392800
H	4.55229700	3.51186400	-1.18986000	H	0.81920400	-4.43717300	2.53416300
C	4.28708500	5.00835900	0.35280900	H	2.38808300	-5.20172200	2.88478700
H	4.32055700	5.84702000	-0.34667100	N	-4.59169800	-1.01958500	-0.66505400
C	4.08480600	5.23403400	1.71801700	N	-2.77428700	-1.15750500	1.20191900
H	3.96256600	6.25132200	2.09741200	N	4.58378100	1.28216400	0.26492700
C	4.02976200	4.15195400	2.59778400	N	2.48929700	0.54577000	1.66640300
H	3.86076300	4.32432400	3.66336400	O	-3.41369600	1.14974100	0.43938700
C	4.17601700	2.83063900	2.13995900	O	3.99531000	-1.15775700	0.24725700
C	4.13241500	1.69822600	3.09777100	P	-3.14511400	-0.31075900	-0.22067000
C	4.87300500	1.72679700	4.29159700	P	3.23263000	0.27233800	0.17986100
H	5.50899600	2.59015000	4.50065100	Cl	0.22494200	0.14880700	-3.51130900
C	4.82322900	0.66224000	5.19447400	Cl	0.17748600	-1.19120500	-0.50761400
H	5.41458500	0.70187600	6.11249200	Cl	-3.18958700	0.85648600	-3.21414400
C	4.02579200	-0.45364100	4.92030900	Cl	3.20286800	1.73287800	-1.73287800
H	3.98581700	-1.28991000	5.62226800	Pd	-1.60808400	-0.19875500	-1.85589300
C	3.27733800	-0.49645600	3.74142800	Pd	1.79617200	0.31152800	-1.56873100
H	2.64083700	-1.35174500	3.51224900				
C	3.32744400	0.56810300	2.83616300				
C	5.78712300	1.01621400	-0.53544500				
H	6.57065600	1.71676200	-0.21629800				
H	5.61020400	1.14016300	-1.61460000				
H	6.13484600	-0.00645400	-0.33859800				
C	1.20857000	1.24050000	1.81701000				
H	0.66169000	0.81176500	2.66843400				
H	0.60021600	1.11012700	0.91880100				

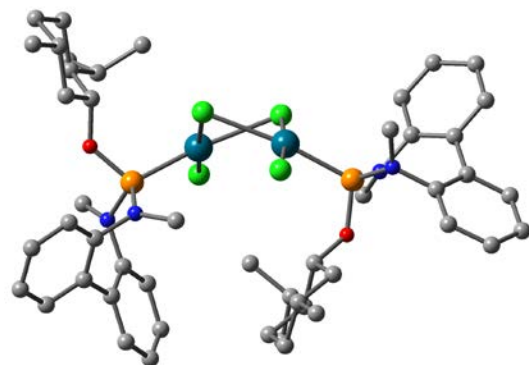


Vib (+8.1 vs. Va)

C	-4.53725700	0.74728700	-1.79267600
C	-4.07343200	1.98508800	-2.24798300
H	-2.99744200	2.16624000	-2.25869600
C	-4.97337100	2.95927200	-2.68258600
H	-4.60570000	3.92892700	-3.02618600
C	-6.34565300	2.68768100	-2.66235400
H	-7.05975000	3.44833500	-2.98689600
C	-6.80901500	1.44337100	-2.22923700
H	-7.88152400	1.23619900	-2.21788300
C	-5.91706300	0.44741500	-1.79335000
C	-6.39974600	-0.90597500	-1.41337500
C	-7.31533800	-1.57307500	-2.24752000
H	-7.65172900	-1.07779300	-3.16138600
C	-7.78427000	-2.85088600	-1.93947300
H	-8.49373700	-3.34590500	-2.60680700
C	-7.32897200	-3.49704200	-0.78601700
H	-7.67386100	-4.50526300	-0.54439800
C	-6.41645800	-2.85788300	0.05406300
H	-6.02974100	-3.36186800	0.94047400
C	-5.95602900	-1.56574300	-0.23990700
C	-3.06867500	-1.11230700	-2.44545400
H	-3.90030900	-1.58075600	-2.99733900
H	-2.44194000	-1.90713400	-2.02184100
H	-2.45598000	-0.52344600	-3.14538100
C	-5.51666500	-0.86269000	2.09511400
H	-6.57811900	-0.57781800	2.14160700
H	-4.92948800	-0.10342500	2.62586400
H	-5.36841300	-1.83236400	2.59221000
C	-2.09104900	1.45029300	1.49958200
H	-1.42399400	1.50502300	0.62412100
C	-2.47203000	2.88221200	1.92118700
H	-3.08532300	2.79496700	2.83805400
C	-1.16099900	3.59700000	2.31753800
H	-1.38423400	4.61830500	2.65749000
H	-0.51885900	3.69738400	1.42565500
C	-0.39356800	2.85963600	3.41994600
H	-0.98816800	2.87255800	4.35255800

H	0.54746100	3.39207600	3.64151600
C	-0.09501700	1.40320400	3.04910000
H	0.56699300	1.40870000	2.16271800
C	-1.39248600	0.70502200	2.63194800
H	-1.16877500	-0.32835100	2.32492300
H	-2.08356300	0.63748000	3.49058400
C	-3.32771700	3.62079100	0.84758800
H	-3.01946200	3.22412400	-0.13302100
C	-4.82741400	3.32751900	1.01266900
H	-5.03718000	2.25156100	1.00723900
H	-5.40590700	3.78792600	0.19593700
H	-5.19596200	3.74598600	1.96556100
C	-3.11704700	5.14077400	0.80620800
H	-3.38915800	5.61034000	1.76670700
H	-3.76036600	5.58645400	0.03000600
H	-2.07957900	5.42081000	0.57649300
C	0.60831900	0.63814500	4.17017400
H	1.51577900	1.16479200	4.50592000
H	0.90558400	-0.36876000	3.83846500
C	-0.05570500	0.52976300	5.04419800
C	1.58447300	2.52602100	-1.24771100
C	0.20564800	2.68170800	-1.47737100
H	-0.38646800	1.80247300	-1.73287500
C	-0.40238100	3.93170400	-1.38259100
H	-1.47239600	4.03182800	-1.57189000
C	0.35415600	5.04845200	-1.01491900
H	-0.11720000	6.02901800	-0.91903300
C	1.71657500	4.90120200	-0.76167100
H	2.30800700	5.76991000	-0.46409900
C	2.36127400	3.65555600	-0.88731700
C	3.83106400	3.57731800	-0.69856500
C	4.67621700	4.54031600	-1.28245000
H	4.23768500	5.31984200	-1.90941400
C	6.05697200	4.50401000	-1.08744400
H	6.69141600	5.25978600	-1.55660600
C	6.62625200	3.49786200	-0.29870300
H	7.70699200	3.46150300	-0.14306100
C	5.80646300	2.52988400	0.28156400
H	6.23218300	1.73517800	0.89525100
C	4.42006000	2.56361200	0.08458700
C	1.99275200	0.59769200	-2.77533200
H	1.16381500	1.07944300	-3.30716900
H	1.73713700	-0.46340300	-2.64928700
H	2.90231900	0.67398600	-3.39114800
C	3.42367100	1.71331400	2.17580600
H	4.40368000	1.71488500	2.67745700
H	2.85086000	0.86883300	2.56693100
H	2.89752000	2.65257000	2.41147300
C	4.88059100	-1.48897200	-0.79040800
H	4.23738600	-2.17620100	-0.22212400
C	5.32009400	-2.17632600	-2.08715800
H	5.98803500	-1.46808000	-2.61362800
C	6.16319800	-3.40945100	-1.70442300

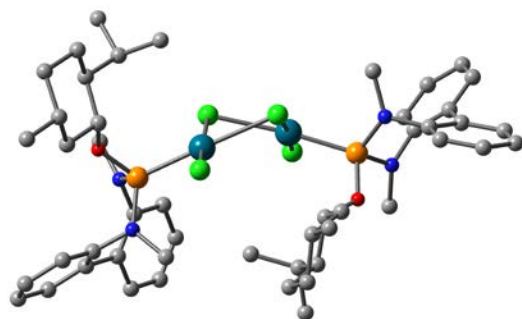
H	6.52863000	-3.90642200	-2.61557800
H	5.52327500	-4.14286400	-1.18302600
C	7.35055200	-3.04905200	-0.80446700
H	8.05120700	-2.40256200	-1.36590500
H	7.91158200	-3.96043300	-0.53645100
C	6.91038100	-2.31091200	0.46707000
H	6.25993400	-2.99207700	1.04734300
C	6.06057600	-1.09138500	0.08774000
H	5.67793400	-0.60641200	0.99797800
H	6.67723300	-0.35499500	-0.45731100
C	4.14415300	-2.47550300	-3.05238300
H	3.72643500	-1.49270700	-3.31647800
C	4.62636000	-3.11778300	-4.36007400
H	4.94983800	-4.16065900	-4.21036800
H	5.47366200	-2.56209800	-4.79525600
H	3.81504300	-3.13292000	-5.10561600
C	3.00870700	-3.29721600	-2.42674000
H	2.21008000	-3.47239700	-3.16563500
H	2.54489300	-2.78808800	-1.56803300
H	3.35741800	-4.28391300	-2.08106800
C	8.09444600	-1.91411500	1.34958800
H	8.68713200	-2.79546000	1.64370200
H	7.75519900	-1.41132800	2.26984200
H	8.76671300	-1.22069100	0.81514900
N	-3.59126000	-0.24924800	-1.37921500
N	-5.10290900	-0.88815000	0.68586400
N	2.19562500	1.25666100	-1.47626000
N	3.59069300	1.58337500	0.72650200
O	-3.29799600	0.75591100	1.09884600
O	4.10291600	-0.30830600	-1.13186800
P	-3.49351800	-0.61486700	0.25586900
P	2.93682400	0.37906900	-0.23078500
Cl	-0.27127300	-0.70615700	-0.62130000
Cl	0.27933900	-3.13960500	1.54284300
Cl	-3.25134400	-3.47499500	1.85709900
Cl	3.38480100	-1.70877500	2.26620200
Pd	-1.82053700	-2.03713600	0.70679100
Pd	1.66147700	-1.18510600	0.77633800



VIIa (+2.1 vs. Va)

C	-4.78498100	-2.23879300	-1.11074000
C	-4.28485000	-3.45259700	-1.60937900
H	-3.25844000	-3.48477200	-1.97727900
C	-5.07680000	-4.60051000	-1.62487100
H	-4.66726000	-5.53557900	-2.01436600
C	-6.38249100	-4.55216200	-1.12605900
H	-7.00781300	-5.44806500	-1.12515700
C	-6.88169300	-3.35441700	-0.61432200
H	-7.89465200	-3.31895500	-0.20664800
C	-6.10426700	-2.18175600	-0.59580000
C	-6.68183800	-0.92808900	-0.04965900
C	-7.97108200	-0.50328800	-0.41709400
H	-8.53295400	-1.08654500	-1.15025100
C	-8.52940300	0.65531200	0.12612200
H	-9.52986600	0.97004500	-0.18058600
C	-7.80815800	1.41402800	1.05455200
H	-8.24054700	2.32214400	1.48119100
C	-6.52598100	1.00912300	1.43046200
H	-5.94431500	1.58421000	2.15192700
C	-5.96456000	-0.15015600	0.88428700
C	-3.41099500	-0.64579900	-2.46807100
H	-2.34474500	-0.39995600	-2.37537400
H	-3.95254300	0.23049900	-2.85804000
H	-3.49853600	-1.46715900	-3.18936800
C	-4.61851300	-1.38980300	2.53780700
H	-4.95691800	-0.79553200	3.40060800
H	-3.59349300	-1.72479300	2.73352000
H	-5.26950500	-2.27317000	2.42929100
C	-2.60807200	2.26575300	0.33400700
H	-1.65357400	1.85597700	0.69494100
C	-2.32700500	3.31510500	-0.74837700
H	-3.30373600	3.75405100	-1.02786700

C	-1.48616100	4.43424100	-0.10063900	H	1.23247400	2.70985100	1.21798200
H	-1.29037200	5.22655800	-0.83851100	H	3.44019300	-2.30498300	0.94812400
H	-0.50031100	4.02884800	0.18639100	C	5.29595300	-2.92763700	0.03921100
C	-2.16697700	5.03681700	1.13398300	C	5.02905800	-1.58146600	2.20539100
H	-3.09271100	5.55536900	0.82102300	H	2.58095700	1.51524200	-3.92538900
H	-1.51676100	5.80441800	1.58744600	C	2.17912200	3.63293400	-3.74210500
C	-2.53097300	3.97317200	2.17966100	C	2.87125000	4.64697700	-1.66144800
H	-1.59200800	3.50924000	2.53657900	C	5.05396500	4.31141400	0.46849900
C	-3.35635200	2.85972900	1.52082500	C	5.40934700	3.20314000	2.59339700
H	-3.56200900	2.06474100	2.25119700	H	4.20770500	1.42826200	2.92738000
H	-4.32389700	3.26068800	1.17057400	H	6.26466700	-2.43119800	-0.15810200
C	-1.72099000	2.72098100	-2.04351400	C	5.57073700	-4.16140400	0.91945500
H	-2.48525100	2.03123300	-2.43335400	C	4.65648900	-3.27112500	-1.33340400
C	-1.49648400	3.79255600	-3.11783100	C	5.30074200	-2.82956300	3.05454700
H	-0.65886400	4.45915600	-2.86001200	H	4.32310100	-0.91070600	2.72112900
H	-2.39598900	4.41350200	-3.26540600	H	5.96841200	-1.01819000	2.06311500
H	-1.24638500	3.32277300	-4.08254700	H	1.69488400	3.70394400	-4.71869200
C	-0.44949600	1.90052300	-1.81262800	C	2.26546000	4.75607800	-2.91380100
H	-0.07865600	1.46467600	-2.75056900	H	2.93669000	5.52179900	-1.01030700
H	-0.62608600	1.05772600	-1.13006400	H	5.30045200	5.11233900	-0.23241800
H	0.36941700	2.50785700	-1.39705300	C	5.70481200	4.24037400	1.70194600
C	-3.25594700	4.56880200	3.38694000	H	5.91997800	3.14070700	3.55726100
H	-2.64912600	5.35002100	3.87300600	H	6.21762000	-4.86554600	0.37248300
H	-3.47836100	3.79464400	4.13910600	H	4.62297600	-4.69339900	1.10824200
H	-4.21251500	5.02779700	3.08273200	C	6.19665500	-3.79670400	2.26803900
N	-3.97691400	-1.06119300	-1.17669000	H	4.29040600	-2.32308900	-1.75537700
N	-4.66398600	-0.58170600	1.31584500	C	5.69616200	-3.82030800	-2.31772100
O	-3.37137500	1.17735100	-0.25284100	C	3.44487500	-4.20995300	-1.23937400
P	-3.39806800	-0.36618600	0.24693700	H	4.33178600	-3.33682800	3.22555300
Cl	-0.90755100	-2.41870500	-0.95308300	C	5.89344200	-2.45886000	4.41483700
Cl	1.05516100	-1.63269400	1.57047400	H	1.85614400	5.71521900	-3.23949500
Cl	1.55565600	-0.97035200	-3.11736600	H	6.45160500	4.99347500	1.96499500
Cl	-1.61078500	0.23762100	2.92788200	H	7.18337000	-3.32275900	2.10860800
Pd	1.35918200	-1.17119400	-0.79355800	H	6.37750800	-4.70929200	2.86091800
Pd	-1.39936700	-1.06145300	0.99409200	H	6.12332900	-4.77463600	-1.96659200
P	3.11853300	0.16404200	-0.40767600	H	6.52881400	-3.11170300	-2.45949700
N	3.86316600	1.04150900	-1.64702600	H	5.24091100	-4.00702500	-3.30372200
N	2.76587900	1.37575600	0.69284600	H	2.91316600	-4.23976500	-2.20304000
O	4.41755500	-0.67146000	0.07881900	H	2.71824000	-3.87911100	-0.48073400
C	3.28870400	2.28891400	-2.04875300	H	3.74596000	-5.24056000	-0.99110600
C	4.76304400	0.37413300	-2.59857700	H	6.06014400	-3.35436400	5.03504900
C	3.80424800	2.31448800	1.01019700	H	5.22686300	-1.77987700	4.97111700
C	1.46677200	1.63921400	1.32221600	H	6.86471800	-1.94950900	4.29209900
C	4.46041300	-1.91482000	0.83040200				
C	2.68268600	2.40736800	-3.30776800				
C	3.40133600	3.42542500	-1.20953800				
H	4.21782200	-0.25492600	-3.31863300				
H	5.47839700	-0.24760000	-2.04620300				
H	5.32107200	1.14858600	-3.14269800				
C	4.09547100	3.35148900	0.09918400				
C	4.45844400	2.24183500	2.24465800				
H	1.46460300	1.36576400	2.38720700				
H	0.67600600	1.07042000	0.82821200				

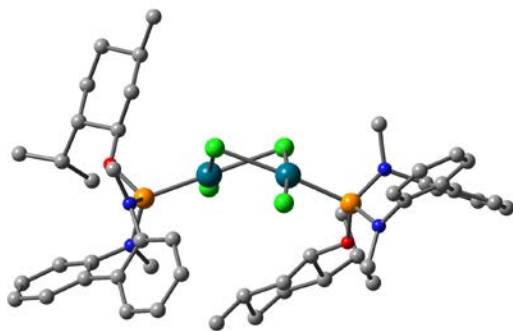


VIIf (+0.8 vs. Va)

C	-5.91682300	0.47846000	-1.44084300
C	-5.94170300	1.00653100	-2.73968300
H	-5.18147200	1.73685600	-3.02022000
C	-6.90403300	0.58430100	-3.65854900
H	-6.90873600	1.00063900	-4.66878800
C	-7.84664400	-0.37983300	-3.28708500
H	-8.59809300	-0.72122900	-4.00307000
C	-7.81894000	-0.91761400	-1.99914300
H	-8.54445800	-1.68289700	-1.71324000
C	-6.86315300	-0.50348600	-1.05500300
C	-6.86212200	-1.07535800	0.31449200
C	-8.04842400	-1.19016700	1.05878500
H	-8.98491000	-0.83276500	0.62416300
C	-8.03878600	-1.72802900	2.34797600
H	-8.97194200	-1.79935500	2.91211000
C	-6.83825400	-2.16254200	2.91964200
H	-6.82601400	-2.57687100	3.93050100
C	-5.64960400	-2.06217900	2.19252500
H	-4.70086000	-2.39684200	2.61514200
C	-5.65941700	-1.52851900	0.90018700
C	-4.95083700	2.43952500	-0.26752900
H	-4.26353600	2.94982100	-0.95929600
H	-4.64378100	2.64626000	0.76553000
H	-5.96800500	2.82921000	-0.41197900
C	-4.19098900	-2.67227400	-0.70108000
H	-3.98956200	-3.55114200	-0.06964600
H	-3.32094800	-2.50586500	-1.34727700
H	-5.06664800	-2.87704300	-1.33936400
C	-2.15338400	0.56164900	2.17708400
H	-1.33547400	0.25605800	1.51023800
C	-1.86125500	1.96737300	2.71044700
H	-2.77327600	2.28313900	3.25099900
C	-0.70741100	1.90330400	3.72795700
H	-0.54781000	2.90181300	4.16499500
H	0.22357000	1.64454800	3.20075100
C	-0.93868100	0.86505700	4.82879700

H	-1.82677200	1.14213100	5.42771500
H	-0.08079100	0.85551300	5.52257900
C	-1.14885800	-0.53509400	4.23577200
H	-0.24122000	-0.79631300	3.66073000
C	-2.32900900	-0.49793400	3.25659900
H	-2.45029800	-1.47535900	2.76292400
H	-3.26351700	-0.28405500	3.80549300
C	-1.62020600	2.97967000	1.55869000
H	-2.39059400	2.77455600	0.80117400
C	-1.82302400	4.42700700	2.02228500
H	-1.08380000	4.71418400	2.78877400
H	-2.82752100	4.57629600	2.45154500
H	-1.70821500	5.12683900	1.17867900
C	-0.26552100	2.82186400	0.85675900
H	-0.24835000	3.40411000	-0.07434700
H	-0.05231100	1.77873900	0.57729300
H	0.56683400	3.17932300	1.48208400
C	-1.35340600	-1.60179000	5.31182700
H	-0.49202200	-1.64584100	5.99790700
H	-1.47964800	-2.60077900	4.86364700
H	-2.25306500	-1.38681600	5.91437800
N	-4.98319700	0.98693400	-0.48211600
N	-4.44360000	-1.49337200	0.13465800
O	-3.39348800	0.62830600	1.41463800
P	-3.69044000	-0.00599100	-0.04219300
Cl	0.52201600	-0.29046300	-2.28382400
Cl	-0.99129000	-1.99591400	0.09284600
Cl	1.96238400	-1.73072400	2.01843000
Cl	-2.36666800	1.73427400	-2.52622800
Pd	1.31045200	-0.86967600	-0.06443000
Pd	-1.79635100	-0.12974400	-1.23311900
P	3.24397200	0.24208100	-0.29099600
N	3.41544700	1.31489900	-1.58641900
N	3.65657800	1.22628700	0.99729800
O	4.47054400	-0.74889500	-0.64975400
C	2.88631400	2.64049200	-1.45358900
C	3.73699100	0.85903900	-2.94424800
C	4.83691100	2.03474100	0.86730300
C	2.88604100	1.43597900	2.22493300
C	4.65997100	-2.13761400	-0.25821800
C	1.75644000	3.02279200	-2.18961800
C	3.55851100	3.58878500	-0.64319600
H	2.84813000	0.52606400	-3.50161700
H	4.45578600	0.03304700	-2.89056900
H	4.20647200	1.69396000	-3.48438000
C	4.78576800	3.22111300	0.10420700
C	6.00038300	1.67725200	1.55688300
H	3.42126100	1.03947800	3.10176700
H	1.91949000	0.92999100	2.15895100
H	2.71337800	2.51482200	2.36335200
H	3.78371900	-2.47394600	0.31371600
C	4.80333400	-2.98270100	-1.53015900
C	5.89216100	-2.17046500	0.63995400

H	1.23663000	2.27614500	-2.78892500
C	1.28194600	4.33381400	-2.13249300
C	3.05679500	4.90116600	-0.59291400
C	5.92978700	4.03757300	0.06923300
C	7.12801700	2.49955000	1.50745200
H	6.00610100	0.75069300	2.13392500
H	5.61986500	-2.51395000	-2.11112100
C	5.25660300	-4.40446400	-1.14852600
C	3.52563800	-2.95408300	-2.41146600
C	6.33019400	-3.59669000	0.99695100
H	5.67531700	-1.59210800	1.55286200
H	6.71457600	-1.65221900	0.11531900
H	0.38855700	4.60652100	-2.69902100
C	1.93120200	5.27575200	-1.32892000
H	3.56019100	5.63378600	0.04238500
H	5.91085900	4.95164400	-0.52876900
C	7.08856000	3.68399300	0.76378100
H	8.03544700	2.21441900	2.04497400
H	5.40834300	-4.99922200	-2.06330600
H	4.45201600	-4.90448900	-0.58320300
C	6.52494100	-4.40854200	-0.29147200
H	3.16020200	-1.91622500	-2.40635000
C	3.83980200	-3.29798900	-3.87241400
C	2.38127100	-3.82866700	-1.87951200
H	5.50715700	-4.06875200	1.56711300
C	7.58073000	-3.59110400	1.87755900
H	1.55729200	6.30054700	-1.26753500
H	7.96793700	4.33085000	0.71563000
H	7.36656500	-3.97583900	-0.86425500
H	6.81197300	-5.44460000	-0.04393900
H	4.22437600	-4.32674800	-3.97366400
H	4.59527800	-2.61395700	-4.29301900
H	2.93334100	-3.22245800	-4.49444700
H	1.44281100	-3.58146500	-2.39906600
H	2.20430300	-3.67431400	-0.80386700
H	2.58206200	-4.90066100	-2.03746800
H	7.87734400	-4.61521700	2.15617400
H	7.41510300	-3.02104400	2.80624300
H	8.43023200	-3.12800600	1.34673200

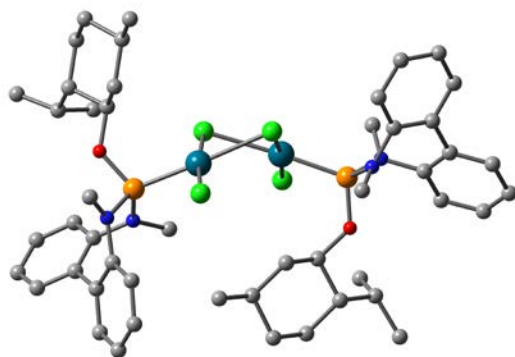


VIIIa (+1.3 vs. Va)

C	-4.81903700	1.98755000	0.92720400
C	-6.04211900	1.62624900	1.50984600
H	-6.12824000	0.66073700	2.00881600
C	-7.13831100	2.48816800	1.46287200
H	-8.08522600	2.18699400	1.91706400
C	-7.01798400	3.72817000	0.82757800
H	-7.87201500	4.40773900	0.77727200
C	-5.80230000	4.09504500	0.25048500
H	-5.71150100	5.05825500	-0.25666800
C	-4.68316600	3.24284200	0.28964900
C	-3.39709500	3.66653500	-0.30994100
C	-2.89504600	4.96440700	-0.10815200
H	-3.45698300	5.65875600	0.52064700
C	-1.68367400	5.36465600	-0.67453300
H	-1.30856600	6.37519500	-0.49571600
C	-0.93961500	4.46115000	-1.44076800
H	0.02890800	4.74463400	-1.85879200
C	-1.42405800	3.17069400	-1.66013700
H	-0.84279100	2.46213100	-2.24896900
C	-2.65284900	2.77490300	-1.11366800
C	-3.33558500	0.76958900	2.45226500
H	-3.29791900	1.70131100	3.03386700
H	-2.35863600	0.28441200	2.49237300
H	-4.06511200	0.08655800	2.91467300
C	-3.54838900	1.27100200	-2.84779800
H	-4.28358600	2.02768300	-3.16621800
H	-3.99699600	0.27923300	-2.96982200
H	-2.65742000	1.33749100	-3.48856300
C	-4.38380700	-2.13551400	-0.88477500
H	-3.75896500	-2.50426100	-0.05744700
C	-5.82393800	-2.61681700	-0.68062000
H	-6.40141200	-2.25557600	-1.55278900
C	-5.81909500	-4.15702600	-0.73289900

H	-5.24523400	-4.55006200	0.12449000
H	-6.84660700	-4.53589500	-0.62096400
C	-5.20760400	-4.69131300	-2.03394800
H	-5.84567000	-4.39342500	-2.88703700
H	-5.19615300	-5.79437200	-2.02160500
C	-3.78774200	-4.15608000	-2.27253300
H	-3.14801500	-4.51746200	-1.44462700
C	-3.79712300	-2.62208200	-2.20489300
H	-2.77501900	-2.22828800	-2.32516300
H	-4.40149800	-2.21612100	-3.03627300
C	-6.49424700	-2.00594200	0.57413900
H	-6.41935900	-0.91634300	0.43487400
C	-7.98819000	-2.34496900	0.64873800
H	-8.50350300	-2.11027500	-0.29728500
H	-8.47701300	-1.76676600	1.44972500
H	-8.15660500	-3.41214700	0.86815500
C	-5.78844000	-2.35133900	1.89249700
H	-5.85739700	-3.42796800	2.11913900
H	-6.26145600	-1.81464100	2.73179500
H	-4.72115600	-2.08283500	1.88626800
C	-3.19030600	-4.65514300	-3.58878100
H	-3.16077400	-5.75629300	-3.62131700
H	-2.16233800	-4.28286300	-3.72678100
H	-3.79120500	-4.30951000	-4.44744200
N	-3.68692400	1.10589100	1.06668500
N	-3.21727200	1.49570100	-1.43784400
O	-4.37987000	-0.67970700	-0.84947400
P	-3.17460500	0.26085600	-0.29922000
Cl	1.06024200	-2.05018200	-0.29785500
Cl	-0.51833600	-0.14252800	-2.39041800
Cl	-1.81221500	-2.06659900	1.75680500
Cl	2.19637200	2.09101400	-2.33102900
Pd	-1.24507000	-0.90560600	-0.19316200
Pd	1.76457600	0.02279800	-1.31995000
P	3.65187400	0.10012100	-0.09845600
N	4.52828100	-1.32308600	-0.18749500
N	4.85035600	1.26149100	-0.35737900
O	3.32785700	0.41892100	1.45902500
C	5.74471100	-1.41212700	0.57068200
C	4.31518300	-2.38881400	-1.17217500
C	5.83629500	1.01358400	-1.36422800
C	4.66329500	2.65018900	0.07853600
C	2.00772000	0.49460700	2.06688300
C	5.78432600	-2.20992700	1.71880200
C	6.90227600	-0.74659800	0.11186300
H	5.19459100	-2.46804800	-1.83234500
H	4.15314000	-3.35368300	-0.66726400
C	6.86453800	0.06709900	-1.12909400
C	5.82921000	1.76255600	-2.55000600
H	5.65313300	3.11780900	0.18178700
H	4.17393100	2.65414800	1.06017500
H	4.05138700	3.23325900	-0.62612500
H	1.36628700	-0.26625700	1.60160500

C	2.13105100	0.18166600	3.56159400
C	1.40521500	1.87528900	1.82853100
H	4.87171400	-2.71637400	2.03548200
C	6.97490700	-2.35190400	2.43476400
C	8.09139600	-0.90279700	0.84544500
C	7.86659500	-0.08611500	-2.10369200
C	6.83775200	1.59698300	-3.50055100
H	5.00897600	2.46015500	-2.72314400
H	2.70347400	1.01419400	4.01359500
C	0.70598500	0.22275000	4.14977100
C	2.92811100	-1.11015100	3.86536900
C	-0.00189500	1.97025000	2.43117500
H	1.36612800	2.08721800	0.74741700
H	2.06256600	2.63645400	2.28591400
H	6.99944500	-2.97080000	3.33474600
C	8.12896400	-1.69382400	1.99584200
H	8.99235600	-0.38189500	0.51307200
H	8.65554600	-0.82311700	-1.93620500
C	7.86149500	0.67103400	-3.27623500
H	6.81594700	2.18397500	-4.42191200
H	0.09374300	-0.57003600	3.68623700
H	0.74013100	0.00711200	5.22853100
C	0.03069400	1.57897800	3.91497500
H	3.91666200	-0.95712800	3.40291500
C	3.15992000	-1.29246500	5.37105100
C	2.32450300	-2.37649500	3.24583100
H	-0.62150300	1.22955100	1.89602100
C	-0.61861400	3.34757300	2.20486200
H	9.06275300	-1.79304500	2.55465300
H	8.65067600	0.52992300	-4.01860300
H	0.57672000	2.36248300	4.47325000
H	-0.99536900	1.56645800	4.31963200
H	3.56531400	-0.37695300	5.83314000
H	3.87809700	-2.10794800	5.55526700
H	2.22892500	-1.55290700	5.90089200
H	1.30414300	-2.56858000	3.61509500
H	2.93551900	-3.25754200	3.50368000
H	2.27120900	-2.31725300	2.14990200
H	-1.64373100	3.39963300	2.60375400
H	-0.66632100	3.58777100	1.13457300
H	-0.02363100	4.13179900	2.70380500
H	3.43566100	-2.17103700	-1.78962000

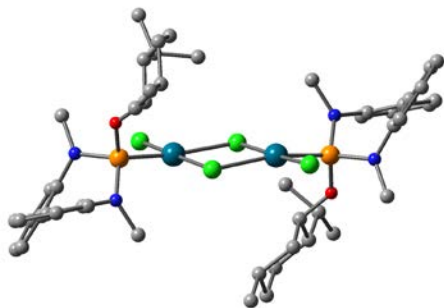


VIIIb (+1.6 vs. Va)

C	-4.39556800	1.92745700	1.13459700
C	-4.87796100	1.66340800	2.42227800
H	-4.34630100	0.94473200	3.04643600
C	-6.01917500	2.31217400	2.89510200
H	-6.39269800	2.09504600	3.89858600
C	-6.68336000	3.23005800	2.07368000
H	-7.58466700	3.73454000	2.43014900
C	-6.19698300	3.50183400	0.79417100
H	-6.72161500	4.21437800	0.15362400
C	-5.04365900	2.86349700	0.30140800
C	-4.50367600	3.19822000	-1.03904000
C	-4.39965700	4.54529400	-1.43167600
H	-4.68787900	5.32356200	-0.72130100
C	-3.93091500	4.90120100	-2.69627300
H	-3.85678500	5.95538100	-2.97353100
C	-3.54552100	3.90337900	-3.59668100
H	-3.16260000	4.16863000	-4.58501100
C	-3.62878700	2.56200200	-3.22563300
H	-3.29553100	1.77935300	-3.90635100
C	-4.10541100	2.19678000	-1.95767600
C	-1.95672600	1.67361700	1.37893600
H	-1.92283100	2.77073400	1.44682300
H	-1.07912500	1.33504200	0.81820900
H	-1.89755000	1.24071800	2.38888100
C	-4.96027700	-0.02377400	-2.63396600
H	-5.76672900	0.56565100	-3.09167200
H	-5.40564800	-0.89239800	-2.13387900
H	-4.27355000	-0.37477800	-3.41981300
C	-4.14980800	-2.43091900	0.39358900
H	-3.19469800	-2.49680900	0.93221500
C	-5.28086800	-2.87966400	1.32601800
H	-6.21381100	-2.82728900	0.73310900
C	-5.04245100	-4.35935000	1.68606100

H	-4.11682900	-4.44690500	2.28130200
H	-5.86075200	-4.72135400	2.32708600
C	-4.92436700	-5.25035100	0.44400800
H	-5.88972100	-5.25614400	-0.09602900
H	-4.72684200	-6.29342800	0.74407000
C	-3.82791200	-4.76486500	-0.51535200
H	-2.86119300	-4.82321400	0.02063900
C	-4.06868900	-3.28940700	-0.86437400
H	-3.26170500	-2.91753900	-1.51742700
H	-5.01336700	-3.19081600	-1.42859500
C	-5.47715700	-1.93823800	2.54066400
H	-5.66502000	-0.94217900	2.10967400
C	-6.71865500	-2.31331300	3.35990300
H	-7.60685800	-2.43065700	2.71719100
H	-6.94269000	-1.52966600	4.10179200
H	-6.57737400	-3.25600000	3.91382700
C	-4.24168100	-1.81892100	3.44316100
H	-3.96567800	-2.78821900	3.88930400
H	-4.44280600	-1.12730600	4.27770300
H	-3.36241000	-1.43779500	2.90231100
C	-3.72878500	-5.62904800	-1.77302200
H	-3.53003200	-6.68262200	-1.51826200
H	-2.91913800	-5.28009200	-2.43416800
H	-4.67050600	-5.59402100	-2.34727700
N	-3.19131200	1.29100200	0.68336800
N	-4.28310500	0.81490700	-1.63529000
O	-4.38932500	-1.04288400	0.03908900
P	-3.32045600	0.07565000	-0.45987200
Cl	-0.93337800	-1.48644400	1.35897200
Cl	0.96165600	-1.94913600	-1.28215800
Cl	-1.48771700	-0.26088200	-3.20589300
Cl	1.78150400	0.31217700	2.81881600
Pd	-1.32835900	-0.84518100	-0.94992800
Pd	1.50440300	-0.85973000	0.81068000
P	3.56023600	-0.23835200	0.17147800
N	4.75407200	-0.66124600	1.26041200
N	4.19037200	-0.82628500	-1.28476100
O	3.65964200	1.34359200	-0.15088900
C	6.11032400	-0.32462700	0.93180600
C	4.57909700	-1.54937600	2.41440100
C	4.85338900	-2.09368100	-1.29540400
C	3.74523100	-0.28590500	-2.57575800
C	2.68345100	2.38558900	0.13154800
C	6.74575600	0.72074900	1.60995900
C	6.80555400	-1.09435700	-0.02504700
H	5.20340200	-2.44881000	2.28492500
H	4.86942100	-1.03682000	3.34435400
C	6.13945900	-2.22776400	-0.71426000
C	4.26812300	-3.18345700	-1.95721200
H	4.52324300	-0.49268000	-3.32439600
H	3.62765000	0.80094800	-2.48897600
H	2.79160600	-0.72062300	-2.91133700
H	2.25963800	2.19898100	1.12846500

C	3.42921000	3.72452800	0.13188500
C	1.56217300	2.35200200	-0.89939400
H	6.17754600	1.28610400	2.34966500
C	8.08179100	1.02371800	1.33979900
C	8.15027000	-0.77447800	-0.28323700
C	6.79339400	-3.46847300	-0.81735300
C	4.93917900	-4.40338700	-2.05248100
H	3.27333800	-3.06612400	-2.38800700
H	3.82198800	3.86289400	-0.89353500
C	2.40562500	4.84880800	0.38766800
C	4.65589600	3.73028800	1.07868700
C	0.53644100	3.45909500	-0.62662400
H	1.06768200	1.36685900	-0.88576000
H	1.98836400	2.48117000	-1.91006900
H	8.57201300	1.84565500	1.86678900
C	8.78238100	0.27411100	0.38838400
H	8.69828800	-1.34945200	-1.03327300
H	7.77831500	-3.58336700	-0.38755200
C	6.20631600	-4.54771700	-1.47929600
H	4.46576900	-5.24320500	-2.56666600
H	2.00121300	4.75004400	1.41033500
H	2.91141900	5.82549400	0.34519900
C	1.24415500	4.82058300	-0.61388400
H	5.30421400	2.91593400	0.71799500
C	5.46244200	5.02994000	0.96398500
C	4.31401600	3.42301500	2.54318200
H	0.13905000	3.29220100	0.39062300
C	-0.62945900	3.39451800	-1.60972800
H	9.82560700	0.50986900	0.16446600
H	6.73538900	-5.50162800	-1.54145900
H	1.62689900	5.03350300	-1.62947900
H	0.52026500	5.61894200	-0.37722600
H	5.68377500	5.27716300	-0.08760100
H	6.42313100	4.93680100	1.49608900
H	4.92715900	5.88684100	1.40520000
H	3.63773100	4.18088200	2.97190600
H	5.22972500	3.42536300	3.15733800
H	3.83513300	2.43929800	2.66403400
H	-1.40617800	4.13727200	-1.37183100
H	-1.10172000	2.40096600	-1.60721900
H	-0.28717700	3.58471200	-2.64084700
H	3.53148900	-1.85748500	2.50447200

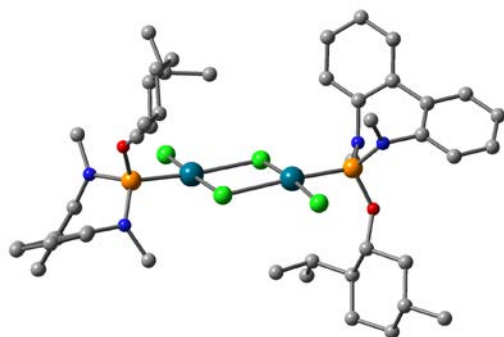


TS_Va-Vb (+6.9 vs. Va)

C	-4.53725700	0.74728700	-1.79267600
C	-4.07343200	1.98508800	-2.24798300
H	-2.99744200	2.16624000	-2.25869600
C	-4.97337100	2.95927200	-2.68258600
H	-4.60570000	3.92892700	-3.02618600
C	-6.34565300	2.68768100	-2.66235400
H	-7.05975000	3.44833500	-2.98689600
C	-6.80901500	1.44337100	-2.22923700
H	-7.88152400	1.23619900	-2.21788300
C	-5.91706300	0.44741500	-1.79335000
C	-6.39974600	-0.90597500	-1.41337500
C	-7.31533800	-1.57307500	-2.24752000
H	-7.65172900	-1.07779300	-3.16138600
C	-7.78427000	-2.85088600	-1.93947300
H	-8.49373700	-3.34590500	-2.60680700
C	-7.32897200	-3.49704200	-0.78601700
H	-7.67386100	-4.50526300	-0.54439800
C	-6.41645800	-2.85788300	0.05406300
H	-6.02974100	-3.36186800	0.94047400
C	-5.95602900	-1.56574300	-0.23990700
C	-3.06867500	-1.11230700	-2.44545400
H	-3.90030900	-1.58075600	-2.99733900
H	-2.44194000	-1.90713400	-2.02184100
H	-2.45598000	-0.52344600	-3.14538100
C	-5.51666500	-0.86269000	2.09511400
H	-6.57811900	-0.57781800	2.14160700
H	-4.92948800	-0.10342500	2.62586400
H	-5.36841300	-1.83236400	2.59221000
C	-2.09104900	1.45029300	1.49958200
H	-1.42399400	1.50502300	0.62412100
C	-2.47203000	2.88221200	1.92118700
H	-3.08532300	2.79496700	2.83805400
C	-1.16099900	3.59700000	2.31753800

H	-1.38423400	4.61830500	2.65749000
H	-0.51885900	3.69738400	1.42565500
C	-0.39356800	2.85963600	3.41994600
H	-0.98816800	2.87255800	4.35255800
H	0.54746100	3.39207600	3.64151600
C	-0.09501700	1.40320400	3.04910000
H	0.56699300	1.40870000	2.16271800
C	-1.39248600	0.70502200	2.63194800
H	-1.16877500	-0.32835100	2.32492300
H	-2.08356300	0.63748000	3.49058400
C	-3.32771700	3.62079100	0.84758800
H	-3.01946200	3.22412400	-0.13302100
C	-4.82741400	3.32751900	1.01266900
H	-5.03718000	2.25156100	1.00723900
H	-5.40590700	3.78792600	0.19593700
H	-5.19596200	3.74598600	1.96556100
C	-3.11704700	5.14077400	0.80620800
H	-3.38915800	5.61034000	1.76670700
H	-3.76036600	5.58645400	0.03000600
H	-2.07957900	5.42081000	0.57649300
C	0.60831900	0.63814500	4.17017400
H	1.51577900	1.16479200	4.50592000
H	0.90558400	-0.36876000	3.83846500
H	-0.05570500	0.52976300	5.04419800
C	1.58447300	2.52602100	-1.24771100
C	0.20564800	2.68170800	-1.47737100
H	-0.38646800	1.80247300	-1.73287500
C	-0.40238100	3.93170400	-1.38259100
H	-1.47239600	4.03182800	-1.57189000
C	0.35415600	5.04845200	-1.01491900
H	-0.11720000	6.02901800	-0.91903300
C	1.71657500	4.90120200	-0.76167100
H	2.30800700	5.76991000	-0.46409900
C	2.36127400	3.65555600	-0.88731700
C	3.83106400	3.57731800	-0.69856500
C	4.67621700	4.54031600	-1.28245000
H	4.23768500	5.31984200	-1.90941400
C	6.05697200	4.50401000	-1.08744400
H	6.69141600	5.25978600	-1.55660600
C	6.62625200	3.49786200	-0.29870300
H	7.70699200	3.46150300	-0.14306100
C	5.80646300	2.52988400	0.28156400
H	6.23218300	1.73517800	0.89525100
C	4.42006000	2.56361200	0.08458700
C	1.99275200	0.59769200	-2.77533200
H	1.16381500	1.07944300	-3.30716900
H	1.73713700	-0.46340300	-2.64928700
H	2.90231900	0.67398600	-3.39114800
C	3.42367100	1.71331400	2.17580600
H	4.40368000	1.71488500	2.67745700
H	2.85086000	0.86883300	2.56693100
H	2.89752000	2.65257000	2.41147300
C	4.88059100	-1.48897200	-0.79040800

H	4.23738600	-2.17620100	-0.22212400
C	5.32009400	-2.17632600	-2.08715800
H	5.98803500	-2.46808000	-2.61362800
C	6.16319800	-3.40945100	-1.70442300
H	6.52863000	-3.90642200	-2.61557800
H	5.52327500	-4.14286400	-1.18302600
C	7.35055200	-3.04905200	-0.80446700
H	8.05120700	-2.40256200	-1.36590500
H	7.91158200	-3.96043300	-0.53645100
C	6.91038100	-2.31091200	0.46707000
H	6.25993400	-2.99207700	1.04734300
C	6.06057600	-1.09138500	0.08774000
H	5.67793400	-0.60641200	0.99797800
H	6.67723300	-0.35499500	-0.45731100
C	4.14415300	-2.47550300	-3.05238300
H	3.72643500	-1.49270700	-3.31647800
C	4.62636000	-3.11778300	-4.36007400
H	4.94983800	-4.16065900	-4.21036800
H	5.47366200	-2.56209800	-4.79525600
H	3.81504300	-3.13292000	-5.10561600
C	3.00870700	-3.29721600	-2.42674000
H	2.21008000	-3.47239700	-3.16563500
H	2.54489300	-2.78808800	-1.56803300
H	3.35741800	-4.28391300	-2.08106800
C	8.09444600	-1.91411500	1.34958800
H	8.68713200	-2.79546000	1.64370200
H	7.75519900	-1.41132800	2.26984200
H	8.76671300	-1.22069100	0.81514900
N	-3.59126000	-0.24924800	-1.37921500
N	-5.10290900	-0.88815000	0.68586400
N	2.19562500	1.25666100	-1.47626000
N	3.59069300	1.58337500	0.72650200
O	-3.29799600	0.75591100	1.09884600
O	4.10291600	-0.30830600	-1.13186800
P	-3.49351800	-0.61486700	0.25586900
P	2.93682400	0.37906900	-0.23078500
Cl	-0.27127300	-0.70615700	-0.62130000
Cl	0.27933900	-3.13960500	1.54284300
Cl	-3.25134400	-3.47499500	1.85709900
Cl	3.38480100	-1.70877500	2.26620200
Pd	-1.82053700	-2.03713600	0.70679100
Pd	1.66147700	-1.18510600	0.77633800

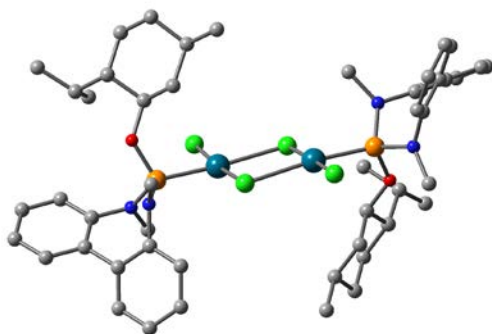


TS_VIIa-VIIb (+6.6 vs. Va)

C	-4.18137500	-1.97224100	-1.81326800
C	-3.18519800	-2.64543600	-2.53481900
H	-2.30198700	-2.09203200	-2.85554700
C	-3.31400100	-4.00532800	-2.82354300
H	-2.52594200	-4.51746400	-3.38077100
C	-4.44293400	-4.70618900	-2.38780300
H	-4.54765400	-5.77216300	-2.60366200
C	-5.43545800	-4.04284000	-1.66400900
H	-6.31062300	-4.59265200	-1.30964100
C	-5.32790700	-2.67365400	-1.36435300
C	-6.39778100	-1.98277200	-0.60244600
C	-7.75314300	-2.14402800	-0.93519300
H	-8.02013500	-2.77838300	-1.78372300
C	-8.75268100	-1.48577000	-0.21448400
H	-9.80013800	-1.61805500	-0.49632200
C	-8.41406100	-0.65121000	0.85583500
H	-9.19290600	-0.12927400	1.41677000
C	-7.07170400	-0.48475700	1.20569300
H	-6.78166300	0.15604500	2.04028600
C	-6.07108700	-1.14687800	0.48818800
C	-3.97633400	0.29788600	-2.77776700
H	-2.97095100	0.28849600	-3.22499500
H	-4.23347000	1.32740000	-2.50273500
H	-4.70658900	-0.05336900	-3.52207300
C	-4.22801900	-2.05257600	1.83143200
H	-4.75294100	-1.95831000	2.79424400
H	-3.15432800	-1.93936200	2.01505600
H	-4.41697500	-3.05569900	1.41301500
C	-4.00615100	2.64124800	0.63087400
H	-3.17824400	2.40414200	1.31383400
C	-3.56940300	3.72917100	-0.35927900
H	-4.40334700	3.82975900	-1.07927200
C	-3.43332200	5.06905700	0.38871700
H	-3.16653000	5.86272300	-0.32722800

H	-2.59637900	5.00283300	1.10442800
C	-4.70056700	5.44747500	1.15954600
H	-5.54042200	5.59069700	0.45400100
H	-4.55604300	6.41105900	1.67702100
C	-5.08211300	4.35978700	2.17342200
H	-4.24216800	4.25978100	2.88743700
C	-5.23813400	3.01785100	1.44697400
H	-5.44023900	2.20843900	2.16701900
H	-6.10358400	3.06709100	0.76222700
C	-2.30047600	3.34159600	-1.16727400
H	-2.39908100	2.27838200	-1.42902400
C	-2.22217300	4.10763900	-2.49346200
H	-2.13029200	5.19464200	-2.33025800
H	-3.11906000	3.93545100	-3.11114900
H	-1.34455300	3.78591400	-3.07712600
C	-0.98673600	3.47977700	-0.38407000
H	-0.17284600	2.96732500	-0.92060300
H	-1.04481800	3.02369900	0.61599500
H	-0.69789400	4.53581400	-0.25791400
C	-6.34243100	4.71516700	2.96379000
H	-6.21806300	5.66570100	3.50738400
H	-6.58837100	3.93261300	3.69993100
H	-7.20873400	4.82500900	2.28896900
N	-4.07723700	-0.56019000	-1.59211300
N	-4.69958200	-1.02240500	0.89933500
O	-4.36382000	1.44469000	-0.12032100
P	-3.71598700	-0.03171300	-0.02676400
Cl	-0.75194600	-0.16898800	-1.62065000
Cl	0.86339700	0.33696300	1.27852300
Cl	2.31612600	-0.21345900	-3.21244500
Cl	-2.25404400	0.48939400	2.83450500
Pd	1.68778100	0.03442100	-0.97268700
Pd	-1.58102500	0.06202700	0.63067300
P	3.80895200	-0.03323900	-0.25380200
N	5.11996200	-0.11607800	-1.31769400
N	4.19614600	1.28411600	0.70597000
O	4.10981600	-1.40248400	0.55338600
C	5.65601400	1.10301500	-1.83994500
C	5.40941100	-1.35606300	-2.05063100
C	5.51786500	1.33828300	1.26501700
C	3.43472200	2.53825000	0.74498000
C	3.23472700	-2.21751800	1.38388200
C	5.50460700	1.40673400	-3.20136600
C	6.41130600	1.96426000	-1.00471100
H	5.33033300	-2.20741900	-1.36297800
H	6.44227500	-1.30371500	-2.42304200
H	4.72298300	-1.51367500	-2.89649500
C	6.61058600	1.67897200	0.43860700
C	5.69974200	1.11063900	2.63296700
H	3.22103600	2.82033400	1.78719600
H	2.47974200	2.42252500	0.21813700
H	4.00866400	3.34562000	0.26039300
H	2.23604300	-1.76268200	1.41713800

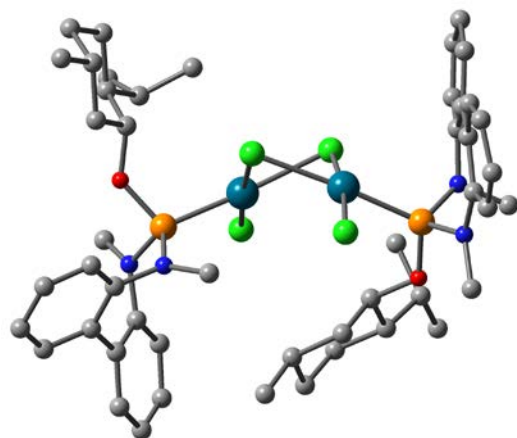
C	3.14063700	-3.62151300	0.77133700
C	3.84187800	-2.20576100	2.78318500
H	4.89401800	0.74851300	-3.81943100
C	6.09814300	2.54513500	-3.74796300
C	6.99270600	3.11023200	-1.57662000
C	7.88365400	1.77398600	1.02777000
C	6.97191300	1.20899900	3.20021900
H	4.82965000	0.86446400	3.24390000
H	4.18466700	-3.96807000	0.65418900
C	2.44104200	-4.56639600	1.76736800
C	2.48560800	-3.61944700	-0.63586300
C	3.13143700	-3.15979500	3.75130000
H	3.81449000	-1.17489700	3.16845400
H	4.90607800	-2.48955300	2.69916100
H	5.96471600	2.76869500	-4.80918900
C	6.84529000	3.40147700	-2.93329300
H	7.56346400	3.78577900	-0.93512900
H	8.74206400	2.02114000	0.39888600
C	8.06532100	1.53913100	2.39227600
H	7.10908300	1.02537500	4.26842500
H	2.41609300	-5.58527100	1.34922500
H	1.38969500	-4.25476800	1.88779500
C	3.10338900	-4.57009900	3.14685100
H	2.88931800	-2.74658600	-1.17203400
C	2.89260900	-4.85402800	-1.44954500
C	0.95687200	-3.46563000	-0.60873000
H	2.08291900	-2.81904800	3.85176100
C	3.77910200	-3.13025200	5.13654100
H	7.30569000	4.30007000	-3.35085900
H	9.06584800	1.61031300	2.82580800
H	4.14030300	-4.94665800	3.06561500
H	2.56925800	-5.25984500	3.82218600
H	2.54103300	-5.78626000	-0.97634600
H	3.98785700	-4.92272000	-1.55507700
H	2.45857000	-4.81433900	-2.46166000
H	0.57842600	-3.21983500	-1.61254600
H	0.62794700	-2.65502000	0.05917900
H	0.46229000	-4.39426100	-0.28069400
H	3.25090800	-3.79579200	5.83830800
H	3.77094700	-2.11341800	5.56174900
H	4.82989400	-3.46329000	5.08367200



TS_VIIIa-VIIIb (+7.9 vs. Va)

C	-5.62089500	-1.15577200	0.32607900
C	-6.75488300	-0.34153000	0.25778400
H	-6.80274000	0.42477100	-0.51798400
C	-7.79835200	-0.51079000	1.16982000
H	-8.67991800	0.13207700	1.11541400
C	-7.70132000	-1.49614100	2.15760700
H	-8.50827000	-1.62747500	2.88254500
C	-6.57039300	-2.31300900	2.22469200
H	-6.49508700	-3.07537400	3.00356900
C	-5.51358400	-2.16293900	1.30997800
C	-4.33581100	-3.06576000	1.34223000
C	-4.52156200	-4.45472200	1.46714100
H	-5.54013200	-4.84579100	1.52142400
C	-3.43888800	-5.33394400	1.50724500
H	-3.61271900	-6.40841500	1.60144400
C	-2.13638200	-4.83397800	1.41510300
H	-1.27909600	-5.50995400	1.43648000
C	-1.92883600	-3.46040600	1.28502000
H	-0.91554300	-3.06737700	1.19989400
C	-3.01216900	-2.56863700	1.25064600
C	-4.80993700	-1.77791800	-1.90325200
H	-5.01252700	-2.83361500	-1.65735400
H	-3.92411000	-1.72819100	-2.54552800
H	-5.66447900	-1.36566300	-2.46104900
C	-1.89870600	-0.60057100	2.23443400
H	-2.28328200	-0.89032300	3.22466700
H	-1.90920100	0.49306700	2.16732900
H	-0.85946200	-0.94727800	2.13505000
C	-3.02786700	-2.44089100	-0.12285400
H	-3.27021700	2.42197500	-1.19567900
C	-3.85243300	3.55207200	0.53929300
H	-3.54056500	3.60873300	1.59933300
C	-3.41954200	4.87773000	-0.12540800
H	-3.70764000	4.86162200	-1.19175800

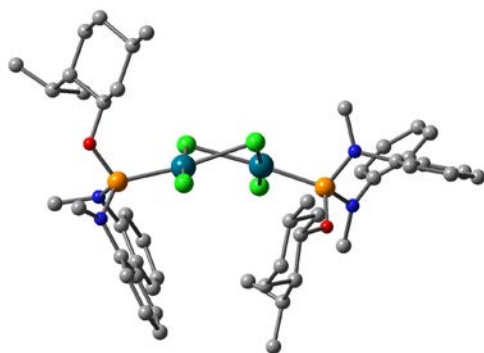
H	-3.96394000	5.71646400	0.33186900	C	4.47494100	-3.29754200	-0.78039800
C	-1.91085700	5.13297400	-0.00998500	H	5.28457300	-3.40715900	-0.03427300
H	-1.64555700	5.26578000	1.05594400	C	3.88318100	-4.69553900	-1.04656300
H	-1.65007900	6.07719100	-0.51719900	H	4.65844700	-5.34843200	-1.47657200
C	-1.07445400	3.98066200	-0.58199200	H	3.08756700	-4.61477800	-1.80702500
H	-1.29038300	3.90673100	-1.66446600	C	3.29261100	-5.33774000	0.21278900
C	-1.53092100	2.66492400	0.05800300	H	4.09409000	-5.50410800	0.95677800
H	-0.97356500	1.82915300	-0.39321100	H	2.87660500	-6.33055500	-0.02860900
H	-1.29782100	2.67073500	1.13755700	C	2.20765500	-4.45391500	0.84438200
C	-5.38288300	3.25003700	0.50943700	H	1.39500700	-4.33554600	0.10207100
H	-5.56115500	2.56599200	-0.34035100	C	2.78401200	-3.06059900	1.12314800
C	-5.80959000	2.52841000	1.79638400	H	1.99758100	-2.39032100	1.50457000
H	-5.21607400	1.62033200	1.96423400	H	3.56482400	-3.12740200	1.90111100
H	-6.87019000	2.23589100	1.75802200	C	5.09216400	-2.62230200	-2.03394200
H	-5.67623000	3.19471500	2.66670900	H	5.35216400	-1.59776900	-1.72670900
C	-6.27560700	4.47934800	0.29063900	C	6.39691700	-3.30779800	-2.45923700
H	-6.14585100	5.22117400	1.09665400	H	6.21981700	-4.33577500	-2.81660900
H	-7.33565100	4.17770200	0.29153800	H	7.11556800	-1.62477600	-1.62477600
H	-6.07753200	4.98241400	-0.66726600	H	6.87696400	-2.75482400	-3.28261200
C	0.43086600	4.19800300	-0.41204500	C	4.12719000	-2.50291000	-3.22253300
H	0.75760900	5.12521300	-0.90911600	H	4.57394300	-1.88015300	-4.01338300
H	1.01161100	3.36639700	-0.84301000	H	3.17230600	-2.02960500	-2.94623500
H	0.70204900	4.28064500	0.65426700	H	3.90111400	-3.48646200	-3.66528900
C	4.37536200	2.61267200	0.75426300	C	1.61306700	-5.07315500	2.11008500
C	4.42787100	3.70451400	-0.12448300	H	1.17963100	-6.06527200	1.90392800
H	4.55229700	3.51186400	-1.18986000	H	0.81920400	-4.43717300	2.53416300
C	4.28708500	5.00835900	0.35280900	H	2.38808300	-5.20172200	2.88478700
H	4.32055700	5.84702000	-0.34667100	N	-4.59169800	-1.01958500	-0.66505400
C	4.08480600	5.23403400	1.71801700	N	-2.77428700	-1.15750500	1.20191900
H	3.96256600	6.25132200	2.09741200	N	4.58378100	1.28216400	0.26492700
C	4.02976200	4.15195400	2.59778400	N	2.48929700	0.54577000	1.66640300
H	3.86076300	4.32432400	3.66336400	O	-3.41369600	1.14974100	0.43938700
C	4.17601700	2.83063900	2.13995900	O	3.99531000	-1.15775700	0.24725700
C	4.13241500	1.69822600	3.09777100	P	-3.14511400	-0.31075900	-0.22067000
C	4.87300500	1.72679700	4.29159700	P	3.23263000	0.27233800	0.17986100
H	5.50899600	2.59015000	4.50065100	Cl	0.22494200	0.14880700	-3.51130900
C	4.82322900	0.66224000	5.19447400	Cl	0.17748600	-1.19120500	-0.50761400
H	5.41458500	0.70187600	6.11249200	Cl	-3.18958700	0.85648600	-3.21414400
C	4.02579200	-0.45364100	4.92030900	Cl	3.20286800	1.73287800	-2.76320800
H	3.98581700	-1.28991000	5.62226800	Pd	-1.60808400	-0.19875500	-1.85589300
C	3.27733800	-0.49645600	3.74142800	Pd	1.79617200	0.31152800	-1.56873100
H	2.64083700	-1.35174500	3.51224900				
C	3.32744400	0.56810300	2.83616300				
C	5.78712300	1.01621400	-0.53544500				
H	6.57065600	1.71676200	-0.21629800				
H	5.61020400	1.14016300	-1.61460000				
H	6.13484600	-0.00645400	-0.33859800				
C	1.20857000	1.24050000	1.81701000				
H	0.66169000	0.81176500	2.66843400				
H	0.60021600	1.11012700	0.91880100				
H	1.35447600	2.31906600	1.99415000				
C	3.39839700	-2.43128700	-0.12205600				
H	2.60168700	-2.25078400	-0.85807200				



t-TS_Va-VIIa (+18.7 vs. Va)

Cl	-1.47833100	-0.82540600	-1.76241500
Cl	0.27161100	-1.95717000	0.74679700
Cl	1.21710500	1.26578500	-2.62489400
Cl	-1.93805400	-0.28177200	2.90186900
Pd	0.85398400	-0.31510900	-0.94309200
Pd	-1.86185300	-0.64180900	0.59789200
P	2.91867200	-0.02884100	-0.10250200
N	4.00987200	1.08057000	-0.75490600
N	2.92182100	0.42009900	1.51142300
O	3.81435100	-1.36147600	-0.33356100
C	4.03188200	2.43350700	-0.29288500
C	4.65725700	0.80581000	-2.04640200
C	4.19465400	0.53998500	2.16257700
C	1.73366400	0.48207800	2.37402200
C	3.42679000	-2.75695700	-0.43853700
C	3.64264400	3.46838200	-1.15607300
C	4.56057600	2.73879800	0.98525700
H	3.96558500	0.92824500	-2.89397500
H	5.05191300	-0.21777200	-2.04681700
H	5.49854300	1.50229100	-2.16336100
C	4.99964200	1.67441200	1.91983900
C	4.60267100	-0.44057600	3.07563400
H	1.54654300	-0.46283200	2.90419300
H	0.84110100	0.71768000	1.78402400
H	1.88615500	1.28654600	3.10591700
H	2.33330600	-2.84088100	-0.38033600
C	3.90158200	-3.29377600	-1.79485900
C	4.04981200	-3.47079800	0.75681900
H	3.20731100	3.20775300	-2.12091100
C	3.79477900	4.80314800	-0.77976900
C	4.69211500	4.09170700	1.34710200

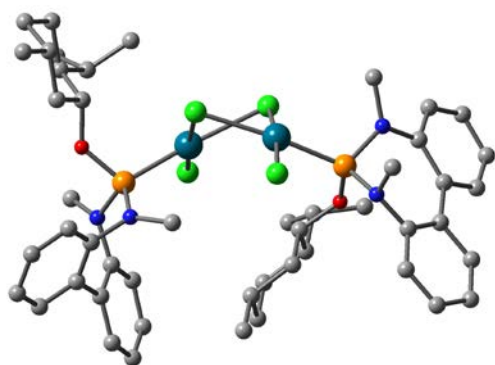
C	6.21963700	1.78194100	2.61269800	H	-4.17741000	1.71655300	3.39945600
C	5.81329700	-0.31167300	3.75743300	H	-4.46253900	2.75193100	1.97593900
H	3.95775000	-1.30416500	3.24717200	C	-2.13281600	3.93598200	-1.15499200
H	4.98320600	-3.06722800	-1.84519600	C	-1.22788400	3.09997000	1.06444200
C	3.74124400	-4.82551300	-1.82401400	C	-5.39819600	-3.35396500	-0.69825300
C	3.21518000	-2.57627800	-2.98844000	C	-4.94665000	-2.76320700	-3.00147100
C	3.88116100	-4.99405200	0.69665800	H	-4.41643000	-0.68451000	-3.27302800
H	3.60043400	-3.06779100	1.67860400	C	-6.01187500	-1.74059300	4.09219200
H	5.12477400	-3.21876300	0.78542500	H	-5.68789200	0.34652900	3.98441000
H	3.48907300	5.59736600	-1.46482900	C	-5.55402600	-2.93956700	2.07762800
C	4.32335700	5.11735200	0.47612600	C	-0.71487200	4.44196300	-1.49087200
H	5.08394500	4.33640400	2.33695600	H	-2.63996500	4.72886700	-0.57213100
H	6.86226200	2.64439500	2.42188000	C	-3.03037100	3.65370500	-2.38636200
C	6.62514900	0.80322100	3.52094900	C	0.17532300	3.64447900	0.76249100
H	6.12519800	-1.08325900	4.46527300	H	-1.17084600	2.21505800	1.71743900
H	4.13256900	-5.21670600	-2.77658200	H	-1.81432800	3.86311700	1.60752200
H	2.66835300	-5.08097700	-1.80144100	C	-5.30125400	-3.71086700	-2.03880200
C	4.42595400	-5.51415000	-0.64090300	H	-5.71022300	-0.14879600	-0.02935700
H	3.17202400	-1.50738500	-2.73130200	H	-4.85361300	-3.03022200	-4.05632400
C	4.05271500	-2.68498700	-4.26832700	C	-5.90208000	-2.95373900	3.42095500
C	1.76993200	-3.02962400	-3.24144100	H	-6.31123400	-1.69199800	5.14176100
H	2.79658900	-5.21431900	0.72333100	H	-5.47670300	-3.91454300	1.61032600
C	4.53753200	-5.67449700	1.89890000	C	0.07640100	4.81021500	-0.23200600
H	4.43505800	6.15969200	0.78358800	H	-0.16891100	3.66064600	-2.04431800
H	7.57999700	0.90809900	4.04168600	H	-0.78248200	5.31804800	-2.15332200
H	5.51636100	-5.33212200	-0.67926100	H	-4.01931800	3.39025200	-1.97763700
H	4.28622700	-6.60653200	-0.70570000	C	-2.56619000	2.47185500	-3.24649800
H	4.16003200	-3.73293000	-4.59504900	C	-3.22651700	4.91306100	-3.24152700
H	5.06508200	-2.27348100	-4.12232600	H	0.75083800	2.83496200	0.27504900
H	3.57914300	-2.12970700	-5.09398000	C	0.90231000	4.05629800	2.04299600
H	1.27067400	-2.33590000	-3.93569600	H	-5.51270500	-4.74329300	-2.32753200
H	1.16922100	-3.04860100	-2.31905900	H	-6.08866300	-3.90469600	3.92422400
H	1.73192100	-4.03570700	-3.68942500	H	-0.41536000	5.66284300	0.27369700
H	4.39130000	-6.76631500	1.86845400	H	1.08844900	5.14689800	-0.50570500
H	4.11948300	-5.30231500	2.84838200	H	-2.57709200	1.52440900	-2.69130000
H	5.62394100	-5.48116500	1.91205500	H	-3.23341100	2.34982900	-4.11572200
P	-3.64771600	0.68276500	0.34585100	H	-1.54333400	2.61783700	-3.62802100
N	-4.61709400	0.27988800	-0.95591500	H	-3.51521100	5.78210900	-2.62684700
N	-4.78978000	0.71911500	1.60927200	H	-2.30932700	5.17989300	-3.79128900
O	-3.30684200	2.24288600	0.14649000	H	-4.01882300	4.75180500	-3.99021900
C	-4.82344400	-1.10474100	-1.21905200	H	0.92897600	3.23408100	2.77315500
C	-5.76153100	1.15545500	-1.24954800	H	1.93870000	4.35627100	1.82917900
C	-5.26503300	-0.54579200	2.06209500	H	0.39082300	4.90848000	2.52272100
C	-4.81862200	1.87090900	2.51649700	H	-1.43673300	1.93697800	-0.74039700
C	-1.97420900	2.73994700	-0.21335800				
C	-5.15229100	-2.04196100	-0.20239600				
C	-4.71106900	-1.46642800	-2.57123600				
H	-5.98838200	1.10557600	-2.32436900				
H	-6.65600600	0.85728400	-0.67598800				
H	-5.50886000	2.19327600	-0.99957900				
C	-5.67381500	-0.57797800	3.41689700				
C	-5.29956900	-1.78004700	1.29825800				
H	-5.85251500	2.06434800	2.83720300				



t-TS_Vb-VIIb (+21.0 vs. Va)

Cl	1.11931400	-1.69061800	-1.14047400
Cl	-0.52367800	-0.92230300	1.59210000
Cl	-1.88290000	-1.29085300	-2.93839700
Cl	2.13088000	1.22711000	2.44661400
Pd	-1.33701300	-1.07725200	-0.68113800
Pd	1.67573100	-0.14416000	0.60338400
P	-3.39521500	-0.33951800	-0.12779400
N	-4.65081600	-0.28798800	-1.25778100
N	-4.06865300	-1.22841900	1.12230100
O	-3.38082600	1.23332200	0.27169000
C	-5.42116400	-1.47442600	-1.47569200
C	-4.65368800	0.72802900	-2.31907800
C	-5.38107200	-0.85832000	1.57631500
C	-3.57297700	-2.52469600	1.59625100
C	-2.30229300	1.91934000	0.96981200
C	-5.32152900	-2.15820000	-2.69687700
C	-6.34797600	-1.91166700	-0.49622100
H	-3.91399300	0.51472200	-3.10564700
H	-4.43526600	1.70760100	-1.87796700
H	-5.65913400	0.76171200	-2.76086700
C	-6.50712700	-1.20473400	0.79884100
C	-5.53448900	-0.21797900	2.81059200
H	-3.41650000	-2.49887200	2.68577100
H	-2.61741900	-2.76809200	1.11617400
H	-4.29865200	-3.31837500	1.35323100
H	-1.35260700	1.44514700	0.68513200
C	-2.25272100	3.38369500	0.52725800
C	-2.48713000	1.78121300	2.47521800
H	-4.58284900	-1.82427000	-3.42524100
C	-6.12995800	-3.26399600	-2.96246300
C	-7.14534700	-3.03423900	-0.78317300
C	-7.78251400	-0.88630900	1.29779100
C	-6.80953300	0.09031300	3.28932100
H	-4.64433200	0.03122600	3.38888700

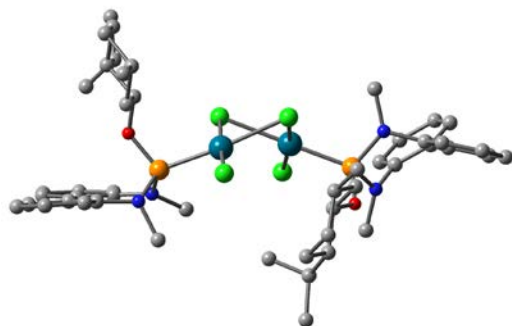
H	-3.16955100	3.87474800	0.90514400	C	4.49113000	-1.82507900	2.49741700
C	-1.05181900	4.02714600	1.25315900	C	1.53027500	2.53914200	-3.56637800
C	-2.25446500	3.55992000	-1.01199000	C	1.59677800	0.40317600	-4.69989000
C	-1.33417100	2.44910800	3.23510400	H	2.89036400	-1.03927300	-3.73821100
H	-2.53147400	0.71334600	2.73420400	C	2.86636000	5.23287900	0.58470000
H	-3.45365800	2.23570400	2.75760300	H	4.15500600	3.92321800	1.63886100
H	-6.03384200	-3.78776900	-3.91660700	C	1.99409200	4.34674900	-1.45749800
C	-7.04511400	-3.70590300	-2.00204800	C	5.29597000	-4.31834000	1.18300100
H	-7.85071100	-3.38503000	-0.02620000	H	6.57881700	-2.60884700	0.93515000
H	-8.66288800	-1.13389900	0.70025900	C	5.78979800	-3.02389300	-1.01812100
C	-7.93468400	-0.24454300	2.52842600	C	4.17834400	-3.17245700	3.16270000
H	-6.92317500	0.59411600	4.25207500	H	3.73245600	-1.07465000	2.76637200
H	-0.97068000	5.08819900	0.97600800	H	5.46524900	-1.44692900	2.85646300
C	-0.11464700	3.54796400	0.92059700	C	1.13318400	1.71657500	-4.61451900
C	-1.17071000	3.90465600	2.77704400	H	1.11555300	3.53987300	-3.58825600
H	-3.25921500	3.25357800	-1.34614800	H	1.27266100	-0.26519700	-5.49997100
C	-2.07893300	5.02802600	-1.42349100	C	2.06102200	5.38419700	-0.53894200
C	-1.24152900	2.66805300	-1.73545800	H	2.93419100	6.00885300	1.33057200
H	-0.41112000	1.91203800	2.96134600	H	1.33073200	4.52554000	-2.29405000
C	-1.51897800	2.33268100	4.74793000	C	5.20508000	-4.22012400	2.71006800
H	-7.67492800	-4.57700300	-2.19776600	H	4.33861600	-4.70080500	0.78793900
H	-8.93567300	0.00010500	2.89208900	H	6.06421200	-5.05487000	0.90340300
H	-2.04237700	4.49278700	3.12250400	H	6.06049100	-2.00244000	-1.32536600
H	-0.28124100	4.34644500	3.25776100	C	4.51562500	-3.40171000	-1.78486300
H	-1.04673200	5.37480100	-1.25461500	C	6.96029200	-3.93152500	-1.41976400
H	-2.75386500	5.69332200	-0.85968200	H	3.18376800	-3.49665400	2.80001400
H	-2.29669100	5.15636200	-2.49604200	C	4.11001200	-3.04173100	4.68478200
H	-1.20535600	2.91162700	-2.80763000	H	0.44439000	2.11270600	-5.36439300
H	-1.49027600	1.60024500	-1.66740300	H	1.47415600	6.29024100	-0.70374900
H	-0.22674400	2.79615000	-1.33305300	H	6.19538100	-3.94524900	3.11911300
H	-0.66709700	2.77778700	5.28738400	H	4.95231700	-5.20554300	3.13675000
H	-1.59982200	1.27800200	5.05866400	H	3.69237400	-2.69623900	-1.60561300
H	-2.43554000	2.85249800	5.07794200	H	4.71156600	-3.39799800	-2.86953700
P	3.71617300	0.33129200	-0.18557900	H	4.16336900	-4.41205300	-1.52026900
N	3.91349400	0.24993800	-1.84586300	H	7.87489400	-3.68898500	-0.85353000
N	4.35364600	1.87152700	0.14805500	H	6.73103100	-4.99586500	-1.24838200
O	4.85620800	-0.64519800	0.40790800	H	7.18762700	-3.81688200	-2.49182000
C	2.89889600	0.81175000	-2.67982300	H	3.34975400	-2.30407800	4.98810800
C	5.27839800	0.46090500	-2.35991900	H	3.85798200	-4.00507900	5.15694300
C	3.53594100	2.98757000	-0.20247500	H	5.08064500	-2.71121000	5.09278200
C	5.38914900	2.02292300	1.17669000	H	3.56991100	-2.28019400	0.60450500
C	4.55428600	-1.95837700	0.98159300				
C	2.40881500	2.13703800	-2.52191200				
C	2.48610000	-0.02638200	-3.72689900				
H	5.38331800	-0.06900200	-3.31779000				
H	5.48916100	1.53311500	-2.51363000				
H	6.01359400	0.05375100	-1.65527200				
C	3.57087000	4.04910100	0.73271700				
C	2.69523200	3.11312000	-1.37676600				
H	5.98977900	2.91572200	0.95191600				
H	4.96874400	2.10584000	2.19194100				
H	6.04639300	1.14855300	1.14662500				
C	5.61526200	-2.96185800	0.52097000				



c-TS_Va-VIIa (+21.5 vs. **Va**)

Cl	0.94639800	-2.27676100	0.98454200
Cl	-1.33331600	-1.98863600	-1.38774000
Cl	-0.96676600	0.06930100	2.89832600
Cl	1.10844600	-0.65568000	-3.45403600
Pd	-1.22506900	-0.85460900	0.77061100
Pd	1.12528300	-1.55544100	-1.30930000
P	-2.99376800	0.44300000	0.30917800
N	-3.53362200	1.63519500	1.37535000
N	-2.77974000	1.32141900	-1.09681400
O	-4.36023500	-0.42384300	0.24839400
C	-2.94114200	2.93685600	1.34366200
C	-4.26744400	1.26100000	2.59345900
C	-3.85706800	2.16800700	-1.52303100
C	-1.61425100	1.26203300	-1.98888400
C	-4.56702200	-1.81698100	-0.10923200
C	-2.17439300	3.37842300	2.43251200
C	-3.21409600	3.81752100	0.26770300
H	-3.60941100	0.81917700	3.35737400
H	-5.05617000	0.54298900	2.33729300
H	-4.73846000	2.16567600	3.00124700
C	-4.06187900	3.40572200	-0.87728200
C	-4.64901500	1.79039400	-2.61364800
H	-1.80323900	0.64352800	-2.87795700
H	-0.74874100	0.84149600	-1.46847600
H	-1.36096900	2.28587800	-2.29855800
H	-3.59723400	-2.29059300	-0.31268900
C	-5.23562400	-2.52893700	1.07299300
C	-5.40511200	-1.81896300	-1.38318800
H	-1.95423700	2.67730100	3.23707700
C	-1.68487900	4.68338000	2.47509200
C	-2.69341700	5.12310500	0.32455100
C	-5.08242000	4.24470200	-1.36041500
C	-5.65510900	2.63805900	-3.07994900
H	-4.46178500	0.82834900	-3.09396400

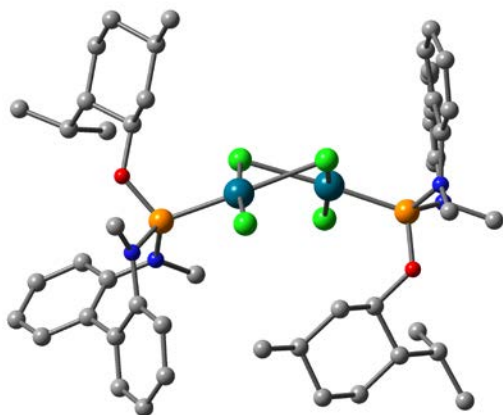
H	-6.13891600	-1.93570600	1.30928100	C	2.14879900	2.10651400	-0.65171300
C	-5.69705900	-3.93019300	0.62969300	H	1.37111200	0.59668600	0.67893900
C	-4.33826800	-2.54218000	2.33977700	C	7.30297400	1.25989800	-0.87590700
C	-5.85794600	-3.22521700	-1.79569200	C	6.33087000	2.59338000	-2.64189000
H	-4.81805200	-1.34927800	-2.18872100	H	4.46656400	1.79369800	-3.39437300
H	-6.29002700	-1.18026600	-1.21342100	C	6.72338300	-2.69171700	2.33591000
H	-1.08300500	5.00744600	3.32718700	H	4.95189800	-3.63621500	1.62871600
C	-1.94235200	5.55961400	1.41610800	C	7.33137200	-0.69954100	1.14937700
H	-2.88411500	5.80232800	-0.50947900	C	1.61401900	2.92588300	2.10874200
H	-5.26515500	5.19891400	-0.86106700	H	3.63926500	2.34852300	1.68886100
C	-5.87107800	3.86822600	-2.44884600	C	2.84861200	0.79331000	3.00186700
H	-6.27184600	2.33684100	-3.92994100	C	1.10002600	3.18517000	-0.35321600
H	-6.22514000	-4.42220400	1.46182700	H	1.86600100	1.53791200	-1.55323900
H	-4.81342600	-4.55353800	0.41149400	H	3.12360300	2.57975300	-0.86189600
C	-6.58237500	-3.89313200	-0.61853400	C	7.35747400	2.35973600	-1.72585400
H	-3.87714700	-1.54567200	2.40962200	H	8.15072900	1.15193000	-0.20781000
C	-5.16745000	-2.73194600	3.61562200	H	6.34353000	3.46174900	-3.30430200
C	-3.18841900	-3.55843500	2.28010400	C	7.57300100	-1.60016400	2.17790800
H	-4.95036500	-3.82154200	-2.01047900	H	6.86661200	-3.41642000	3.14070900
C	-6.71481100	-3.18448000	-3.06191100	H	8.00952500	0.14506200	1.11199100
H	-1.54819000	6.57832600	1.43370300	C	1.48231300	3.90768400	0.94270400
H	-6.66189500	4.53460900	-2.80165800	H	0.63747700	2.44738500	2.29063900
H	-7.51130500	-3.33221800	-0.40404400	H	1.87223300	3.47414100	3.02641100
H	-6.88878800	-4.91587600	-0.89606400	H	2.29045300	-0.11129100	2.70579600
H	-5.67775300	-3.70963300	3.62623800	C	2.27975900	1.23747700	4.35633200
H	-5.93813800	-1.94972400	3.71383200	C	4.32382400	0.40482200	3.16683100
H	-4.52511300	-2.68634600	4.50979200	H	0.13368900	2.67880500	-0.17097500
H	-2.46873100	-3.36456500	3.09061900	C	0.92184400	4.14246800	-1.53110600
H	-2.62965500	-3.50377200	1.33275100	H	8.21282200	3.03671000	-1.66260000
H	-3.55240500	-4.59199100	2.39655400	H	8.41303000	-1.43287700	2.85546100
H	-7.01548800	-4.19795100	-3.37297500	H	2.44119800	4.43774100	0.78789800
H	-6.17050600	-2.71955400	-3.89996300	H	0.72890500	4.67398300	1.17994300
H	-7.63427700	-2.59822000	-2.89260100	H	1.19711100	1.41901600	4.31384500
P	3.25146500	-0.96705100	-0.91275800	H	2.45011700	0.44771600	5.10620800
N	4.18097200	-0.34722500	-2.16260700	H	2.77456800	2.15169900	4.72609200
N	4.23388000	-2.22369000	-0.34741100	H	4.76150100	0.06204200	2.22279600
O	3.35170700	0.16596300	0.22612800	H	4.91411000	1.26913600	3.51978000
C	5.25355500	0.54360400	-1.85584000	H	4.44224100	-0.40313500	3.90726100
C	4.44275500	-1.26917900	-3.27459400	H	0.66298500	3.59979000	-2.45479600
C	5.40129800	-1.91967200	0.40482200	H	0.12192900	4.87260500	-1.32752000
C	3.77292500	-3.61063700	-0.46339400	H	1.85273300	4.70242000	-1.72486500
C	2.31152200	1.14878300	0.52319900				
C	6.24769400	0.30531900	-0.86097900				
C	5.29249900	1.67438200	-2.69038200				
H	4.67607200	-0.69307000	-4.18127200				
H	5.28845000	-1.94457500	-3.04913300				
H	3.54398200	-1.86493800	-3.48205300				
C	5.65264400	-2.82004800	1.46526600				
C	6.28597700	-0.79923500	0.19233200				
H	4.63985500	-4.26357600	-0.63860500				
H	3.21963900	-3.96280500	0.42168200				
H	3.10397900	-3.70089500	-1.33078600				
C	2.67237500	1.83410600	1.84664700				



c-TS_Vb-VIIb (+24.1 vs. Va)

Cl	0.70570500	-1.78474600	0.96019800
Cl	-1.14356100	0.78130900	1.79932700
Cl	-1.87792800	-2.87822400	-1.12290900
Cl	1.25209900	2.85758600	0.27053700
Pd	-1.66841700	-1.09187700	0.35906000
Pd	1.00546800	0.55849000	0.52591800
P	-3.73477600	-0.32099200	-0.10881900
N	-4.80429500	-1.20963700	-1.06520300
N	-4.62542700	-0.06172200	1.28632000
O	-3.70036400	1.02205300	-1.01274600
C	-5.57458600	-2.24603600	-0.44914700
C	-4.63386100	-1.23648900	-2.52568700
C	-5.98082200	0.39710100	1.14956300
C	-4.23132000	-0.47800300	2.63626300
C	-2.76121800	2.12933600	-0.90573400
C	-5.31322500	-3.58990000	-0.75714500
C	-6.65153300	-1.91581500	0.41041700
H	-3.65120000	-1.63451600	-2.82211700
H	-4.75526400	-0.22194000	-2.92823500
H	-5.41664900	-1.87680200	-2.95182700
C	-6.98351700	-0.50751200	0.73881700
C	-6.30567200	1.71365800	1.49505800
H	-4.22987000	0.38469200	3.32059600
H	-3.22398400	-0.91092800	2.62646800
H	-4.93498200	-1.23768600	3.01396200
H	-1.78151900	1.73146300	-0.60947900
C	-2.63148700	2.78738300	-2.28213400
C	-3.24108500	3.10112400	0.16456000
H	-4.46372400	-3.82200900	-1.39940200
C	-6.10730700	-4.60888400	-0.23025800
C	-7.43181400	-2.96072400	0.93772800
C	-8.31041100	-0.04570800	0.67738200
C	-7.62937900	2.15292300	1.42955400
H	-5.51069000	2.38525500	1.82010000

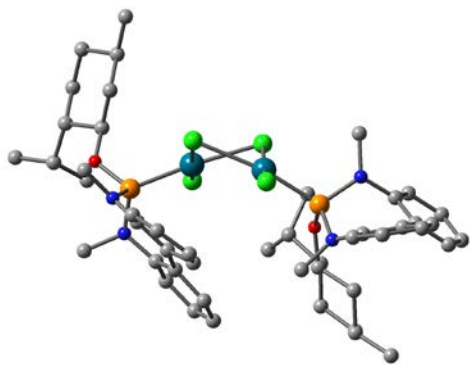
H	-3.62861000	3.19476500	-2.53674000	C	4.56639800	1.34304100	2.05631700
C	-1.66159400	3.97819300	-2.14216100	H	3.02428200	-0.14392500	2.32915400
C	-2.26284000	1.78252500	-3.40286100	C	7.30031600	0.24902600	-1.95516300
C	-2.30397700	4.30834800	0.29605300	C	7.20063700	2.57954400	-1.32520600
H	-3.30167800	2.56855600	1.12540100	H	5.20218500	3.25880900	-0.86170300
H	-4.26043800	3.43620100	-0.09744900	C	4.74844400	-4.15107200	-2.61140000
H	-5.88567900	-5.65012000	-0.47652000	H	2.72671800	-3.59497900	-2.23555400
C	-7.16976400	-4.29445300	0.62299100	C	6.33603300	-2.37499300	-2.33424300
H	-8.25445200	-2.71357900	1.61281100	C	4.95028900	-0.63361700	4.18348500
H	-9.09459400	-0.72958000	0.34465300	H	5.93270300	-1.04485700	2.31927600
C	-8.63244800	1.26967300	1.01632000	C	4.38481800	-2.56817400	2.50690900
H	-7.87542700	3.18329800	1.69675200	C	4.63465400	1.80224000	3.51733800
H	-1.56207400	4.49122300	-3.11064100	H	3.90685600	2.01149800	1.47968500
H	-0.65976300	3.60586600	-1.86935600	H	5.56748200	1.39799000	1.59525800
C	-2.12285400	4.97629600	-1.07381300	C	7.93671500	1.46462000	-1.72894700
H	-3.08991700	1.05648200	-3.43695200	H	7.95279400	-0.55730700	-2.27130200
C	-2.19860700	2.45484200	-4.78010700	H	7.68137800	3.53952400	-1.12442900
C	-0.98455500	0.98525400	-3.12152200	C	6.06856000	-3.70811500	-2.61620500
H	-1.31768800	3.92513500	0.61029800	H	4.49383700	-5.19338400	-2.81678200
C	-2.80506100	5.28636600	1.35903100	H	7.38712600	-2.11116600	-2.33455400
H	-7.78975400	-5.08681200	1.04906300	C	5.46916000	0.80128900	4.32627300
H	-9.66976300	1.60740800	0.95368500	H	3.93787900	-0.69928300	4.62143300
H	-3.08351300	5.43022200	-1.38376600	H	5.58637100	-1.31219900	4.76960800
H	-1.39607900	5.80246200	-0.99301800	H	3.31184000	-2.49787700	2.25245200
H	-1.31706000	3.10951800	-4.87519300	C	4.49210300	-3.46586600	3.74815700
H	-3.09464300	3.06794500	-4.97260400	C	5.10235900	-3.24390500	1.32897700
H	-2.13036700	1.69781800	-5.57795100	H	3.60363100	1.78416700	3.92031300
H	-0.77307600	0.28681200	-3.94670000	C	5.16503000	3.23232100	3.62692800
H	-1.07191200	0.38390600	-2.20502100	H	9.01847100	1.53079700	-1.86794900
H	-0.10744600	1.64158800	-3.00981500	H	6.89453600	-4.39045200	-2.82827900
H	-2.11504700	6.13801700	1.47428200	H	6.51736100	0.84827400	3.97570100
H	-2.90056200	4.79416800	2.34087600	H	5.48107000	1.09191700	5.39051300
H	-3.79587900	5.69127000	1.08816800	H	3.90461900	-3.09041100	4.59894500
P	2.93486000	0.07568300	-0.51327200	H	4.11829500	-4.47507400	3.51138700
N	3.75989600	1.29149000	-1.32269000	H	5.53887800	-3.57416200	4.07936900
N	2.84594100	-1.1295900	-1.69182500	H	5.04453300	-2.64333600	0.41424300
O	4.01724900	-0.48710400	0.54039500	H	6.16968100	-3.39690700	1.56726500
C	5.17986500	1.20447300	-1.44007100	H	4.66447600	-4.23212300	1.11364400
C	3.05719600	1.88076200	-2.46735700	H	4.53584500	3.93531400	3.05742300
C	4.00913900	-1.87763100	-2.01836000	H	5.19031800	3.57030300	4.67559300
C	1.54627600	-1.50435300	-2.26065100	H	6.19119500	3.29958900	3.22655700
C	4.08577800	-0.08861600	1.94138100				
C	5.90070600	0.03128800	-1.81505600				
C	5.82990200	2.42531400	-1.18292900				
H	3.48747500	2.86610300	-2.69441300				
H	3.13110000	1.24046400	-3.36575500				
H	2.00075800	2.03339600	-2.21077200				
C	3.75281400	-3.23887700	-2.29991300				
C	5.36245500	-1.37872500	-2.05409200				
H	1.66911200	-1.70137700	-3.33550600				
H	1.08178400	-2.37258500	-1.77171500				
H	0.85093500	-0.66565000	-2.14899700				
C	4.90178000	-1.10782000	2.71548100				



t-TS_Vb-VIIIb (+19.5 vs. Va)

C	-4.26243800	1.46779100	1.59361400
C	-4.59700900	0.95435900	2.85211700
H	-3.93851300	0.21575800	3.31015800
C	-5.75212800	1.38657400	3.50506600
H	-6.01046900	0.97656300	4.48423700
C	-6.57708900	2.33753800	2.89389500
H	-7.48946600	2.67420100	3.39209000
C	-6.23872800	2.85682900	1.64327200
H	-6.88969100	3.59315100	1.16644000
C	-5.07555800	2.43803300	0.97124700
C	-4.69724100	3.02812300	-0.33649300
C	-4.76565800	4.42173100	-0.51766700
H	-5.06127300	5.04750000	0.32760800
C	-4.45879900	5.01296600	-1.74323800
H	-4.51723800	6.09822800	-1.85492200
C	-4.06592500	4.21047300	-2.81861000
H	-3.80923700	4.66158800	-3.78005600
C	-3.97775700	2.82821300	-2.65904900
H	-3.63448800	2.19932400	-3.47984900
C	-4.28943900	2.22613200	-1.43070700
C	-1.80203900	1.55733400	1.56110400
H	-1.89226900	2.64514400	1.70069600
H	-0.95048100	1.36284000	0.90055900
H	-1.59382300	1.07837800	2.52984300
C	-4.97003600	0.04412900	-2.37669800
H	-5.88490700	0.58537200	-2.65548300
H	-5.25391700	-0.94225800	-1.99034400
H	-4.33803100	-0.08852000	-3.26833300
C	-3.57609300	-2.66586300	0.14733600
H	-2.57533400	-2.68120200	0.60062600

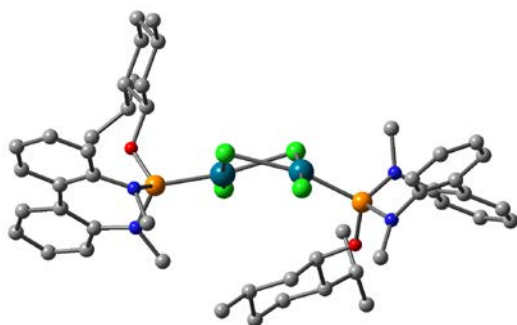
C	-4.55285800	-3.40080200	1.07210900	H	5.13308000	0.29949700	-3.59161900
H	-5.53490300	-3.38831900	0.56209800	H	3.34135500	0.16401400	-3.50270600
C	-4.09990300	-4.87085900	1.17154800	H	4.18881900	1.52842300	-2.72874400
H	-3.12099400	-4.91847700	1.67964100	C	3.29760900	4.23726200	0.07174000
H	-4.80561300	-5.43433400	1.80089900	C	1.46502800	2.83831600	-0.99856500
C	-3.98263800	-5.54011400	-0.20285000	C	5.31219500	-3.37427800	1.75287800
H	-4.98406000	-5.59817300	-0.66907000	C	5.73250000	-1.96181300	3.67290700
H	-3.62937400	-6.57897600	-0.08868500	H	5.56279800	0.15191500	3.24683300
C	-3.04641400	-4.76911000	-1.14483800	C	4.43503300	-3.63945900	-3.25204200
H	-2.03592800	-4.77233200	-0.69290400	H	4.42288800	-1.62231400	-3.88693700
C	-3.50180800	-3.30589600	-1.23490500	C	4.54093000	-3.95395300	-0.88648800
H	-2.81053300	-2.73184400	-1.87385900	C	2.20248500	5.19058000	0.59371300
H	-4.49857600	-3.25506700	-1.70860800	H	3.57116800	4.57404500	-0.94635300
C	-4.75374200	-2.68891600	2.43354900	C	4.60415400	4.23653100	0.90751100
H	-5.09972500	-1.67355500	2.18298700	C	0.37423700	3.76936700	-0.45343500
C	-5.86179500	-3.34821800	3.26464100	H	1.07711500	1.81210700	-1.09597800
H	-6.78269100	-3.48553800	2.67402000	H	1.76997100	3.16254600	-2.00945600
H	-6.11298900	-2.72404300	4.13755200	C	5.63572800	-3.23098100	3.09767000
H	-5.55705400	-4.33627500	3.64718300	H	5.29316900	-4.39506600	1.38617900
C	-3.46678200	-2.54189500	3.25667000	H	5.97292300	-1.83354400	4.73049300
H	-3.03534400	-3.52115100	3.52056500	C	4.40757100	-4.49635000	-2.15697100
H	-3.67628000	-2.01795800	4.20368900	H	4.36682800	-4.01551400	-4.27545800
H	-2.69227800	-1.96773000	2.72625700	H	4.50637900	-4.66835000	-0.07179700
C	-2.95165700	-5.41252900	-2.52878300	C	0.94666900	5.18309400	-0.28682400
H	-2.59920100	-6.45444900	-2.46082700	H	1.92381100	4.89765400	1.62114100
H	-2.25496400	-4.85922600	-3.17905700	H	2.60517200	6.21253600	0.65920300
H	-3.93780300	-5.42292000	-3.02402700	H	5.30381000	3.58758000	0.35707500
N	-3.04294800	1.05499400	0.96077400	C	4.45050400	3.64284900	2.31493500
N	-4.28917700	0.80038200	-1.31688700	C	5.24424600	5.62976200	0.96550500
O	-4.01782400	-1.28623100	0.03825900	H	0.11168500	3.40526700	0.55643600
P	-3.13859400	0.02371700	-0.35215100	C	-0.88534000	3.72734700	-1.31421200
Cl	-0.41426200	-1.43662500	1.04030300	H	5.81944100	-4.12686200	3.69570800
Cl	1.25995400	-1.22827900	-1.78372900	H	4.29169800	-5.57536100	-2.27814100
Cl	-1.56498900	0.29635200	-3.24741600	H	1.19312400	5.58817200	-1.28601700
Cl	2.20578900	0.36626800	2.57934400	H	0.18111200	5.85139800	0.14274300
Pd	-1.09938000	-0.53900700	-1.11709100	H	4.09333700	2.60259200	2.29782900
Pd	1.85974400	-0.52103400	0.45239300	H	5.42197500	3.64851800	2.83577500
P	3.77987900	0.37752600	-0.25362500	H	3.74846300	4.23094700	2.92885600
N	5.08713400	0.21153400	0.77113700	H	5.32589200	6.08086500	-0.03743800
N	4.40484000	-0.27956900	-1.69839200	H	4.66385400	6.32071100	1.59843400
O	3.70351600	1.94504700	-0.61518100	H	6.25848200	5.57203700	1.39232900
C	5.20119400	-1.01136300	-1.49328100	H	-1.26089300	2.69974400	-1.42566200
C	6.35961000	0.82155000	0.35913700	H	-1.69373700	4.33768900	-0.88290300
C	4.56452800	-1.69613900	-1.73130300	H	-0.68309200	4.10735900	-2.32976000
C	4.25085100	0.46102300	-2.95538300	H	2.38185100	2.46991900	0.91001800
C	2.67882300	2.84554900	-0.08033400				
C	5.05747100	-2.28265000	0.87503500				
C	5.51100000	-0.86474000	2.85430800				
H	6.94303800	1.07867000	1.25514100				
H	6.95082000	0.13785700	-0.27414700				
H	6.16528100	1.74452800	-0.20111100				
C	4.48904400	-2.27338800	-3.02168400				
C	4.71161800	-2.57665800	-0.58603000				



t-TS_Va-VIIIa (+27.5 vs. Va)

Cl	0.20035400	2.09723000	-0.45624200
Cl	1.46935100	-0.31031600	-2.32428400
Cl	-1.94142400	-1.55472400	-2.60386300
Cl	2.88606100	1.66970200	1.73639600
Pd	-0.86351400	0.10918000	-1.36835600
Pd	2.14409200	0.55580700	-0.16864800
P	3.65190500	-1.05746600	0.16909900
N	3.79385800	-1.62717400	1.73129300
N	3.32359600	-2.49948200	-0.68206500
O	5.16177500	-0.74010400	-0.29742800
C	2.60574000	-1.69718100	2.51377000
C	4.78923600	-2.67656000	1.99211200
C	2.04674600	-3.10497100	-0.48167100
C	4.07296900	-2.78605500	-1.91015900
C	5.63226300	0.61634700	-0.57970900
C	1.42273700	-2.33183400	2.05007800
C	2.70814400	-1.12076200	3.78950000
H	5.09727100	-2.62149900	3.04642000
H	4.38422500	-3.68257800	1.78593400
H	5.67474400	-2.51381900	1.36490300
C	1.58236000	-3.86462500	-1.58331100
C	1.18825000	-2.97900400	0.68281000
H	4.23136600	-3.87019000	-2.00298400
H	3.55820300	-2.41225700	-2.81042500
H	5.05302200	-2.30709500	-1.84322100
C	7.12058600	0.69202700	-0.23207000
C	5.35434800	0.95040100	-2.03987800
C	0.38172900	-2.35913800	3.02100700
C	1.65975200	-1.16642400	4.69552400
H	3.64732200	-0.62352200	4.03533200
C	0.33492000	-4.46270200	-1.64293800
H	2.21365200	-3.95801100	-2.45975900
C	-0.09134900	-3.57545500	0.52959200
C	7.60470900	2.11822900	-0.56402300

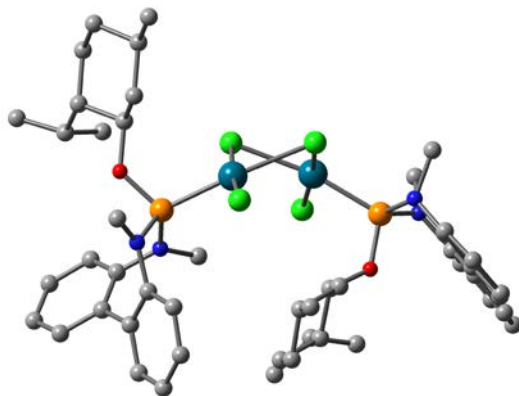
H	7.64096500	-0.00228100	-0.91917700	C	-5.51203800	-2.26839300	-0.37958900
C	7.44216600	0.21481500	1.20765700	C	-6.12223100	0.14867000	-0.81142800
C	5.83722300	2.36633400	-2.38444900	H	-3.82515700	-0.62805200	3.08577300
H	4.27518400	0.85491100	-2.24131300	C	-5.48944900	0.64723200	3.59442200
H	5.87037300	0.21058500	-2.67789000	C	-5.51671000	2.81498600	2.52434400
C	0.48507300	-1.80474200	4.29182600	C	-3.49520600	4.86264800	1.53397700
H	-0.56664200	-2.83771200	2.80588400	C	-2.46032400	5.61550500	-0.50699800
H	1.75076300	-0.71285200	5.68474600	H	-2.23973500	4.13866600	-2.04995800
C	-0.53199400	-4.29229100	-0.57128600	H	-5.88437700	-2.07800600	0.64453100
H	0.03881200	-5.01626200	-2.53650000	C	-6.73624900	-2.68308400	-1.22146700
H	-0.81703000	-3.47803000	1.32525500	C	-4.37032200	-3.32920600	-0.27496000
C	7.32276800	2.50514900	-2.02097100	C	-7.36971600	-0.24610800	-1.61369200
H	7.10518200	2.83917900	0.10646000	H	-5.75137800	1.12482500	-1.14832100
H	8.68325200	2.19942600	-0.36156200	H	-6.37893800	0.26745300	0.25621600
H	7.10308400	-0.83282800	1.25187800	H	-5.94434400	-0.08897500	4.26148900
C	6.69120600	0.97865600	2.30663200	C	-6.10709400	1.88472600	3.37981400
C	8.95251400	0.20446800	1.47822200	H	-5.99730400	3.78123400	2.35516400
H	5.26762000	3.07163800	-1.74940400	H	-3.83212400	5.06086800	2.55406300
C	5.55958100	2.71188200	-3.84796000	C	-2.90535600	5.88421800	0.78950300
H	-0.37062600	-1.87286100	4.96805700	H	-1.98472800	6.39813700	-1.10291800
H	-1.54438900	-4.69762800	-0.58668400	H	-6.42480500	-2.84739400	-2.26898100
H	7.91347300	1.85431300	-2.69263100	H	-7.12980400	-3.64358100	-0.85986800
H	7.66085200	3.53821300	-2.20917300	C	-7.85246500	-1.63392400	-1.17474000
H	5.59912700	0.90931300	2.19664800	H	-3.59244300	-3.05045600	-1.00428700
H	6.94910400	0.56796500	3.29655700	C	-3.73381100	-3.29408700	1.12398300
H	6.96323000	2.04711100	2.31647800	C	-4.80563400	-4.76532600	-0.59899900
H	9.50525900	-0.31378500	0.67697500	H	-7.07097000	-0.31690200	-2.67750200
H	9.36019500	1.22514400	1.56173200	C	-8.46590800	0.81402000	-1.49478800
H	9.17186500	-0.31158700	2.42677000	H	-7.04922400	2.12417800	3.87859100
H	4.48550400	2.63041700	-4.08032900	H	-2.78742000	6.87999600	1.22273700
H	5.88198700	3.73908500	-4.08313200	H	-8.23817000	-1.56225200	-0.14046200
H	6.10228500	2.02663600	-4.52154900	H	-8.70019400	-1.95498300	-1.80360300
H	5.07368000	1.31044600	0.06662800	H	-3.29052900	-2.31312900	1.33719000
P	-2.72213200	0.61153400	-0.25202600	H	-2.94711300	-4.05797500	1.22245500
N	-2.48844700	0.97082300	1.37849800	H	-4.49032300	-3.50378800	1.90018800
N	-3.41677000	2.02876800	-0.90469100	H	-5.58429800	-5.12407200	0.09559600
O	-3.86523200	-0.51616000	-0.15867500	H	-3.94590900	-5.44869500	-0.50374900
C	-3.70308900	1.27761500	2.07661600	H	-5.19144400	-4.86926900	-1.62388600
C	-1.42047800	0.29637600	2.13152400	H	-9.35294000	0.54053400	-2.08882000
C	-3.20680600	3.30453400	-0.30318500	H	-8.11249500	1.79773000	-1.84437800
C	-3.59153000	1.98461600	-2.36477600	H	-8.78570400	0.92743100	-0.44479900
C	-5.02720000	-0.91169700	-0.92211600				
C	-4.29565100	0.34464000	2.94006200				
C	-4.30723300	2.53445200	1.86212600				
H	-1.27608100	0.82955400	3.08103100				
H	-0.47688100	0.33899500	1.57611800				
H	-1.64619100	-0.75893700	2.35096900				
C	-3.65848200	3.56670900	1.01448800				
C	-2.60821800	4.33725800	-1.04450100				
H	-4.37331500	2.70048100	-2.65520700				
H	-3.90564400	0.97849500	-2.67218500				
H	-2.66359400	2.21314300	-2.91500700				
H	-4.70715900	-1.04551000	-1.96910700				



c-TS_Va-VIIIfa (+23.1 vs. Va)

C	5.87050800	0.43459300	1.48445400
C	5.84900000	1.60578600	2.24809300
H	4.89151100	1.96719800	2.62521300
C	7.03720900	2.28802300	2.51937000
H	7.01587600	3.20597100	3.11137900
C	8.24851500	1.79196300	2.02530900
H	9.18161500	2.32356200	2.22726600
C	8.27024800	0.61988400	1.26584900
H	9.21696700	0.24427000	0.87067800
C	7.08497000	-0.07930000	0.97942100
C	7.10329200	-1.33795200	0.19221800
C	8.04058300	-2.34331000	0.48880400
H	8.73783900	-2.18585700	1.31507500
C	8.08421200	-3.53329300	-0.23947800
H	8.82073600	-4.29951900	0.01395200
C	7.17516200	-3.74448400	-1.28103100
H	7.19070400	-4.67909500	-1.84682700
C	6.23233700	-2.76301100	-1.59074400
H	5.49822300	-2.92386200	-2.38121900
C	6.19304800	-1.56001200	-0.87118900
C	4.29557400	-1.27508300	2.28760900
H	5.15324700	-1.94192100	2.47466200
H	3.44864300	-1.88754200	1.95569900
H	4.01493600	-0.77196900	3.22564900
C	5.29165200	-0.11088800	-2.66807600
H	6.33643700	-0.04576800	-3.00464600
H	4.83814000	0.88451800	-2.75017400
H	4.73769600	-0.80825700	-3.31422700
C	2.45185400	1.99308400	-0.90203200
H	1.71489900	1.56733400	-0.20737100
C	2.55447400	3.49607200	-0.62616500
H	3.22243200	3.91894800	-1.40058300
C	1.14618300	4.08798900	-0.84961800
H	0.44939200	3.66352100	-0.10595100
H	1.16623500	5.17479000	-0.67811800
C	0.61342200	3.79941600	-2.25934300

H	1.24182300	4.32154200	-3.00454300	C	-7.03639000	-1.29036100	-2.21453700
H	-0.40461400	4.20981500	-2.37058400	C	-5.79774300	-3.31913800	-2.65283100
C	0.61428700	2.29940900	-2.58749100	H	-3.67092300	-3.11538700	-2.32499900
H	-0.06487000	1.79623200	-1.87431600	C	-6.89049300	3.59918200	-0.68346200
C	2.00845600	1.71478300	-2.33560400	H	-4.81481500	3.95662800	-0.39002400
H	2.00210900	0.62967600	-2.52529500	C	-7.43457500	1.35402600	-1.32002100
H	2.73798900	2.16263200	-3.03381800	C	-4.67249800	-2.05329800	3.94636800
C	3.19779300	3.83662200	0.74042500	H	-5.95831300	-1.31880300	2.39201400
H	4.19721100	3.37184100	0.71502500	C	-5.11313300	0.45820200	3.32939900
C	3.40741700	5.34738900	0.90648600	C	-3.52666500	-3.61601700	2.29507100
H	3.91306000	5.78623800	0.03025300	H	-3.03801500	-2.62368300	0.42444100
H	4.02895000	5.55591200	1.79232500	H	-4.77699400	-2.83582800	0.69573400
H	2.45270900	5.88050200	1.04641400	C	-7.00783100	-2.62473000	-2.60530600
C	2.45264200	3.24989500	1.94572600	H	-8.01980000	-0.83326800	-2.21766100
H	1.41441800	3.61303100	2.00816800	H	-5.75436500	-4.37214700	-2.93957000
H	2.95692400	3.53769500	2.88314500	C	-7.84890000	2.63729900	-0.98907700
H	2.41187800	2.15230000	1.91416500	H	-7.16986400	4.61975100	-0.41176400
C	0.11405600	2.00531300	-4.00085900	H	-8.23648400	0.65456300	-1.52478700
H	-0.91351700	2.37724200	-4.14400100	C	-4.57412600	-3.48523600	3.40823700
H	0.11607700	0.92295500	-4.20757700	H	-3.71855000	-1.78130000	4.43323200
H	0.75655800	2.49180200	-4.75419600	H	-5.44384100	-2.00904300	4.72853300
N	4.64944900	-0.28871100	1.26114600	H	-4.13766700	0.94121900	3.13881900
N	5.28389500	-0.52542600	-1.26048300	C	-5.40615400	0.61490300	4.82849800
O	3.73756100	1.36423600	-0.64346000	C	-6.17821800	1.21598000	2.52235300
P	3.96388900	-0.19998400	-0.26163500	H	-2.54067600	-3.36114500	2.72919700
Cl	1.16359000	-0.28520900	1.60664100	C	-3.44531100	-5.03322800	1.72672000
Cl	-0.46800300	-1.91727100	-0.72593200	H	-7.94522300	-3.11955700	-2.87046700
Cl	2.66431000	-2.37907000	-2.37750100	H	-8.91542300	2.87125600	-0.96655700
Cl	-1.49625900	1.97284300	1.78982100	H	-5.55793000	-3.79390600	3.00738100
Pd	2.00509900	-1.29352300	-0.42073300	H	-4.33905100	-4.18040600	4.23204200
Pd	-1.02924200	0.11194900	0.45956000	H	-4.61811800	0.18530500	5.46443700
P	-3.10473300	0.25526900	-0.38683800	H	-5.48627500	1.68414200	5.08292700
N	-3.37360900	-0.71923700	-1.72747700	H	-6.36283700	0.14027600	5.10549700
N	-3.71038400	1.74063500	-0.91754600	H	-6.00861800	1.13662100	1.44237900
O	-4.20096100	-0.23672700	0.68480600	H	-7.18266300	0.81103400	2.73807400
C	-4.66992600	-1.26623600	-1.95029300	H	-6.18744300	2.28607100	2.78645300
C	-2.59365300	-0.38285500	-2.92267800	H	-2.66832400	-5.10528800	0.94853500
C	-5.11880600	1.91947600	-1.02623700	H	-3.20825100	-5.76712600	2.51395100
C	-2.81311100	2.88335300	-1.09798800	H	-4.40631700	-5.32678400	1.27054800
C	-3.92011200	-1.17906900	1.75951000				
C	-5.88810200	-0.53217300	-1.85011100				
C	-4.64591600	-2.62408300	-2.31741700				
H	-2.54232700	-1.25516300	-3.58868800				
H	-3.03700600	0.46649300	-3.47434400				
H	-1.56375400	-0.12817300	-2.63810600				
C	-5.55701500	3.22130100	-0.69180900				
C	-6.08591800	0.91500800	-1.40191000				
H	-3.10712700	3.43448600	-2.00342600				
H	-2.79402200	3.56404700	-0.23418600				
H	-1.79177800	2.51702700	-1.23694300				
C	-4.99273400	-1.02226600	2.84324200				
C	-3.82399800	-2.59055400	1.19515300				
H	-2.94971700	-0.89167000	2.20296900				

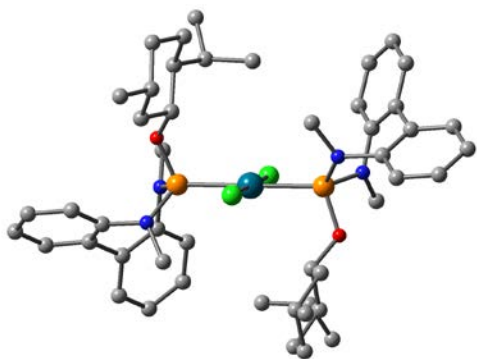


c-TS_Vb-VIIIb (+21.6 vs. Va)

C	3.48317300	2.17614000	-1.58150500
C	4.14576200	1.81268500	-2.76023800
H	3.94473300	0.83403400	-3.19707500
C	5.04462300	2.69274500	-3.36415200
H	5.56205500	2.39905200	-4.28045800
C	5.28328500	3.94382600	-2.78440700
H	5.99325100	4.63582700	-3.24371900
C	4.61724900	4.30984700	-1.61390100
H	4.81316400	5.28370000	-1.15956000
C	3.70275800	3.43926200	-0.99256300
C	2.96979600	3.85257100	0.22861900
C	2.40220700	5.13776400	0.30462000
H	2.47138700	5.79590000	-0.56447900
C	1.75749100	5.58089900	1.45932200
H	1.32666200	6.58429300	1.49221900
C	1.65392500	4.73002900	2.56425100
H	1.13859400	5.06011800	3.46908100
C	2.18697000	3.44303300	2.50399800
H	2.07807800	2.75869100	3.34485500
C	2.85129000	2.99723900	1.35140000
C	1.30258200	1.05581500	-1.80361300
H	0.94817300	2.02353400	-2.18628600
H	0.51174500	0.62914800	-1.18112500
H	1.47105600	0.36899100	-2.64570300
C	4.37121700	1.42491000	2.50422500
H	4.90546400	2.34366800	2.78353700
H	5.11014000	0.66917900	2.21178000
H	3.80277000	1.05499900	3.37111500
C	4.57011600	-1.75717200	0.18483800
H	3.73176800	-2.25509500	-0.32136300
C	5.85575300	-2.02294000	-0.60566600
H	6.67514500	-1.53703800	-0.04251900
C	6.11846800	-3.54151500	-0.58808600

H	5.31744500	-4.05861100	-1.14481500	C	-2.52512700	2.57790900	-0.74111600
H	7.05804600	-3.76154600	-1.11742400	C	-2.40423600	1.40355300	1.54434400
C	6.18290100	-4.10480400	0.83675300	H	-1.37223300	0.82999800	-0.25376800
H	7.05599700	-3.67358200	1.36144300	C	-6.89113500	0.48153400	1.84678300
H	6.34384200	-5.19572000	0.80521700	C	-5.62712900	0.07129600	3.86404200
C	4.91716800	-3.78576100	1.64611000	H	-3.85562000	-1.11852500	3.54156900
H	4.06265600	-4.27700500	1.14229300	C	-7.32335800	-0.28138500	-3.20757800
C	4.65701700	-2.27301100	1.61697300	H	-5.63507100	-1.50296600	-3.65277600
H	3.72346700	-2.03620600	2.15382100	C	-7.47503700	0.40534100	-0.91370200
H	5.47433000	-1.74519300	2.14022100	C	-1.50306900	3.58975200	-0.18161300
C	5.84681900	-1.37772000	-2.01449500	H	-3.53093100	2.96347800	-0.48864400
H	5.69247600	-0.30087300	-1.84060400	C	-2.45446800	2.35888600	-2.28678500
C	7.20023500	-1.52921800	-2.72041800	C	-1.40140200	2.43854400	2.06579700
H	8.03276400	-1.21328000	-2.07016500	H	-2.20984200	0.42070500	2.00138000
H	7.23218700	-0.90966500	-3.63130400	H	-3.42871400	1.69696700	1.82944000
H	7.39009000	-2.57086000	-3.02759700	C	-6.72039100	0.64898900	3.21639600
C	4.70237400	-1.86143100	-2.91538600	H	-7.77115900	0.96212500	1.43420500
H	4.76220800	-2.94512100	-3.10739400	H	-5.46257500	0.20254400	4.93574600
H	4.74797700	-1.35836100	-3.89520000	C	-7.97318000	0.44050600	-2.20996200
H	3.71185100	-1.65318500	-2.48386000	H	-7.67670800	-0.27473400	-4.24127200
C	4.99316600	-4.31354500	3.07932600	H	-8.02634200	1.00351600	-0.19770900
H	5.15309800	-5.40376500	3.09491100	C	-1.62267800	3.76466500	1.33342600
H	4.06574400	-4.09752800	3.63394300	H	-0.47765100	3.25530500	-0.42217300
H	5.82881700	-3.84346100	3.62569600	H	-1.63673800	4.56102100	-0.67885500
N	2.51488900	1.28595800	-1.00802300	H	-1.83164600	1.46486300	-2.46047000
N	3.50525500	1.72565100	1.35554000	C	-1.80738900	3.51530300	-3.06297300
O	4.33253700	0.32505400	0.17939200	C	-3.84297500	2.06905400	-2.87656400
P	2.92840800	0.46487800	0.39214300	H	-0.38592000	2.07985100	1.81997600
Cl	1.30129100	-2.18983800	-0.98138600	C	-1.48753800	2.57565000	3.58465100
Cl	-0.70536600	-2.38584500	1.59100900	H	-7.45066700	1.24053200	3.77371900
Cl	1.19452600	0.08857100	3.18610300	H	-8.86193700	1.03618700	-2.42939200
Cl	-1.40229800	-1.25152200	-2.94370400	H	-2.62771100	4.15460900	1.58314900
Pd	1.27980300	-0.90840100	1.07873900	H	-0.89484900	4.51352500	1.67987700
Pd	-1.15867900	-1.92202100	-0.72274700	H	-0.76567400	3.70296700	-2.76242400
P	-3.26790000	-1.26741700	-0.36202500	H	-1.80034400	3.28314100	-4.14018200
N	-3.92476000	-1.68877400	1.12634700	H	-2.36910700	4.45610700	-2.93381300
N	-4.46764800	-1.78938800	-1.42650900	H	-4.33805500	1.23344200	-2.36944700
O	-3.38521400	0.33518400	-0.40982600	H	-4.49526000	2.95527000	-2.78361000
C	-4.92493000	-0.85713100	1.71098900	H	-3.76938500	1.81932300	-3.94772500
C	-4.04329400	-3.12709700	1.38415900	H	-1.26584300	1.61575900	4.07548700
C	-5.66729400	-1.03778500	-1.54959500	H	-0.76130200	3.31717500	3.95452700
C	-4.21672400	-2.93077200	-2.31100500	H	-2.49488700	2.90252500	3.89577900
C	-2.34715600	1.26247000	0.02871500				
C	-6.01828700	-0.26738100	1.00776800				
C	-4.74286800	-0.66688700	3.09360600				
H	-4.06208300	-3.31344900	2.46708600				
H	-4.96028900	-3.54699700	0.93140400				
H	-3.16960900	-3.65351900	0.97359300				
C	-6.18171800	-0.98874400	-2.86474200				
C	-6.34112200	-0.33572100	-0.48540900				
H	-5.13528500	-3.53042900	-2.38997500				
H	-3.87544000	-2.63439800	-3.31406100				
H	-3.43207300	-3.56304200	-1.87370200				

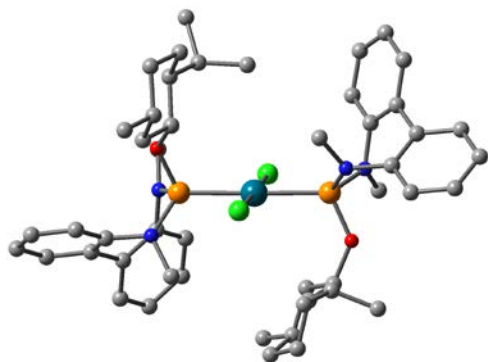
8.4 Mononuclear complex 2a



IXa (0.0)

Pd	0.00001700	-0.00007900	-0.20260500
Cl	0.00010800	-0.00107400	-2.57008200
Cl	0.00015800	0.00037300	2.18901300
P	-2.32684000	0.39437900	-0.22008700
N	-3.24104400	-0.54844800	0.83697000
N	-3.26812700	0.27695200	-1.63460400
O	-2.62273300	1.96795800	0.09946800
C	-4.66562400	-0.37147000	0.84759700
C	-2.77197400	-1.78376000	1.46954000
C	-3.71419700	-1.02808200	-2.01300600
C	-3.25508600	1.31645100	-2.66962100
C	-1.77669600	2.78612800	0.94573200
C	-5.44652800	-0.93928300	-0.18278800
C	-5.27301300	0.30276000	1.91170400
H	-1.68168900	-1.85054100	1.41309100
H	-3.05416500	-1.79122400	2.53391300
H	-3.21411400	-2.66587000	0.97495600
C	-4.79416900	-1.63224900	-1.32137500
C	-3.13194800	-1.68636800	-3.10614200
H	-3.39136100	2.29794700	-2.19808500
H	-2.32333300	1.32551600	-3.25597000
H	-4.10423700	1.13968800	-3.34546700
C	-1.60200700	4.15952800	0.28881000
C	-2.40929900	2.84517200	2.33185300
H	-0.78995100	2.30833700	1.03313800
C	-6.84452600	-0.82659800	-0.10078800
C	-6.66466900	0.41304900	1.97294800
H	-4.63901100	0.73506100	2.68771700
C	-5.25062400	-2.88974400	-1.75203000
C	-3.60664400	-2.93130400	-3.52332500
H	-2.28566700	-1.21507300	-3.60680500
C	-0.85035600	5.08545700	1.26414200
H	-2.62225600	4.56529800	0.15295500

C	-0.94823700	4.07174100	-1.11739200	H	0.79012100	-2.30806300	1.03348100
C	-1.65309200	3.78098700	3.28202500	C	6.84459000	0.82654700	-0.10102900
H	-2.43532500	1.82300900	2.74135100	C	6.66476600	-0.41309700	1.97271100
H	-3.45402000	3.18743200	2.22242600	H	4.63912400	-0.73500300	2.68757800
C	-7.45008000	-0.15804000	0.96617300	C	5.25055000	2.88983400	-1.75211800
H	-7.45930500	-1.25210300	-0.89763000	C	3.60609700	2.93162200	-3.52298500
H	-7.13391300	0.94476300	2.80425200	H	2.28513000	1.21536600	-3.60637700
C	-4.66720700	-3.53759700	-2.84275300	C	0.85019700	-5.08539800	1.26392100
H	-6.07410800	-3.36439200	-1.21287800	H	2.62178300	-4.56514200	0.15228200
H	-3.13637300	-3.43416600	-4.37199900	C	0.94735800	-4.07104400	-1.11735700
C	-1.52223500	5.16821200	2.63775600	C	1.65357800	-3.78151000	3.28189800
H	0.17788000	4.70863900	1.40175100	H	2.43585000	-1.82345000	2.74150600
H	-0.75558000	6.09009700	0.82217100	H	3.45429400	-3.18784100	2.22202400
H	-1.43377600	3.22761300	-1.62912000	C	7.45016100	0.15795800	0.96590700
C	0.55726500	3.77333400	-1.09617300	H	7.45935000	1.25203200	-0.89789600
C	-1.23726000	5.32746800	-1.94963400	H	7.13402000	-0.94483000	2.80399600
H	-0.63244600	3.37086800	3.40676700	C	4.66685500	3.53780700	-2.84262400
C	-2.31694800	3.83622900	4.65857000	H	6.07413300	3.36444500	-1.21308500
H	-8.53896500	-0.07412800	1.00571500	H	3.13559200	3.43461300	-4.37145200
H	-5.03699400	-4.51679700	-3.15648600	C	1.52247200	-5.16856400	2.63731300
H	-2.53044700	5.61160300	2.53455500	H	-0.17795900	-4.70852400	1.40194700
H	-0.94941500	5.83992300	3.29977300	H	0.75519000	-6.08990900	0.82170300
H	0.80051800	2.89664900	-0.47904000	H	1.43241300	-3.22651800	-1.62889200
H	0.92155000	3.55238800	-2.11078700	C	-0.55823000	-3.77313000	-1.09549800
H	1.14067400	4.62681300	-0.71441600	C	1.23649400	-5.32630100	-1.95026300
H	-2.32061400	5.51000500	-2.04101200	H	0.63298600	-3.37136200	3.40699600
H	-0.78224400	6.22601100	-1.50002000	C	2.31776600	-3.83714100	4.65826900
H	-0.82531100	5.22648600	-2.96692400	H	8.53904400	0.07399800	1.00540400
H	-2.38164700	2.83352600	5.11155200	H	5.03656400	4.51704500	-3.15633400
H	-1.75425300	4.48539400	5.34906300	H	2.53063200	-5.61198000	2.53371200
H	-3.34258800	4.23663800	4.58213300	H	0.94980100	-5.84041900	3.29931300
P	2.32692200	-0.39441400	-0.22017100	H	-0.80155100	-2.89687500	-0.47779200
N	3.24111200	0.54849800	0.83689400	H	-0.92289600	-3.55170700	-2.10986800
N	3.26821200	-0.27695400	-1.63465800	H	-1.14124600	-4.62701200	-0.71404200
O	2.62283100	-1.96793400	0.09955300	H	2.31987700	-5.50837500	-2.04222300
C	4.66569900	0.37151100	0.84745700	H	0.78204200	-6.22520900	-1.50080300
C	2.77215200	1.78436800	1.46847100	H	0.82402800	-5.22505800	-2.96731800
C	3.71410000	1.02818800	-2.01298800	H	2.38264800	-2.83455600	5.11148700
C	3.25583900	-1.31631000	-2.66977500	H	1.75519200	-4.48643900	5.34873400
C	1.77674100	-2.78607300	0.94580200	H	3.34335800	-4.23760400	4.58148100
C	5.44659800	0.93928000	-0.18297100				
C	5.27310900	-0.30273900	1.91153300				
H	1.68183900	1.85098000	1.41232900				
H	3.05469200	1.79278000	2.53274200				
H	3.21403900	2.66610300	0.97298700				
C	4.79419300	1.63229200	-1.32150600				
C	3.13153100	1.68660900	-3.10586300				
H	3.38882200	-2.29807700	-2.19790300				
H	2.32562700	-1.32351700	-3.25858700				
H	4.10723800	-1.14132000	-3.34328600				
C	1.60163100	-4.15928400	0.28859500				
C	2.40963100	-2.84551600	2.33177600				

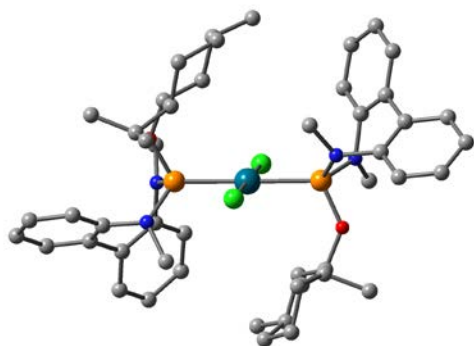


Ixb (+3.9 vs. **Ixa**)

Pd	0.03872700	-0.07699400	-0.22003100
Cl	0.02007000	-0.14426500	-2.59017500
Cl	0.02507200	0.05034100	2.16427600
P	2.34347900	-0.60395700	-0.25919900
N	3.32068300	0.28028400	0.79526000
N	3.25173100	-0.45747900	-1.69845000
O	2.66194200	-2.17169500	0.05154500
C	4.73742700	0.04292100	0.76574200
C	2.93212100	1.55196600	1.41228000
C	3.74474800	0.83820800	-2.04523000
C	3.22184100	-1.46470500	-2.75853000
C	1.80462600	-3.30248600	0.34211100
C	5.51881500	0.60467100	-0.26865700
C	5.34182600	-0.68189300	1.79739200
H	1.85067200	1.69722700	1.34031600
H	3.20193700	1.55034800	2.47996900
H	3.44119400	2.39534400	0.91458100
C	4.87354300	1.36443000	-1.36827600
C	3.16249300	1.56282200	-3.09544700
H	3.10306200	-2.45766400	-2.30712100
H	2.40679800	-1.30543500	-3.48118600
H	4.18720800	-1.44833600	-3.28831700
C	1.26539700	-3.29610200	1.77826700
C	0.67870100	-3.47283700	-0.67600500
H	2.49901800	-4.15190200	0.23060100
C	6.91186000	0.42753100	-0.22587900
C	6.72807000	-0.85676900	1.81918500
H	4.71139300	-1.10237300	2.58135200
C	5.37994300	2.61209400	-1.77096100
C	3.68657300	2.79661000	-3.48603200
H	2.27861600	1.15143400	-3.58401600
C	0.56068900	-4.64569400	2.01416100
H	0.49355300	-2.51238300	1.82468000
C	2.32456600	-2.90187800	2.83425900

C	-0.09617000	-4.78093700	-0.45375500
H	1.08554900	-3.43741100	-1.69858200
H	-0.02263700	-2.62477000	-0.58776000
C	7.51334900	-0.29672800	0.80651200
H	7.52518000	0.84757000	-1.02675100
H	7.19223900	-1.42999600	2.62537400
C	4.79742900	3.32496700	-2.82094900
H	6.24114900	3.02755700	-1.24195600
H	3.21622200	3.35216800	-4.30115600
C	-0.57008300	-4.87789200	1.00453100
H	1.29385800	-5.46926700	1.94198600
H	0.15252400	-4.68043500	3.03562400
H	2.63786800	-1.88243600	2.55751800
C	3.57401100	-3.79084000	2.82737400
C	1.71489900	-2.80414400	4.23797800
H	0.60330800	-5.62005000	-0.63471600
C	-1.26200600	-4.89703400	-1.43845000
H	8.59789400	-0.43086400	0.81486000
H	5.20677200	4.29480400	-3.11408700
H	-1.35864300	-4.12252900	1.16657900
H	-1.04167700	-5.86027500	1.17719000
H	4.09562300	-3.75413700	1.85881300
H	4.29023200	-3.45749300	3.59647800
H	3.32670100	-4.84290900	3.04707600
H	0.80656400	-2.18091400	4.22863700
H	1.44987500	-3.79454200	4.64374300
H	2.43120200	-2.34591500	4.93937300
H	-0.91303700	-4.85848300	-2.48305200
H	-1.81277100	-5.84133800	-1.29826500
H	-1.97585900	-4.06758900	-1.30139900
P	-2.25813100	0.45902700	-0.24441400
N	-3.21008200	-0.41416500	0.83798200
N	-3.20928800	0.35030200	-1.65337200
O	-2.47868300	2.05129500	0.03343400
C	-4.62433200	-0.17096400	0.85723400
C	-2.78906600	-1.65546300	1.48920300
C	-3.72195600	-0.94024800	-1.99526200
C	-3.14205800	1.36077800	-2.71514200
C	-1.62125400	2.84972200	0.88768500
C	-5.43718900	-0.72302700	-0.15696000
C	-5.19344500	0.54874800	1.91249300
H	-1.72017100	-1.82267500	1.33042500
H	-2.96598900	-1.60132100	2.57479400
H	-3.34716000	-2.51322700	1.07591200
C	-4.82524500	-1.47349800	-1.28169400
C	-3.18205100	-1.65397500	-3.07575000
H	-3.25413600	2.35873600	-2.27225800
H	-2.19975900	1.32249900	-3.28314000
H	-3.98360400	1.19388800	-3.40261400
C	-1.41019300	4.21811800	0.23174900
C	-2.26083500	2.92647700	2.26949500
H	-0.64705100	2.34944400	0.98305700
C	-6.82788300	-0.54417500	-0.06999400

C	-6.57830800	0.72370000	1.97922400
H	-4.53638600	0.96451300	2.67789000
C	-5.34555600	-2.71779900	-1.67740800
C	-3.72108600	-2.88353000	-3.45865000
H	-2.31907300	-1.23727200	-3.59558400
C	-0.63382200	5.12123300	1.20950000
H	-2.41817400	4.65335300	0.09456500
C	-0.75907500	4.11197700	-1.17334500
C	-1.48072700	3.83790100	3.22390700
H	-2.31793800	1.90568900	2.67836500
H	-3.29410900	3.30020600	2.15505400
C	-7.39533500	0.17184100	0.98714100
H	-7.46664900	-0.95649100	-0.85478700
H	-7.01744700	1.29061300	2.80367600
C	-4.80385300	-3.42039700	-2.75561500
H	-6.18683600	-3.13789600	-1.12075700
H	-3.28198000	-3.43018300	-4.29674600
C	-1.30541100	5.22129500	2.58228300
H	0.38359000	4.71598100	1.34717200
H	-0.51144500	6.12386100	0.77019700
H	-1.30553700	3.31669400	-1.70242500
C	0.71959100	3.70118500	-1.15233700
C	-0.94990700	5.40121200	-1.98256000
H	-0.47375900	3.39641100	3.35195800
C	-2.14829800	3.91098000	4.59779500
H	-8.47892000	0.30673000	1.03086100
H	-5.22265800	-4.38834900	-3.04120300
H	-2.29927100	5.69573300	2.47760000
H	-0.71372100	5.87411100	3.24661400
H	0.89251600	2.78750500	-0.56483300
H	1.07614100	3.48962700	-2.17136200
H	1.36188700	4.49516000	-0.73806200
H	-2.01486400	5.67619400	-2.05806200
H	-0.41524500	6.25112700	-1.52648800
H	-0.55925100	5.28137000	-3.00617000
H	-2.24444000	2.90992400	5.04886500
H	-1.56948700	4.54210200	5.29169100
H	-3.16133700	4.34169700	4.51786900

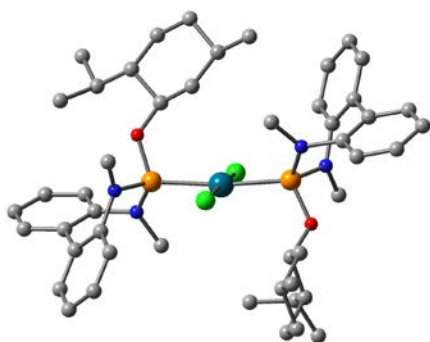


IXc (+7.2 vs. IXa)

Pd	-0.00000600	-0.00006900	-0.23166900
Cl	0.00000600	-0.00054800	-2.60528400
Cl	-0.00003900	0.00027700	2.15225700
P	2.26852300	-0.65895300	-0.27295800
N	3.27960900	0.16209800	0.79856300
N	3.19236700	-0.53774700	-1.70486200
O	2.50463700	-2.24385800	0.01532400
C	4.68275100	-0.14391700	0.78168400
C	2.93977700	1.43448200	1.43964000
C	3.75736300	0.73324600	-2.03174200
C	3.10810600	-1.52636600	-2.77995200
C	1.59769600	-3.34104100	0.28564200
C	5.49995600	0.39029500	-0.23931800
C	5.24127000	-0.90782900	1.81099900
H	1.87886300	1.65936900	1.30121700
H	3.13667200	1.38400300	2.52197200
H	3.53563200	2.25476100	1.00351500
C	4.90414000	1.19345300	-1.33619300
C	3.23119900	1.49483200	-3.08601300
H	2.94664300	-2.51951400	-2.34225600
H	2.29619800	-1.31831200	-3.49358800
H	4.06935300	-1.54624100	-3.31671900
C	1.07578800	-3.34636400	1.72799000
C	0.45458300	-3.43193300	-0.72327500
H	2.25043000	-4.21847000	0.14327700
C	6.88217600	0.14378700	-0.18672500
C	6.61702600	-1.15051900	1.84306900
H	4.58411100	-1.30483200	2.58514300
C	5.48216600	2.41475700	-1.72362700
C	3.82876000	2.69884700	-3.46303700
H	2.33480400	1.13478900	-3.59170200
C	0.30876200	-4.66481400	1.94054500
H	0.34315200	-2.52853200	1.80222100
C	2.16444900	-3.02858000	2.77938500

C	-0.37964700	-4.70671900	-0.51971400
H	0.85278800	-3.39476900	-1.74933800
H	-0.20334000	-2.55241500	-0.60945600
C	7.43789500	-0.61985900	0.84290900
H	7.52282900	0.54085200	-0.97781300
H	7.04510200	-1.75386100	2.64723300
C	4.95581000	3.16322800	-2.77831500
H	6.35707700	2.77980400	-1.18014600
H	3.40086300	3.28359000	-4.28093600
C	-0.84462200	-4.81128700	0.94086200
H	0.99750300	-5.52271300	1.83657800
H	-0.08713200	-4.70514800	2.96662400
H	2.52432400	-2.02018800	2.52002000
C	3.36817100	-3.97754800	2.73905800
C	1.57543500	-2.93063600	4.19185600
H	0.27849400	-5.57358300	-0.72362300
C	-1.55808300	-4.74911800	-1.49408700
H	8.51437100	-0.80756500	0.85884100
H	5.42077200	4.11137900	-3.05891400
H	-1.58837800	-4.01670200	1.12912900
H	-1.36793400	-5.77007200	1.09633800
H	3.88079900	-3.94560500	1.76549600
H	4.10836700	-3.69683700	3.50649200
H	3.07110900	-5.02063200	2.93912300
H	0.69996800	-2.26212000	4.20620400
H	1.26436300	-3.91480600	4.57971100
H	2.32151300	-2.52482400	4.89455900
H	-1.21873200	-4.69985300	-2.54134100
H	-2.14784000	-5.67194700	-1.37036700
H	-2.23362800	-3.89374100	-1.32952200
P	-2.26848300	0.65889500	-0.27308100
N	-3.27954400	-0.16207300	0.79854900
N	-3.19242900	0.53766200	-1.70492600
O	-2.50457400	2.24381400	0.01521300
C	-4.68268000	0.14398200	0.78168100
C	-2.93972700	-1.43449700	1.43953300
C	-3.75743500	-0.73333500	-2.03174100
C	-3.10800300	1.52623300	-2.78006500
C	-1.59761900	3.34104300	0.28538700
C	-5.49991600	-0.39038600	-0.23921300
C	-5.24114600	0.90808600	1.81087100
H	-1.87883700	-1.65942700	1.30098700
H	-3.13648900	-1.38406000	2.52189300
H	-3.53565300	-2.25474400	1.00344700
C	-4.90411700	-1.19359900	-1.33605400
C	-3.23135300	-1.49490100	-3.08606200
H	-2.94727900	2.51949900	-2.34235400
H	-2.29559800	1.31852000	-3.49323300
H	-4.06894100	1.54555900	-3.31739100
C	-1.07582300	3.34662400	1.72777300
C	-0.45448900	3.43179000	-0.72349400
H	-2.25033900	4.21845100	0.14283300
C	-6.88213500	-0.14390200	-0.18660200

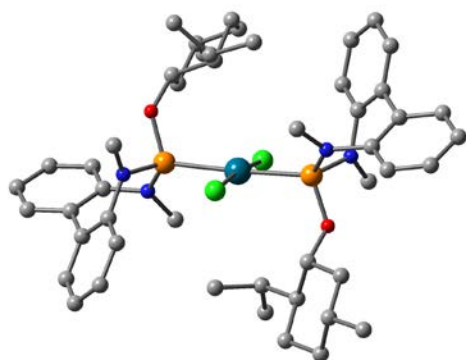
C	-6.61691000	1.15077600	1.84294700
H	-4.58396300	1.30524000	2.58490700
C	-5.48208200	-2.41495700	-1.72338600
C	-3.82886400	-2.69898100	-3.46298300
H	-2.33504200	-1.13481900	-3.59187000
C	-0.30887000	4.66513500	1.94017300
H	-0.34314900	2.52884000	1.80220500
C	-2.16458200	3.02894600	2.77914800
C	0.37969400	4.70662500	-0.52005700
H	-0.85266300	3.39451000	-1.74956700
H	0.20344500	2.55229100	-0.60958300
C	-7.43781800	0.61991700	0.84293200
H	-7.52282600	-0.54110000	-0.97759300
H	-7.04494000	1.75426700	2.64702400
C	-4.95578500	-3.16343300	-2.77810500
H	-6.35691000	-2.78005100	-1.17980000
H	-3.40102900	-3.28370000	-4.28093200
C	0.84457900	4.81145400	0.94052600
H	-0.99761100	5.52301200	1.83602100
H	0.08699800	4.70567000	2.96625200
H	-2.52442900	2.02052000	2.51986200
C	-3.36831900	3.97793100	2.73851200
C	-1.57573100	2.93121300	4.19166000
H	-0.27846300	5.57343400	-0.72414400
C	1.55819900	4.74891300	-1.49435300
H	-8.51429900	0.80759000	0.85888000
H	-5.42069700	-4.11163700	-3.05860300
H	1.58834700	4.01692400	1.12899900
H	1.36785400	5.77029000	1.09581700
H	-3.88078800	3.94576900	1.76488300
H	-4.10860900	3.69735800	3.50590200
H	-3.07126300	5.02104200	2.93843000
H	-0.70034400	2.26259400	4.20625100
H	-1.26453000	3.91540900	4.57934500
H	-2.32192300	2.52566300	4.89439300
H	1.21893100	4.69947400	-2.54162500
H	2.14793500	5.67176700	-1.37073300
H	2.23373800	3.89356600	-1.32962200



Xa (+4.1 vs. IXa)

Pd	-0.05337800	0.15921100	-0.06331900
Cl	0.31120000	-1.11310300	-2.03882600
Cl	-0.37626800	1.53618200	1.85010300
P	-2.39117300	-0.10596500	-0.27847700
N	-3.14528200	-0.71681400	1.09719500
N	-3.05504300	-1.12723700	-1.46927200
O	-3.15226300	1.26028000	-0.75404800
C	-4.56003700	-0.94898400	1.06658800
C	-2.47401600	-1.05187500	2.35495100
C	-3.16080800	-2.52662300	-1.20445700
C	-3.08825300	-0.68625400	-2.87058500
C	-2.76997900	2.60051100	-0.35993800
C	-5.06736300	-2.08200000	0.39462700
C	-5.42205500	-0.08967600	1.75872100
H	-1.38699800	-1.00781400	2.23182000
H	-2.75291500	-0.35321000	3.16008900
H	-2.75052200	-2.07536900	2.65395600
C	-4.15709500	-3.01010500	-0.31959900
C	-2.33724200	-3.43769900	-1.88442000
H	-3.70671300	0.21733900	-2.95875000
H	-2.08382600	-0.48053200	-3.27301600
H	-3.54954100	-1.48020400	-3.47279300
C	-2.99113900	3.53811500	-1.55161900
C	-3.57282900	2.99031300	0.87641900
H	-1.70374600	2.60629200	-0.09490100
C	-6.45318600	-2.31778500	0.43733200
C	-6.79504300	-0.34100700	1.79199700
H	-5.00174000	0.77694100	2.27082600
C	-4.29112900	-4.39956600	-0.15092200
C	-2.49468200	-4.81300300	-1.70991500
H	-1.55761600	-3.04553200	-2.53720900
C	-2.73619200	4.98860800	-1.09841300
H	-4.06043600	3.45069600	-1.82289900
C	-2.16755900	3.11323600	-2.79536500

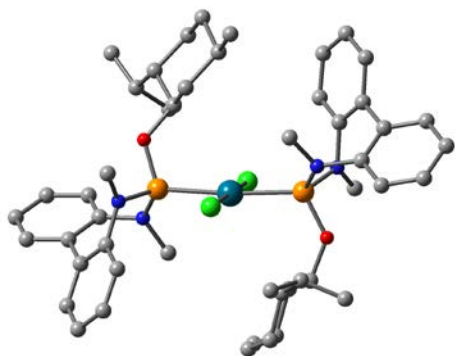
C	-3.31417300	4.43843000	1.30804200	C	6.74348000	-0.16998900	-1.69224200
H	-3.30548100	2.30019000	1.69174300	H	4.80887100	-0.91949600	-2.32941300
H	-4.64609600	2.84965300	0.65640000	C	4.86003700	4.10067100	0.40791200
C	-7.31064600	-1.45894800	1.12736700	C	3.05627600	4.78615600	1.85813200
H	-6.85992100	-3.18222700	-0.09269800	H	1.77998000	3.19385300	2.57167800
H	-7.46082300	0.33785900	2.33037700	C	2.82928000	-5.00999200	0.32899800
C	-3.47503400	-5.29784500	-0.83939100	H	3.53246500	-3.62444500	1.80978600
H	-5.04831300	-4.77479500	0.54162100	C	4.78849000	-3.29505900	0.07100300
H	-1.83792400	-5.50500800	-2.24283600	C	0.44356000	-4.22837600	0.74766200
C	-3.57225800	5.37996400	0.12382900	H	1.20434900	-2.79523100	2.19803400
H	-1.66832900	5.10920600	-0.84636900	H	0.28931400	-2.07452600	0.85992900
H	-2.93847000	5.67852900	-1.93263700	C	7.40363700	0.77803700	-0.90309900
H	-2.37192600	2.04166600	-2.93760700	H	7.18795000	2.44758000	0.44927900
C	-0.64998100	3.25930000	-2.61616100	H	7.31290100	-0.89925400	-2.27327400
C	-2.63808700	3.83266300	-4.06564600	C	4.16256300	5.11395100	1.06816000
H	-2.24238500	4.51679400	1.57279600	H	5.71439900	4.35419800	-0.22422300
C	-4.13979700	4.81014000	2.54048100	H	2.49204200	5.56954700	2.37036300
H	-8.38480400	-1.65940900	1.14087300	C	1.49485300	-5.30964000	1.02138300
H	-3.59656100	-6.37283100	-0.68639000	H	2.69115300	-5.05529800	-0.76687000
H	-4.64748900	5.34373400	-0.13402500	H	3.55239600	-5.79793700	0.58398300
H	-3.35364600	6.42185100	0.41421700	H	4.58443000	-2.74009900	-0.86129800
H	-0.29085800	2.76569700	-1.70008900	C	5.62542300	-4.52384400	-0.31428500
H	-0.11924900	2.79852700	-3.46437400	C	5.62262000	-2.38566400	0.98715500
H	-0.34155400	4.31642200	-2.57092300	H	0.23722400	-4.21926600	-0.33877300
H	-3.72182700	3.70471400	-4.22264900	C	-0.87731800	-4.48586700	1.47148600
H	-2.43035300	4.91473400	-4.02339700	H	8.49548100	0.79294200	-0.86101300
H	-2.12018400	3.43574800	-4.95392200	H	4.47676800	6.15375300	0.95789500
H	-3.92340800	4.13535200	3.38477600	H	1.65861700	-5.37787700	2.11344800
H	-3.92989000	5.84149600	2.86778300	H	1.11708400	-6.29524000	0.69934200
H	-5.21972200	4.74014700	2.32354300	H	5.13287300	-5.15835700	-1.06592800
P	2.27947000	0.19253400	0.26385200	H	6.59018800	-4.20072300	-0.73812900
N	3.17973400	0.71887800	-1.05343400	H	5.84871200	-5.15142000	0.56539700
N	2.99756900	1.06319900	1.54306100	H	5.08099100	-1.46970500	1.25162300
O	2.83804800	-1.27204300	0.72647000	H	5.87859100	-2.91863000	1.91987100
C	4.60993500	0.73039300	-0.97094300	H	6.56419800	-2.09208400	0.49735600
C	2.60338200	1.41820100	-2.20371800	H	-1.63559200	-3.74169200	1.18395900
C	3.36118800	2.42772800	1.33031200	H	-1.28205300	-5.47875000	1.22238500
C	2.81435200	0.62732700	2.93180400	H	-0.74289300	-4.43613700	2.56586700
C	2.33061300	-2.57856600	0.37538700				
C	5.26258400	1.70949400	-0.19180500				
C	5.34831200	-0.19031400	-1.72195000				
H	2.88656100	2.48475300	-2.18859500				
H	1.51228000	1.33869000	-2.18556500				
H	2.96073900	0.96642400	-3.14221400				
C	4.48311100	2.75048400	0.52563000				
C	2.65870900	3.45428400	1.98187400				
H	2.78105400	-0.46866000	2.95975400				
H	1.88916800	1.01694100	3.38268900				
H	3.67989100	0.96091600	3.52445600				
C	3.40555600	-3.62942100	0.71031900				
C	1.02220700	-2.85788400	1.10989300				
H	2.14646300	-2.59657500	-0.71113500				
C	6.66883900	1.70862400	-0.16563900				



Xb (+5.1 vs. **Ixa**)

Pd	0.07593300	0.04325300	0.06532500
Cl	0.26714800	-1.12937000	-2.00001700
Cl	-0.13836800	1.44546800	1.96823600
P	-2.26018600	0.11690200	-0.27296400
N	-3.26976200	-0.17586000	1.05248600
N	-2.96047900	-0.94095800	-1.40310600
O	-2.68444200	1.51332800	-1.01043800
C	-4.68649500	-0.31272500	0.86100500
C	-2.83413600	-0.32746600	2.44430400
C	-3.19283100	-2.28942800	-0.98152000
C	-2.99505000	-0.68211000	-2.84387100
C	-2.38135500	2.86317200	-0.56601700
C	-5.21260500	-1.49339500	0.29041500
C	-5.55249800	0.67274000	1.35116500
H	-1.75200100	-0.46696400	2.49364900
H	-3.09186200	0.55666100	3.04977000
H	-3.32486500	-1.21335000	2.87531800
C	-4.31118500	-2.57779100	-0.16513800
C	-2.35867900	-3.33155000	-1.41229800
H	-2.80492600	0.38077200	-3.02867100
H	-2.24128100	-1.26986300	-3.38825400
H	-3.99825000	-0.92776400	-3.23065400
C	-1.65052500	3.60829300	-1.69565800
C	-3.72567400	3.49961100	-0.21455600
H	-1.73870600	2.81768800	0.32731100
C	-6.60870800	-1.63147000	0.19913500
C	-6.93690100	0.51893600	1.25489500
H	-5.12882700	1.55927100	1.82517400
C	-4.55452000	-3.91253500	0.20343700
C	-2.62074100	-4.65189900	-1.04338600
H	-1.49045600	-3.08600800	-2.02261700
C	-1.60058400	5.11698600	-1.38389600
H	-2.28459900	3.47133100	-2.59166300

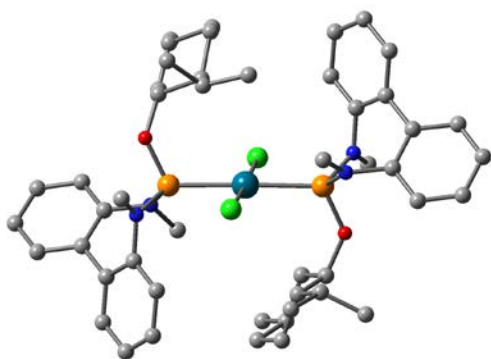
C	-0.25332000	3.01067700	-2.01258900	C	6.90792500	1.17330200	0.20750700
C	-3.64369400	4.99967600	0.08822800	C	7.01200100	-0.81595700	-1.16521500
H	-4.15844600	2.95779900	0.63782900	H	5.10512000	-1.54803300	-1.88259300
H	-4.40636100	3.33718500	-1.06936600	C	5.14922400	3.64519500	0.54023600
C	-7.46635500	-0.63581400	0.67013100	C	3.33256200	4.44042700	1.91515300
H	-7.02088800	-2.53442700	-0.25755500	H	1.99104500	2.91951500	2.65871000
H	-7.59909600	1.30075500	1.63464100	C	0.76471400	-4.80610000	0.49334000
C	-3.72036500	-4.94445700	-0.23027900	H	0.38861800	-2.73614900	0.15383700
H	-5.40698400	-4.13568000	0.84946800	C	0.49563400	-2.94270700	2.28224700
H	-1.95434000	-5.44913000	-1.38101200	C	2.64159600	-4.74931100	-1.21619400
C	-2.97724300	5.71593700	-1.09272900	H	2.37899100	-2.62075600	-1.51108200
H	-0.95927800	5.28558200	-0.50271100	H	3.98640400	-3.07216900	-0.89783500
H	-1.11861000	5.64580500	-2.22178200	C	7.65614300	0.16953400	-0.40964800
H	-0.35752700	1.91563100	-1.93770000	H	7.41124700	1.94240900	0.79810100
C	0.83422900	3.44468900	-1.01844700	H	7.59013300	-1.60125700	-1.65825200
C	0.17674800	3.31059700	-3.45399700	C	4.46348300	4.70405800	1.13638500
H	-2.98982900	5.13421600	0.97164800	H	6.03217900	3.84499500	-0.07162300
C	-5.02161100	5.57452600	0.42115800	H	2.78331400	5.25952300	2.38621600
H	-8.54813200	-0.76264300	0.58237100	C	1.17052100	-5.09735400	-0.95403000
H	-3.92469000	-5.97422000	0.07286500	H	1.34220400	-5.45827800	1.17345300
H	-3.62722600	5.62246200	-1.98286000	H	-0.29480900	-5.06287600	0.63450600
H	-2.88538600	6.79482200	-0.88030800	H	0.61107200	-1.84799900	2.35932500
H	0.52132000	3.30872400	0.02539200	C	1.31096500	-3.56319000	3.42353500
H	1.74631900	2.84666000	-1.15059500	C	-0.99945300	-3.24407500	2.45091600
H	1.11621800	4.50003400	-1.16140200	H	3.25757000	-5.39853700	-0.56358800
H	-0.55335800	2.92114300	-4.18222700	C	3.04686600	-5.00647200	-2.66877100
H	0.28268200	4.39471300	-3.62864300	H	8.74351300	0.15738400	-0.30179200
H	1.15187700	2.84679000	-3.67477400	H	4.81002300	5.73020100	0.99150800
H	-5.47448400	5.05895900	1.28390100	H	0.53841300	-4.49923300	-1.63453800
H	-4.95966600	6.64835300	0.66138600	H	0.98519800	-6.15799200	-1.19663500
H	-5.70898800	5.46074800	-0.43461700	H	2.37059600	-3.26634900	3.38523200
P	2.41659000	-0.16165100	0.42769500	H	0.91489500	-3.23777400	4.39916100
N	3.44522900	0.24910700	-0.84443600	H	1.26741600	-4.66488000	3.40289500
N	3.14722000	0.70953700	1.70444800	H	-1.58760100	-2.83628500	1.61374500
O	2.82940200	-1.64113500	0.99327000	H	-1.19467700	-4.32729100	2.49841000
C	4.86587600	0.19951200	-0.65195700	H	-1.38237100	-2.80242400	3.38351700
C	3.02075400	0.67127400	-2.18114800	H	4.11049000	-4.77062900	-2.83745200
C	3.56500400	2.05683600	1.47420500	H	2.88383000	-6.05953400	-2.95051200
C	2.94347800	0.30686500	3.10083900	H	2.45186900	-4.37848500	-3.35364700
C	2.46362300	-2.98654200	0.60943100				
C	5.50651600	1.21171100	0.09320200				
C	5.62119300	-0.79581300	-1.28477100				
H	3.53255700	1.61105600	-2.44392700				
H	1.94101000	0.83749200	-2.20623900				
H	3.26120900	-0.09136200	-2.93958200				
C	4.72512700	2.31425600	0.70325800				
C	2.88833100	3.12789500	2.07825000				
H	2.94974700	-0.78767000	3.16581700				
H	1.99591200	0.67967700	3.51908400				
H	3.78129500	0.69237200	3.70121400				
C	0.98657600	-3.32746500	0.86437700				
C	2.91129200	-3.29091600	-0.81831400				
H	3.07571600	-3.59807400	1.29325500				



Xc (+2.9 vs. IXa)			
Pd	-0.04752900	-0.19427900	0.01130700
Cl	0.19636700	0.88940300	2.11328200
Cl	-0.20858300	-1.31921000	-2.07182200
P	-2.37372900	-0.38120600	0.42752900
N	-3.39618700	-0.10122800	-0.88912400
N	-3.08791400	0.66695100	1.57092200
O	-2.86511600	-1.79775400	1.06867500
C	-4.81197400	-0.06074500	-0.64502200
C	-2.99217800	0.53049300	-2.14789600
C	-3.38011500	1.99752800	1.13625200
C	-3.08321500	0.42197500	3.01134200
C	-2.14919000	-3.02932100	1.34150400
C	-5.38802200	1.10466700	-0.09041700
C	-5.61803600	-1.13700600	-1.02663400
H	-1.90326800	0.60682500	-2.21005100
H	-3.34038000	-0.06832300	-3.00444900
H	-3.42676200	1.54172300	-2.22026600
C	-4.52278100	2.23436700	0.33179600
C	-2.57608600	3.07408400	1.53893700
H	-3.00749500	-0.65697800	3.19176600
H	-2.25027300	0.92306000	3.52761800
H	-4.03871700	0.77014500	3.43659900
C	-1.68547900	-3.75939200	0.07337400
C	-1.00636100	-2.81594100	2.33194600
H	-2.92113400	-3.64027100	1.83749800
C	-6.78405100	1.16056500	0.05012200
C	-7.00536000	-1.06943600	-0.86900100
H	-5.14489500	-2.02290400	-1.45077000
C	-4.81989300	3.55435800	-0.04724200
C	-2.89239800	4.37987100	1.15716200
H	-1.68615800	2.86602600	2.13386300
C	-1.06484300	-5.10481600	0.49516100
H	-0.87170200	-3.16003800	-0.36321600
C	-2.78125300	-3.85275700	-1.01663700

C	-0.35467400	-4.14537900	2.74078700
H	-1.37908500	-2.27983600	3.21906600
H	-0.24426900	-2.16844200	1.86769600
C	-7.58795300	0.08395900	-0.33458500
H	-7.23864400	2.05303700	0.48708900
H	-7.62875200	-1.91686100	-1.16441800
C	-4.01568800	4.62152400	0.36006000
H	-5.69143800	3.73863200	-0.68016600
H	-2.24817300	5.20630000	1.46751400
C	0.08839000	-4.91068900	1.48576600
H	-1.83540300	-5.75092400	0.95338200
H	-0.69951400	-5.63770800	-0.39553000
H	-3.02488700	-2.80967500	-1.27426600
C	-4.07562400	-4.52756400	-0.54467200
C	-2.25219700	-4.50601600	-2.29966300
H	-1.12779700	-4.75520400	3.24746700
C	0.79893900	-3.92663800	3.72133700
H	-8.67176700	0.14352200	-0.20783800
H	-4.26208700	5.63928300	0.04795600
H	0.89981000	-4.34348500	0.99208000
H	0.51578800	-5.88665500	1.77245500
H	-4.54563600	-3.97971400	0.28641800
H	-4.81083200	-4.56867300	-1.36535400
H	-3.89817400	-5.56508000	-0.21575700
H	-1.30801800	-4.03717800	-2.61753400
H	-2.07695300	-5.58692100	-2.17060900
H	-2.97977800	-4.38984600	-3.11953800
H	0.46792300	-3.37761800	4.61768800
H	1.23001300	-4.88640500	4.04899600
H	1.60575600	-3.34245900	3.24962900
P	2.24755400	0.18675500	-0.39538600
N	3.28571900	-0.23036500	0.86144600
N	3.06464900	-0.50824800	-1.71821800
O	2.51401900	1.75865500	-0.76466000
C	4.69466500	-0.01619000	0.69586200
C	2.91387000	-1.09700800	1.98061100
C	3.59524900	-1.82695500	-1.55946000
C	2.85794700	-0.02868100	-3.08674400
C	1.52532100	2.80900800	-0.60885600
C	5.44691600	-0.89730500	-0.11112900
C	5.32228900	1.02099900	1.39342200
H	3.42631800	-2.07110600	1.89740700
H	1.83322200	-1.26577300	1.98594100
H	3.18725100	-0.62843300	2.93893900
C	4.78081600	-2.02537400	-0.80861900
C	2.98386600	-2.91915700	-2.19409300
H	2.67631500	1.05276100	-3.06194000
H	2.00646800	-0.51519800	-3.58635000
H	3.77567300	-0.20930800	-3.66774500
C	2.23981600	4.14632000	-0.38307200
C	0.61895100	2.86421100	-1.83634200
H	0.91442500	2.58388000	0.27729600
C	6.83496200	-0.69723500	-0.20291900

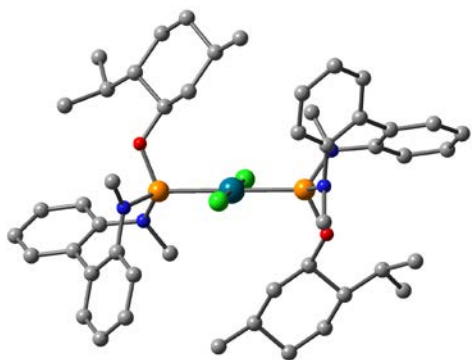
C	6.70279700	1.20725100	1.28837200
H	4.71188300	1.67112000	2.02097600
C	5.31876200	-3.32184300	-0.72837800
C	3.53696300	-4.19797300	-2.10475100
H	2.05528200	-2.75295600	-2.74025400
C	1.14908100	5.21567200	-0.17098300
H	2.76574600	4.38865700	-1.32634200
C	3.32467300	4.09249800	0.71966200
C	-0.47094700	3.93221200	-1.67194800
H	1.23412400	3.08437200	-2.72768200
H	0.15960900	1.87583200	-1.99957000
C	7.45844800	0.34620000	0.48552000
H	7.42652200	-1.36348400	-0.83542700
H	7.18558400	2.02431900	1.82986400
C	4.70989400	-4.40127400	-1.37089500
H	6.22518900	-3.48016100	-0.13903200
H	3.04327300	-5.03752300	-2.60055600
C	0.17184400	5.28984500	-1.35037500
H	0.58601900	4.98335500	0.74998900
H	1.61454600	6.20073000	-0.01249800
H	4.00918800	3.28630500	0.41138700
C	2.78564500	3.72783200	2.10873000
C	4.14733400	5.38637800	0.77259800
H	-1.08852300	3.63663200	-0.80506300
C	-1.38244700	4.00938700	-2.89697700
H	8.53788800	0.48883600	0.39220900
H	5.14534900	-5.40019200	-1.28984800
H	0.71219500	5.64629100	-2.24741700
H	-0.61596900	6.03431500	-1.14283300
H	2.27319400	2.75482000	2.11473500
H	3.61115200	3.67674900	2.83821000
H	2.07545000	4.48440500	2.48141800
H	4.52734800	5.66598200	-0.22404600
H	3.55618400	6.23424900	1.15665800
H	5.01549200	5.26597600	1.44095900
H	-1.83758900	3.03209700	-3.11804600
H	-2.19809000	4.73352900	-2.73884700
H	-0.81655600	4.32586300	-3.78998100



Xd (+5.9 vs. IXa)			
Pd	-0.01891500	0.02701700	-0.07901000
Cl	0.04415800	1.14494700	2.02315500
Cl	-0.03827000	-1.00203400	-2.21233900
P	-2.29140700	-0.53018300	0.37344300
N	-3.44723700	-0.52855900	-0.85926900
N	-3.12665300	0.44213800	1.49438000
O	-2.45639900	-1.97218900	1.12839500
C	-4.82775600	-0.69286700	-0.49744200
C	-3.23984900	-0.24243400	-2.27893700
C	-3.64224900	1.68345400	1.00421200
C	-3.09077000	0.26290100	2.94251500
C	-1.52176500	-3.05237700	1.37544700
C	-5.55447700	0.41185600	0.00045800
C	-5.46767600	-1.91466400	-0.72944200
H	-2.19370700	0.00266100	-2.47026500
H	-3.50805700	-1.11601600	-2.89680700
H	-3.87088100	0.61058500	-2.57861200
C	-4.85727900	1.69056000	0.27696100
C	-2.97976300	2.88908000	1.27264200
H	-2.73075000	-0.74582500	3.17455700
H	-2.43184900	0.99143900	3.43874600
H	-4.11295800	0.36154000	3.34570100
C	-0.89953400	-3.63869000	0.09868000
C	-0.46884000	-2.65202800	2.40576100
H	-2.16761000	-3.81977000	1.83267100
C	-6.93050300	0.25838700	0.23630000
C	-6.83597500	-2.05289400	-0.48099500
H	-4.88048000	-2.75156200	-1.10975400
C	-5.37600200	2.92082500	-0.15944300
C	-3.51269700	4.10335000	0.83423600
H	-2.03475800	2.85152800	1.81516800
C	0.00224300	-4.82532600	0.49124500
H	-0.23402100	-2.86754100	-0.32002000

C	-1.94498900	-3.95636100	-1.00103000
C	0.41980700	-3.84249600	2.79394100
H	-0.96710400	-2.23348700	3.29471700
H	0.15893100	-1.85028000	1.98522700
C	-7.56863000	-0.96144800	-0.00299800
H	-7.49858300	1.10392100	0.63195200
H	-7.32791900	-3.01217300	-0.65955700
C	-4.71296800	4.11948900	0.11604300
H	-6.30630600	2.93029300	-0.73273400
H	-2.98206900	5.03496800	1.04514000
C	1.05842400	-4.42930400	1.52808500
H	-0.61259000	-5.65052700	0.89378700
H	0.50127500	-5.21597600	-0.40820600
H	-2.40740000	-2.99077900	-1.26114500
C	-3.07076800	-4.89165400	-0.53996200
C	-1.28412100	-4.48320700	-2.28132500
H	-0.23555800	-4.62191200	3.22946000
C	1.45908100	-3.45622200	3.84725100
H	-8.63869100	-1.06245900	0.19455200
H	-5.13027700	5.06540300	-0.23791000
H	1.73801100	-3.67775100	1.08572600
H	1.68308700	-5.30119200	1.78699200
H	-3.64990800	-4.46204300	0.29152700
H	-3.77557100	-5.08065300	-1.36644100
H	-2.68102900	-5.87070500	-0.21517200
H	-0.45408800	-3.83060900	-2.59155500
H	-0.89432700	-5.50635100	-2.15192200
H	-2.01423300	-4.51412700	-3.10647900
H	0.98220500	-3.04240000	4.75052000
H	2.06181500	-4.32806300	4.14911800
H	2.14923700	-2.69377300	3.45388500
P	2.26430400	0.53841200	-0.46267800
N	3.32439300	0.33189600	0.83980200
N	3.09965400	-0.32405500	-1.67018800
O	2.50702600	2.02690400	-1.08416500
C	4.73471400	0.49305200	0.61193200
C	3.00624300	-0.39762400	2.06891800
C	3.58324100	-1.62317400	-1.31218500
C	3.04999900	0.00331400	-3.09493800
C	1.92174300	3.30869700	-0.73727500
C	5.46086000	-0.53074400	-0.03732100
C	5.39860600	1.61300900	1.12222800
H	3.53265800	-1.36745900	2.08262800
H	1.93053500	-0.57287000	2.14463900
H	3.31540400	0.18665500	2.95007400
C	4.76020300	-1.74034400	-0.53373000
C	2.92812600	-2.78114400	-1.75828800
H	2.67097300	1.02412500	-3.22048700
H	2.39817900	-0.68082700	-3.65815900
H	4.07038300	-0.03862200	-3.51196400
C	0.40886500	3.38720400	-0.99680100
C	2.30217100	3.70973000	0.68613000
H	2.42877600	3.99312700	-1.43704100

C	6.85202300	-0.38797900	-0.16830100
C	6.78276500	1.74249000	0.97919500
H	4.81671100	2.37388300	1.64476600
C	5.24590500	-3.02373400	-0.22845400
C	3.42680300	-4.04730700	-1.44656000
H	2.00995000	-2.67167500	-2.33444000
C	-0.07263500	4.80671200	-0.64176000
H	-0.07381200	2.70588000	-0.27677900
C	-0.00767500	2.90583700	-2.40800800
C	1.78350500	5.10551300	1.06080600
H	1.88798100	2.96963400	1.38855300
H	3.39827300	3.67786700	0.77550900
C	7.50937200	0.73966500	0.32987300
H	7.41908900	-1.16899400	-0.68059800
H	7.29149400	2.62435000	1.37604700
C	4.58949100	-4.17055500	-0.67936400
H	6.14538200	-3.11559000	0.38518700
H	2.89603000	-4.93779300	-1.79246300
C	0.27347900	5.18527800	0.80061800
H	0.38254900	5.54185300	-1.32961900
H	-1.16054800	4.86909800	-0.79011300
H	0.35495700	1.87016700	-2.50108200
C	0.61336900	3.70687100	-3.55882300
C	-1.53479600	2.84287600	-2.53909200
H	2.27467000	5.84170900	0.39477500
C	2.14014000	5.45325100	2.50725300
H	8.59133200	0.83509800	0.20963800
H	4.98019900	-5.15833800	-0.42315000
H	-0.24176900	4.49524500	1.49268000
H	-0.09543300	6.20013800	1.02847900
H	1.71438700	3.68451400	-3.53247700
H	0.30168600	3.28651400	-4.52877600
H	0.29575500	4.76267300	-3.54228200
H	-1.98303700	2.30904900	-1.68695200
H	-1.98746900	3.84683900	-2.57875000
H	-1.82532800	2.31386600	-3.45997900
H	3.22899300	5.41140700	2.67436100
H	1.79432700	6.46543400	2.77322200
H	1.66655500	4.74111500	3.20433900

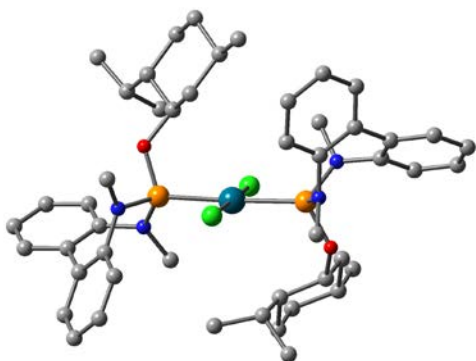


XIa (+7.8 vs. IXa)

Pd	-0.00012100	-0.00001800	0.21243700
Cl	-0.00002000	-0.00045100	-2.16559900
Cl	-0.00023100	0.00086900	2.58663600
P	2.35061500	-0.22265300	0.22930600
N	3.17274400	0.79738300	-0.83169200
N	3.26437300	-0.00269400	1.64991800
O	2.80989100	-1.76197300	-0.07883900
C	4.60716300	0.77073900	-0.86642100
C	2.57788900	1.99817800	-1.42476600
C	3.60408600	1.34077300	2.00710400
C	3.31192600	-1.01016500	2.71199700
C	1.98092200	-2.77390600	-0.70497200
C	5.34495300	1.37855400	0.17373100
C	5.26077400	0.22676900	-1.97550500
H	2.98316200	2.90537100	-0.94475000
H	1.49228900	1.98395800	-1.29763400
H	2.79250400	2.03692300	-2.50399200
C	4.64267300	2.01338800	1.31681000
C	2.94853900	1.98087100	3.07026300
H	3.16635900	-2.00288400	2.26932400
H	2.54005500	-0.85535900	3.48062700
H	4.30812600	-0.98536400	3.18172200
C	2.89128000	-3.89555900	-1.23055400
C	0.94977800	-3.30533300	0.28828400
H	1.46044100	-2.31122200	-1.56128100
C	6.74592500	1.40593600	0.07101500
C	6.65420000	0.26615000	-2.06378500
H	4.65947000	-0.22616700	-2.76562900
C	4.99351200	3.31205600	1.72622900
C	3.31633100	3.26856000	3.46410700
H	2.12990800	1.46100800	3.56823200
C	1.98850100	-4.96788400	-1.87574700
H	3.35882900	-4.36616500	-0.34528300

C	4.03866900	-3.34730500	-2.13588200
C	0.05344400	-4.37723200	-0.34161700
H	1.48076900	-3.72458900	1.16169100
H	0.33038000	-2.47581700	0.66570900
C	7.39696500	0.85351200	-1.03488800
H	7.32842900	1.85901300	0.87680000
H	7.15816900	-0.16790900	-2.93058200
C	4.34328200	3.93759400	2.79115100
H	5.78286300	3.83940100	1.18521600
H	2.78857400	3.75443600	4.28846300
C	0.92708700	-5.50300200	-0.90673400
H	1.48861100	-4.54070900	-2.76390400
H	2.60502900	-5.80328700	-2.23775400
H	3.69283200	-2.38014600	-2.54331400
C	4.39399700	-4.23608300	-3.33612600
C	5.30099700	-3.08370300	-1.30165300
H	-0.46828700	-3.91154500	-1.19742700
C	-1.00590400	-4.86951400	0.64495300
H	8.48796700	0.88006100	-1.09134700
H	4.63042700	4.94960300	3.08658900
H	1.42530600	-6.02491400	-0.06831800
H	0.29733100	-6.25343000	-1.41440500
H	3.54575600	-4.38591100	-4.02044800
H	5.20789700	-3.77239400	-3.91697700
H	4.74835800	-5.22950300	-3.01319000
H	5.09114000	-2.41015300	-0.46092100
H	5.69275800	-4.03327000	-0.89652000
H	6.09507600	-2.62602200	-1.91150300
H	-1.63239700	-4.03885300	1.00820600
H	-1.66948100	-5.61697000	0.18053000
H	-0.53451900	-5.33875100	1.52545300
P	-2.35086100	0.22282500	0.22924300
N	-3.17305200	-0.79718800	-0.83173900
N	-3.26460900	0.00281600	1.64986500
O	-2.81003300	1.76214900	-0.07898100
C	-4.60748500	-0.77086700	-0.86612300
C	-2.57803500	-1.99765000	-1.42538200
C	-3.60381200	-1.34076500	2.00718100
C	-3.31289400	1.01041900	2.71176300
C	-1.98088900	2.77403200	-0.70498800
C	-5.34484800	-1.37921000	0.17403200
C	-5.26152400	-0.22671800	-1.97486300
H	-2.98526600	-2.90503000	-0.94741600
H	-1.49271900	-1.98478700	-1.29566200
H	-2.79020500	-2.03474500	-2.50514900
C	-4.64218000	-2.01383500	1.31696300
C	-2.94800600	-1.98053300	3.07036900
H	-3.16728600	2.00311000	2.26905200
H	-2.54135900	0.85585200	3.48078700
H	-4.30931700	0.98548800	3.18101000
C	-2.89111300	3.89561300	-1.23094400
C	-0.95002600	3.30558400	0.28850300
H	-1.46015800	2.31126500	-1.56110900

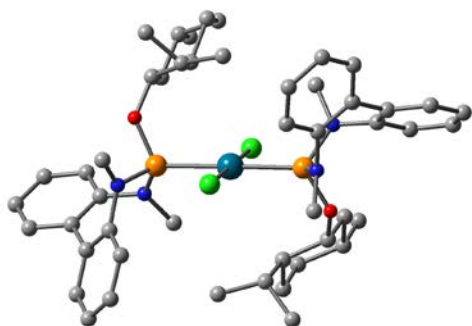
C	-6.74582800	-1.40709500	0.07156300
C	-6.65495900	-0.26653200	-2.06286100
H	-4.66053300	0.22672000	-2.76493300
C	-4.99246000	-3.31262200	1.72646200
C	-3.31527600	-3.26834900	3.46431000
H	-2.12957000	-1.46032400	3.56828900
C	-1.98822200	4.96801000	-1.87586100
H	-3.35897900	4.36621700	-0.34584000
C	-4.03819700	3.34720700	-2.13659500
C	-0.05360100	4.37752700	-0.34117900
H	-1.48127700	3.72481600	1.16176600
H	-0.33067100	2.47612200	0.66610700
C	-7.39729200	-0.85455500	-1.03403400
H	-7.32802900	-1.86061000	0.87732000
H	-7.15925800	0.16769100	-2.92938300
C	-4.34195900	-3.93783800	2.79140800
H	-5.78160000	-3.84033600	1.18549600
H	-2.78731500	-3.75395000	4.28869800
C	-0.92715800	5.50324100	-0.90651400
H	-1.48798400	4.54088300	-2.76384500
H	-2.60471400	5.80334600	-2.23808100
H	-3.69225300	2.37994200	-2.54369400
C	-4.39310000	4.23570300	-3.33716800
C	-5.30079800	3.08379900	-1.30273300
H	0.46835500	3.91187300	-1.19686200
C	1.00550900	4.86979500	0.64565600
H	-8.48829600	-0.88152700	-1.09028400
H	-4.62868900	-4.94995000	3.08689400
H	-1.42567000	6.02509600	-0.06823900
H	-0.29732900	6.25373100	-1.41400400
H	-3.54463700	4.38529200	-4.02126300
H	-5.20684900	3.77191400	-3.91815000
H	-4.74750000	5.22923000	-3.01460300
H	-5.09120900	2.41038500	-0.46182300
H	-5.69267800	4.03349400	-0.89788200
H	-6.09469600	2.62602400	-1.91274900
H	1.63184100	4.03908900	1.00909500
H	1.66925700	5.61720500	0.18140300
H	0.53391800	5.33907000	1.52602500



XIb (+1.3 vs. IXa)

Pd	-0.11026100	-0.19240800	-0.20051000
Cl	0.04677500	0.09718100	2.16644200
Cl	-0.16312300	-0.50065600	-2.54677600
P	-2.44805900	-0.63543500	-0.14233800
N	-3.34226800	0.39060000	0.85731800
N	-3.36917000	-0.55321600	-1.57595400
O	-2.84745800	-2.17466100	0.23429100
C	-4.77078100	0.25184700	0.88096200
C	-2.84550000	1.67086600	1.36713700
C	-3.79244400	0.74130400	-2.01088500
C	-3.41517300	-1.63412000	-2.56300700
C	-2.20081300	-3.10598000	1.13541400
C	-5.54034300	0.76050700	-0.18900300
C	-5.39445200	-0.31691200	1.99576000
H	-3.32048200	2.51099900	0.83162100
H	-1.76181100	1.73518400	1.23559500
H	-3.06363200	1.76356600	2.44266400
C	-4.87600500	1.38382200	-1.36114800
C	-3.18709500	1.35105600	-3.12036500
H	-3.27900000	-2.59435300	-2.05156500
H	-2.64153000	-1.53648300	-3.33941300
H	-4.40993200	-1.63763500	-3.03653800
C	-0.74982200	-3.42145000	0.73476000
C	-2.33882700	-2.62699600	2.57923200
H	-2.80394900	-4.02034700	1.01056800
C	-6.94032400	0.67959800	-0.10278500
C	-6.78009700	-0.39463600	2.06266500
H	-4.77056800	-0.68679100	2.81099600
C	-5.31864000	2.62376600	-1.85386200
C	-3.64859000	2.57847800	-3.59973200
H	-2.33757400	0.85326900	-3.58885800
C	-0.15029400	-4.40460100	1.75526100
H	-0.19386400	-2.47546300	0.84751400
C	-0.59173600	-3.84660100	-0.74633100

C	-1.70049900	-3.59101000	3.58882700	C	6.54216300	0.66923500	1.79202400
H	-1.85751700	-1.64136200	2.67307800	H	4.51503100	0.79240900	2.55732500
H	-3.40943600	-2.49410000	2.80121500	C	5.37152800	-2.71711700	-1.90394900
C	-7.56073700	0.10572600	1.00978500	C	3.70000800	-2.97913800	-3.62719800
H	-7.54577600	1.05797100	-0.92994800	H	2.19367200	-1.42886500	-3.70667400
H	-7.26847000	-0.84481200	2.93476600	C	1.25771800	5.11628800	1.53868100
C	-4.71761500	3.21824600	-2.96487700	H	2.77928300	4.51694100	0.14322500
H	-6.14391600	3.12874900	-1.34600900	C	3.35224800	3.64741700	2.01991500
H	-3.16103400	3.04240500	-4.46066800	C	-0.53856900	4.31894000	-0.06699700
C	-0.24572400	-3.87037800	3.18748000	H	1.00553000	3.71618000	-1.46938800
H	-0.67457200	-5.37505200	1.69345000	H	-0.07635600	2.39933000	-0.97897000
H	0.90163200	-4.60262200	1.49789300	C	7.34966200	0.19759900	0.75130100
H	-1.05562000	-3.04853800	-1.34571100	H	7.41183700	-0.86050900	-1.13095000
C	-1.30342600	-5.15812700	-1.10035600	H	6.98201500	1.21746100	2.62862000
C	0.88209500	-3.88628200	-1.16895100	C	4.83846400	-3.44966900	-2.96575300
H	-2.24986900	-4.55166400	3.54063600	H	6.25483500	-3.08662900	-1.37744500
C	-1.81082300	-3.04396500	5.01337300	H	3.26593600	-3.54893300	-4.45253900
H	-8.65106300	0.04509200	1.05176900	C	0.22562400	5.53044600	0.48280600
H	-5.07675400	4.18463800	-3.32677100	H	0.72690200	4.70648400	2.41591500
H	0.32962400	-2.93036600	3.26745000	H	1.80573500	6.00294200	1.89264300
H	0.20917500	-4.58649600	3.89289400	H	3.99795700	2.94405200	1.47090100
H	-2.37981400	-5.12333500	-0.86844000	C	2.81085300	2.90230700	3.24808300
H	-1.20804000	-5.36566700	-2.17840800	C	4.23142200	4.83192100	2.44023600
H	-0.87007000	-6.01716700	-0.56187100	H	-1.06657300	3.85254100	0.78482800
H	1.38827300	-2.93598900	-0.94429500	C	-1.58412800	4.69168200	-1.11754600
H	1.43660000	-4.69810600	-0.67044600	H	8.42736400	0.37792500	0.76771800
H	0.97121600	-4.04458300	-2.25472100	H	5.30726200	-4.38843700	-3.27059800
H	-2.86150000	-2.86621500	5.29572100	H	0.73717500	6.04077600	-0.35467400
H	-1.37559300	-3.74282800	5.74615400	H	-0.48177100	6.26100900	0.91108000
H	-1.27319800	-2.08457200	5.10091700	H	2.26873700	1.98418800	2.97387000
P	2.17830600	0.33479700	-0.34195900	H	3.63932300	2.61317700	3.91564200
N	3.18490300	-0.53017100	0.69010000	H	2.12698500	3.53272500	3.83996800
N	3.05548800	0.21655800	-1.79869900	H	4.59934900	5.39261500	1.56489100
O	2.42586300	1.92970300	-0.08212800	H	3.68775500	5.53936800	3.08805200
C	4.59143100	-0.25021700	0.68255100	H	5.10934800	4.48032900	3.00635400
C	2.78628000	-1.69966700	1.47488600	H	-2.14163300	3.80518700	-1.45879100
C	3.63115000	-1.04234000	-2.15550600	H	-2.31236700	5.41612700	-0.71788600
C	2.86662500	1.19075500	-2.87743800	H	-1.10777500	5.14732400	-2.00267400
C	1.46705300	2.87176500	0.46144700				
C	5.39523700	-0.73890900	-0.36915700				
C	5.16482900	0.44128800	1.75507800				
H	3.35730300	-2.58364800	1.14500900				
H	1.72112200	-1.90396300	1.34109400				
H	2.96676600	-1.53201800	2.54820600				
C	4.78950900	-1.50792000	-1.48422800				
C	3.10087600	-1.78647100	-3.22013700				
H	2.69272600	2.18102000	-2.43937300				
H	2.01853900	0.94238800	-3.53369200				
H	3.78958400	1.23689900	-3.47540000				
C	2.25563000	4.06782700	1.00880100				
C	0.46115400	3.28843900	-0.60847300				
H	0.92638100	2.38655800	1.28717800				
C	6.77996200	-0.50154900	-0.31507200				

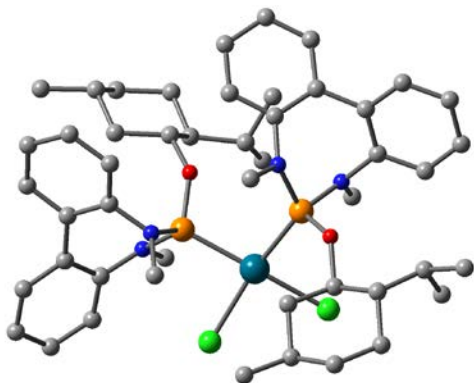


XIc (+4.0 vs. IXa)

Pd	-0.00008400	0.00004400	-0.18929500
Cl	-0.00032600	-0.00005600	2.20452700
Cl	0.00010700	0.00001300	-2.55321600
P	-2.29286100	-0.65318400	-0.23687500
N	-3.30301500	0.24864400	0.76537500
N	-3.18263100	-0.61469700	-1.69560700
O	-2.57035100	-2.23498900	0.06395600
C	-4.70701500	-0.04545300	0.76888200
C	-2.93504500	1.48296600	1.46038500
C	-3.76928100	0.61798900	-2.11412200
C	-3.03939900	-1.65816300	-2.71658600
C	-1.89627800	-3.19864400	0.90425500
C	-5.51534700	0.40267800	-0.29731400
C	-5.27453200	-0.70430100	1.86478600
H	-3.50110000	2.33417200	1.04608300
H	-1.86758700	1.68274300	1.34519000
H	-3.14899900	1.39900000	2.53752300
C	-4.91800000	1.11991000	-1.45122900
C	-3.26983600	1.29112500	-3.23920200
H	-2.92686500	-2.63189400	-2.22525000
H	-2.17580700	-1.49332600	-3.37851600
H	-3.95970100	-1.68350000	-3.31959500
C	-0.41264500	-3.37410300	0.54424500
C	-2.13745800	-2.87629700	2.37724800
H	-2.42405300	-4.13680900	0.66483400
C	-6.89947400	0.16512400	-0.22924000
C	-6.65137900	-0.93365900	1.91495000
H	-4.62104400	-1.02483200	2.67791900
C	-5.51109900	2.30084000	-1.93157000
C	-3.88441500	2.45180800	-3.71008300
H	-2.37403600	0.90262000	-3.72358900
C	0.21599700	-4.40476500	1.49800800
H	0.06844500	-2.40822700	0.76481000

C	-0.17174400	-3.64978400	-0.96127200
C	-1.46828600	-3.88482900	3.32139000
H	-1.74348300	-1.87065500	2.58743200
H	-3.22459200	-2.85017400	2.55321300
C	-7.46396600	-0.49715100	0.86311500
H	-7.53511800	0.49254700	-1.05536100
H	-7.08773300	-1.45353200	2.77127300
C	-5.00528000	2.96480900	-3.05039300
H	-6.38523000	2.70014500	-1.41149500
H	-3.47456300	2.96585400	-4.58306300
C	0.01924300	-4.01696400	2.96677600
H	-0.22924700	-5.40040200	1.32175500
H	1.29008600	-4.50067700	1.27669400
H	-0.65415600	-2.82366300	-1.50613600
C	-0.79554800	-4.95559800	-1.46872500
C	1.31668400	-3.57510300	-1.31953300
H	-1.93850900	-4.87412100	3.15616800
C	-1.68000600	-3.49033300	4.78433400
H	-8.54142400	-0.67769300	0.89037500
H	-5.48382100	3.88156500	-3.40329500
H	0.51629300	-3.04902400	3.15942600
H	0.49885400	-4.76128400	3.62510900
H	-1.88166000	-4.99618600	-1.28960300
H	-0.63981300	-5.05625500	-2.55496800
H	-0.34168000	-5.83874300	-0.98943300
H	1.76025700	-2.62401900	-0.99078100
H	1.89589400	-4.39744700	-0.86891500
H	1.45834800	-3.63166600	-2.40910900
H	-2.75221000	-3.41740900	5.02995100
H	-1.22406100	-4.22488600	5.46800100
H	-1.22158900	-2.50805600	4.98978800
P	2.29286300	0.65315000	-0.23660700
N	3.30293800	-0.24921000	0.76521000
N	3.18267000	0.61500700	-1.69529000
O	2.57045400	2.23484100	0.06467500
C	4.70690600	0.04495300	0.76910600
C	2.93453700	-1.48285200	1.46116100
C	3.76948700	-0.61748600	-2.11415700
C	3.03949300	1.65879100	-2.71599200
C	1.89628600	3.19834400	0.90505600
C	5.51542100	-0.40263500	-0.29718200
C	5.27422800	0.70335700	1.86538800
H	3.50097000	-2.33435100	1.04798900
H	1.86719700	-1.68285100	1.34530900
H	3.14766900	-1.39796900	2.53839300
C	4.91826000	-1.11946000	-1.45143800
C	3.27010700	-1.29030400	-3.23946700
H	2.92749900	2.63244600	-2.22438200
H	2.17561600	1.49440600	-3.37766000
H	3.95959300	1.68388600	-3.31930200
C	0.41275700	3.37406700	0.54475800
C	2.13707900	2.87553500	2.37800700
H	2.42419500	4.13653200	0.66602800

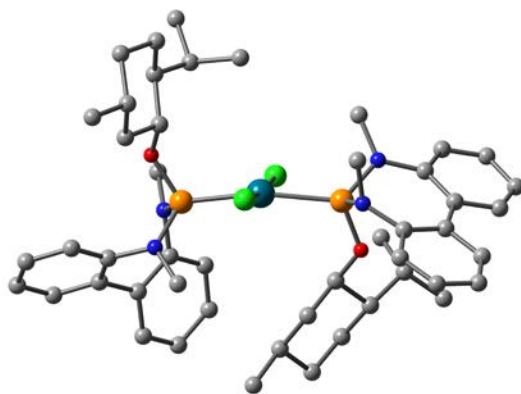
C	6.89952200	-0.16499200	-0.22881600
C	6.65104700	0.93278400	1.91584600
H	4.62061200	1.02350300	2.67857300
C	5.51156800	-2.30010900	-1.93223500
C	3.88485600	-2.45071900	-3.71076700
H	2.37422900	-0.90172700	-3.72365300
C	-0.21594900	4.40459900	1.49862700
H	-0.06852100	2.40821300	0.76498500
C	0.17223100	3.65017800	-0.96075700
C	1.46782300	3.88391900	3.32227000
H	1.74290100	1.86989500	2.58781700
H	3.22416400	2.84923100	2.55425800
C	7.46381300	0.49682200	0.86391400
H	7.53529900	-0.49199500	-1.05500200
H	7.08725500	1.45229700	2.77246100
C	5.00583800	-2.96375200	-3.05128500
H	6.38577400	-2.69946200	-1.41232300
H	3.47507100	-2.96455100	-4.58390500
C	-0.01959200	4.01639400	2.96735400
H	0.22949800	5.40020700	1.32274500
H	-1.28997500	4.50073900	1.27710000
H	0.65459500	2.82411300	-1.50574200
C	0.79649800	4.95594800	-1.46771400
C	-1.31612500	3.57589900	-1.31932400
H	1.93826100	4.87317200	3.15743100
C	1.67912800	3.48896800	4.78515400
H	8.54125100	0.67744700	0.89140900
H	5.48454500	-3.88028400	-3.40454600
H	-0.51686100	3.04849700	3.15965700
H	-0.49921000	4.76063000	3.62577600
H	1.88259500	4.99609500	-1.28838400
H	0.64101500	5.05697400	-2.55396400
H	0.34286500	5.83913100	-0.98827300
H	-1.75991900	2.62477800	-0.99097900
H	-1.89526600	4.39819200	-0.86852700
H	-1.45756900	3.63285300	-2.40890400
H	2.75126000	3.41577500	5.03100500
H	1.22315800	4.22341300	5.46892000
H	1.22048100	2.50671800	4.99022000



Cis isomer of **IXa** (+10.9 vs. **IXa**)

Pd	0.46462000	-1.18237500	-1.14136500
Cl	-0.52737100	-3.26983300	-1.82870200
Cl	2.32021400	-1.56210900	-2.63849800
P	-1.54990000	-0.66864800	-0.19157200
N	-1.85172100	-1.35730900	1.31236600
N	-2.90345000	-1.12155500	-1.15462900
O	-1.68749100	0.93059500	0.01539800
C	-3.00940200	-0.91875500	2.02916500
C	-1.28753600	-2.65863500	1.69645600
C	-3.77695000	-2.19255800	-0.80254500
C	-2.72889900	-0.84276800	-2.58681900
C	-2.65018000	2.00003900	-0.26585300
C	-4.28388300	-1.31920200	1.58319600
C	-2.86389900	-0.10690300	3.16052600
H	-0.76026900	-2.58071800	2.66079700
H	-2.08865200	-3.41009700	1.78233600
H	-0.59092500	-3.01125000	0.92678700
C	-4.44798800	-2.27373000	0.45303900
C	-4.05133800	-3.18232300	-1.76808600
H	-2.04346000	0.00333900	-2.70766900
H	-2.27269300	-1.68596200	-3.12355800
H	-3.69716700	-0.58019300	-3.03834100
C	-2.60429300	2.47613000	-1.72610700
C	-4.06607600	1.67470900	0.19188000
H	-2.26238200	2.81196400	0.36290300
C	-5.40630600	-0.84582900	2.28965300
C	-3.98841800	0.34527700	3.85255700
H	-1.85961500	0.16358600	3.48862600
C	-5.34089100	-3.34445100	0.66769100
C	-4.95000300	-4.21863400	-1.53135100
H	-3.52745900	-3.15797000	-2.71979700
C	-3.53192900	3.70086400	-1.85598100
H	-3.05749900	1.68438400	-2.34068800

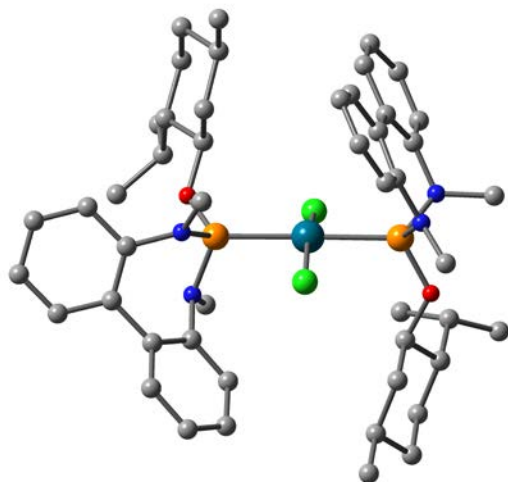
C	-1.16772900	2.71546000	-2.24989200	C	4.18476500	4.11330100	1.19123700
C	-5.01264500	2.87319600	0.01940600	C	5.76174900	3.08033000	-0.32067300
H	-4.04409500	1.38035300	1.24682800	H	4.93616200	1.58875700	-1.64468100
H	-4.45252100	0.81795600	-0.38124100	C	1.28731100	4.88205100	1.36166400
C	-5.26361100	-0.01931200	3.40478300	C	-0.79456100	4.08769900	2.27800000
H	-6.40575700	-1.11491600	1.94192800	H	-1.03511400	1.94758900	2.30692800
H	-3.87106900	0.98593900	4.72952200	C	5.41606900	-3.36064700	0.82848900
C	-5.60411100	-4.30822000	-0.30133000	H	4.94554900	-1.64952300	2.04879700
H	-5.83030700	-3.42021300	1.64101900	C	5.88154800	-0.85893300	0.28809300
H	-5.12252500	-4.96636500	-2.30931100	C	3.03383600	-4.20761200	1.12629100
C	-4.96591100	3.38141600	-1.42685700	H	2.62135400	-2.46709900	2.35030300
H	-3.14761900	4.52518200	-1.23110800	H	1.55644400	-2.62360600	0.94305700
H	-3.51493100	4.06398500	-2.89556500	C	5.48836900	3.98165200	0.71374600
H	-0.57247200	1.85284000	-1.91073000	H	3.97616600	4.81164500	2.00472700
C	-0.51421300	3.97335900	-1.66673400	H	6.77928300	2.96367100	-0.70126500
C	-1.11816800	2.73080400	-3.78251100	C	0.03709100	5.15179300	1.91684100
H	-4.64055700	3.68946500	0.66890500	H	1.93913600	5.71101200	1.07735100
C	-6.43077700	2.51517800	0.46818000	H	-1.77910600	4.27424100	2.71418700
H	-6.15251000	0.34450200	3.92565200	C	4.49861100	-4.34310200	1.56721700
H	-6.30158000	-5.12263200	-0.09336300	H	5.44125700	-3.63166400	-0.24103600
H	-5.38917600	2.60651400	-2.09309200	H	6.44734700	-3.46243600	1.20072700
H	-5.60589700	4.27351200	-1.53524000	H	5.40856900	0.11794100	0.47165900
H	-0.57682600	4.00017600	-0.57118300	C	5.99478200	-1.03062500	-1.23265400
H	0.55285000	4.01535300	-1.92782000	C	7.26949800	-0.81359400	0.93937400
H	-0.98467400	4.88962600	-2.05838200	H	2.97751000	-4.45519900	0.04954000
H	-1.52037300	1.79953200	-4.21374500	C	2.10054600	-5.15517600	1.88088900
H	-1.69844700	3.57054500	-4.19892800	H	6.29121200	4.57963600	1.15158400
H	-0.08174500	2.84101400	-4.13826500	H	-0.28471300	6.18504000	2.06552600
H	-6.44424500	2.17553000	1.51601000	H	4.55873500	-4.15473100	2.65581300
H	-7.10923700	3.37878800	0.37689100	H	4.84689200	-5.37793300	1.40835300
H	-6.83957600	1.69808200	-0.15053900	H	5.01306100	-0.99938300	-1.72976800
P	1.78556300	0.35183200	-0.03568500	H	6.61488300	-0.22625000	-1.66173700
N	2.37190200	1.64221400	-0.94464500	H	6.47665600	-1.98539900	-1.50022500
N	1.30749100	1.14159600	1.40366300	H	7.19914000	-0.70339700	2.03436800
O	3.05863700	-0.43720200	0.62341500	H	7.85364800	-1.72515500	0.73015600
C	3.41969600	2.43379400	-0.36961700	H	7.84925500	0.04101500	0.55362800
C	2.24213700	1.69964700	-2.40611200	H	1.06503100	-5.06620300	1.51417500
C	0.87890500	2.49284800	1.49037200	H	2.41280700	-6.20504800	1.75945100
C	1.06156600	0.28102400	2.56860400	H	2.09828600	-4.92764100	2.96102200
C	3.50110500	-1.81207000	0.48843200				
C	3.12442000	3.35482200	0.65663300				
C	4.72956400	2.30983700	-0.85397700				
H	2.19020500	2.75523200	-2.70809300				
H	1.32224700	1.19511000	-2.71908600				
H	3.07587200	1.20636100	-2.92534900				
C	1.74154600	3.56589900	1.15221900				
C	-0.37567300	2.77667900	2.05774600				
H	0.16133600	-0.34118700	2.45183600				
H	0.94128400	0.91196900	3.45846300				
H	1.92585500	-0.37419700	2.73175600				
C	4.95502700	-1.89556200	0.96934600				
C	2.59582900	-2.74676600	1.28161100				
H	3.45115500	-2.08669600	-0.57293600				



c-TS_IXa-Xa (+17,1 vs. IXa)

Pd	0.26137300	-0.61077400	-0.04143000
Cl	-0.21311900	0.11235200	-2.24754500
Cl	0.81392400	-1.62744100	2.02322700
P	2.43622800	0.23527200	-0.24061000
N	3.01174200	1.04892600	1.11712700
N	2.79372700	1.37477600	-1.45153800
O	3.52530800	-0.89567700	-0.66993800
C	4.27179000	1.73240300	1.02217300
C	2.23863400	1.38467900	2.31448400
C	2.38952500	2.72677100	-1.20836100
C	3.09251000	1.00187000	-2.83738000
C	3.50049700	-2.26773200	-0.19893000
C	4.33593600	2.98274100	0.36924100
C	5.40171100	1.20108100	1.65215100
H	1.24490400	0.93046200	2.27322900
H	2.74521600	1.00967100	3.21782900
H	2.13407900	2.47889400	2.39297900
C	3.14182400	3.53298200	-0.31788600
C	1.29549000	3.27851400	-1.89160300
H	3.68288100	0.07783200	-2.84256900
H	2.18657900	0.84971300	-3.44328600
H	3.70206900	1.80026500	-3.28734300
C	3.84501800	-3.18090900	-1.37976600
C	4.47055800	-2.38538600	0.97198500
H	2.48895300	-2.50555200	0.16162800
C	5.55493800	3.68113600	0.38012500
C	6.60820100	1.90598200	1.64719300
H	5.31992100	0.23336600	2.14897200
C	2.75427600	4.87059600	-0.12744200
C	0.93591000	4.61388200	-1.69851100
H	0.71631000	2.63821400	-2.55668600
C	4.01876400	-4.62392900	-0.87006000
H	4.82552900	-2.83471600	-1.75769300

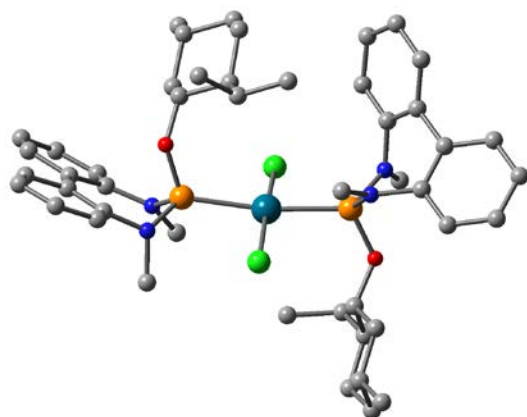
C	2.82627600	-3.04247500	-2.54196400	C	-6.19898400	-1.22196400	2.30901700
C	4.63436400	-3.83107000	1.45648400	C	-4.94166100	-1.34386400	4.36789800
H	4.10239600	-1.74707900	1.79088000	H	-2.82420200	-1.65132700	4.06356400
H	5.44971200	-1.98502200	0.65406800	C	-6.10372900	-1.36039200	-2.81799600
C	6.68171100	3.15030700	1.01285100	H	-4.04500600	-1.68466600	-3.25147700
H	5.61998400	4.64355800	-0.13307000	C	-6.60847000	-1.16588800	-0.48186600
H	7.48849000	1.48332500	2.13745900	C	-2.88306400	4.01342400	-0.46920100
C	1.66206300	5.41148600	-0.80877500	H	-4.16982000	2.72151900	0.67596800
H	3.32131500	5.48941100	0.57213400	C	-4.34399600	2.04561800	-1.34922900
H	0.07355200	5.02438800	-2.22929300	C	-1.08664300	3.63916300	1.30926900
C	5.03165100	-4.72577500	0.27405400	H	-0.87813000	1.53515200	1.82585200
H	3.04697000	-5.00348400	-0.51039400	H	-2.41852400	2.24780700	2.33359300
H	4.31772000	-5.27763100	-1.70468400	C	-6.15630700	-1.18881800	3.69856000
H	2.66393800	-1.96226500	-2.68067900	H	-7.18618400	-1.08976800	1.88024600
C	1.45510100	-3.66241700	-2.23946000	H	-4.88155500	-1.30732600	5.45803600
C	3.39018900	-3.58571200	-3.86050800	C	-7.03317100	-1.14181100	-1.80363600
C	3.64619200	-4.17385700	1.81901800	H	-6.39182200	-1.34218300	-3.87175600
H	5.62713700	-3.92150300	2.61630500	H	-7.38658300	-0.97741200	0.24829600
H	7.62226800	3.70654900	1.00246300	C	-2.16589800	4.58450700	0.75898000
H	1.37514100	6.45211800	-0.64001900	H	-2.16463100	3.93576400	-1.30371800
H	6.03262600	-4.42103900	-0.08500000	H	-3.67022000	4.70938200	-0.79827000
H	5.12253300	-5.77363800	0.60730200	H	-4.66226000	1.04882300	-1.01186300
H	1.05728000	-3.32754300	-1.26869700	C	-3.57629700	1.85482000	-2.66237500
H	0.72686200	-3.36717800	-3.01046000	C	-5.62239200	2.86333600	-1.57477000
H	1.49737000	-4.76349900	-2.22564400	H	-0.29326200	3.55268300	0.54530000
H	4.34508300	-3.09969100	-4.11976300	C	-0.45896700	4.19096700	2.59001900
H	3.56962400	-4.67263400	-3.80944600	H	-7.08437300	-1.03425400	4.25442200
H	2.68621600	-3.40883700	-4.68985500	H	-8.08437100	-0.94927200	-2.02912800
H	5.31373800	-3.28747400	3.46166400	H	-2.90898900	4.77442600	1.55601300
H	5.72013000	-4.95625100	2.98410300	H	-1.71207200	5.56020300	0.51402500
H	6.62977700	-3.58640700	2.29932900	H	-2.69123400	1.21523000	-2.53514300
P	-2.06422700	-1.00566300	0.25677100	H	-4.22482900	1.37248000	-3.41096400
N	-2.58030600	-1.88025900	1.60386500	H	-3.24235400	2.81764500	-3.08451600
N	-2.93598700	-1.78376700	-0.98370100	H	-6.18648000	2.99812300	-0.63684700
O	-2.86686900	0.38267900	0.51212900	H	-5.40684000	3.86427400	-1.98482000
C	-3.84715500	-1.59811100	2.19173900	H	-6.28404800	2.35055900	-2.29142000
C	-2.17871800	-3.28906300	1.59734300	H	0.30399100	3.50739500	2.99175100
C	-4.33238700	-1.59848100	-1.11809900	H	0.02235500	5.16537300	2.40712600
C	-2.20220300	-2.56797900	-1.97683100	H	-1.22422600	4.33258400	3.37230800
C	-2.34431900	1.71115200	0.25476300				
C	-5.06699300	-1.42284000	1.46968900				
C	-3.80491100	-1.53696000	3.59711300				
H	-2.18605700	-3.68224600	2.62428500				
H	-2.85243900	-3.90680700	0.97352400				
H	-1.15062000	-3.37501900	1.21748500				
C	-4.78264200	-1.57198300	-2.45964400				
C	-5.27921400	-1.41325300	-0.04306400				
H	-2.75697900	-3.49280900	-2.19647600				
H	-2.00879700	-2.02022300	-2.91171700				
H	-1.22579500	-2.84603500	-1.56213400				
C	-3.49185900	2.62439200	-0.19328200				
C	-1.67163900	2.23555600	1.51984400				
H	-1.60233700	1.64587700	-0.55490200				



t-TS_IXa-Xa (+21,0 vs. IXa)

C	1.41634000	-1.68341500	-4.27395100
C	1.59620600	-2.10236200	-2.93322700
C	0.63292500	-3.01017300	-2.34239100
C	-0.44806800	-3.34803800	-3.20037700
C	-0.61180400	-2.91716600	-4.51000000
C	0.34945700	-2.07705400	-5.06498100
H	2.12895500	-0.98338500	-4.69964900
H	-1.22295600	-4.01506900	-2.84443800
H	-1.48060300	-3.24809000	-5.08317600
H	0.26519400	-1.71054400	-6.09086900
C	0.61136100	-3.68568600	-0.96425800
C	-0.47497900	-4.55516500	-0.65853600
C	1.56348300	-3.57851100	0.09131900
C	-0.59776700	-5.27737300	0.52191000
H	-1.28260800	-4.70013100	-1.36600400
C	1.43312100	-4.30723200	1.28765200
C	0.37564400	-5.17078600	1.51767600
H	-1.46855700	-5.92312200	0.65896300
H	2.19110700	-4.13790900	2.05442200
H	0.29383800	-5.72173800	2.45715000
P	2.45872100	-1.19012200	-0.60251800
C	3.99953600	-3.36881600	-0.17388600
H	4.12245300	-4.19964400	0.53503300
H	4.08348300	-3.76153800	-1.20343700
H	4.80797500	-2.64608400	-0.00138500
C	3.73830000	-0.82940800	-3.02698800
H	4.09142600	-1.46453900	-3.85308900

H	3.37591500	0.13080700	-3.43140300	H	-1.64099400	1.59073400	2.92811000
H	4.58709700	-0.62409100	-2.36711800	H	0.06389400	1.86794300	2.51504200
N	2.70172300	-2.72241100	0.05697600	H	-1.00423300	3.25906400	2.90514200
N	2.71116800	-1.54131400	-2.26788100	C	-4.14658900	-1.31551700	2.19534800
Pd	0.41902200	-0.12431000	-0.18073500	C	-3.43758600	-1.63299900	-0.23690800
O	3.81744200	-0.40369000	-0.21407200	H	-2.14436600	-1.66272600	1.48188200
C	3.83870100	0.83444300	0.55302900	C	-4.12744200	4.80490300	-0.74664900
C	4.87416000	0.68118800	1.67286800	C	-5.79794400	3.11971000	-1.20774700
C	4.15984000	1.97225600	-0.40939600	H	-5.04841400	1.11293500	-1.48249400
H	2.83796900	0.99184200	0.99174600	C	-1.15900300	5.36329100	-1.27999400
C	5.05111200	2.03795000	2.38078400	C	0.96428200	5.09297300	-0.16253200
H	5.82599300	0.44335000	1.16171800	H	1.10143000	3.42288700	1.19516500
C	4.56124700	-0.49577700	2.63447100	C	-4.50737400	-2.81319000	2.22732400
C	4.35100400	3.31314500	0.31054100	H	-5.04209800	-0.77789600	1.82936400
H	3.35203900	2.04096700	-1.15365700	C	-3.73754500	-0.69066600	3.56858100
H	5.08833500	1.71121600	-0.94853000	C	-3.83938500	-3.11253200	-0.20372200
C	5.41219900	3.16501800	1.40919400	H	-2.58936300	-1.50497900	-0.92964000
H	4.11193300	2.30548600	2.89484600	H	-4.27329600	-1.02282800	-0.62299500
H	5.81832300	1.94630100	3.16584800	C	-5.46330600	4.45171000	-0.94262500
H	4.22526700	-1.33313600	2.00191500	H	-3.86576000	5.84154700	-0.52170300
C	3.42944100	-0.20001100	3.62750500	H	-6.84169600	2.82956800	-1.35073700
C	5.82338000	-0.96463200	3.36992600	C	0.15321600	5.78809600	-1.06424700
H	3.39535200	3.56275400	0.80798900	H	-1.79561000	5.90034900	-1.98720200
C	4.67782300	4.43345300	-0.67733600	H	1.99453000	5.41087900	0.01017500
H	6.39026600	2.95394000	0.93787200	C	-4.93105700	-3.33326200	0.84962900
H	5.52497400	4.11634700	1.95656300	H	-3.63771800	-3.39397000	2.58400000
H	2.51870800	0.15800600	3.12558100	H	-5.31759000	-2.98746300	2.95011500
H	3.14963100	-1.11803800	4.16832600	H	-2.63335100	-0.65875600	3.58772100
H	3.73356400	0.54622900	4.37958000	C	-4.18369900	-1.49360300	4.79851500
H	6.61850900	-1.25405500	2.66316000	C	-4.25583000	0.75179200	3.68480700
H	6.22813200	-0.17515700	4.02533000	H	-2.95059700	-3.68125700	0.12092300
H	5.60444700	-1.83726100	4.00651200	C	-4.24839600	-3.61128500	-1.58986900
H	3.89202300	4.53059500	-1.44335200	H	-6.24352800	5.21405400	-0.87915600
H	4.77512800	5.40371100	-0.16327800	H	0.54167900	6.65721300	-1.60028800
H	5.63029400	4.23168000	-1.19650200	H	-5.85279800	-2.81254600	0.52816300
Cl	0.89159300	1.20344000	-2.08787900	H	-5.18183100	-4.40612600	0.91051000
Cl	0.26498600	-1.08832800	1.97142100	H	-3.75827100	-2.50789600	4.81996100
P	-1.60671100	0.98311500	0.13883000	H	-3.85880900	-0.98138800	5.71880000
N	-2.41731600	1.52289700	-1.23514700	H	-5.28203000	-1.58541200	4.84593100
N	-1.38435600	2.43164900	1.01846700	H	-3.97652400	1.35253500	2.80952600
O	-2.71497900	0.28639000	1.11051000	H	-5.35747000	0.75680600	3.76064100
C	-3.44799900	2.50670600	1.09544800	H	-3.85872900	1.24567700	4.58715900
C	-2.36992400	0.78397300	-2.50004300	H	-3.44925000	-3.43803800	-2.32860200
C	-0.85515300	3.54447700	0.29514100	H	-4.47432600	-4.68994100	-1.57745700
C	-0.95617000	2.27602800	2.41631300	H	-5.14902300	-3.08323100	-1.94736300
C	-3.04249700	-1.12199300	1.14551500				
C	-3.10033700	3.84705900	-0.81635500				
C	-4.79277100	2.15435600	-1.28005200				
H	-1.54032900	0.06820000	-2.48638200				
H	-3.30404800	0.22961700	-2.68610000				
H	-2.19363200	1.48305300	-3.33134600				
C	-1.68635700	4.24718500	-0.60955800				
C	0.46208200	3.97707100	0.50752900				

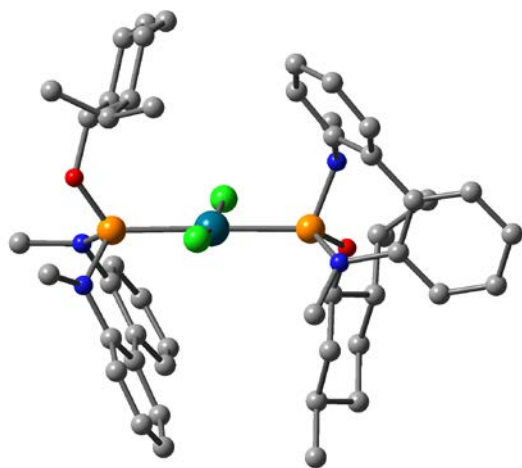


c-TS_IXb-Xc (+20,2 vs. IXa)

Pd	0.14544900	-0.48551600	-0.07702800
Cl	-0.25021500	0.54733500	-2.18044300
Cl	0.61884800	-1.81033400	1.82994700
P	2.39113600	0.18855100	-0.17417000
N	3.03532400	0.81975000	1.24942900
N	2.87050100	1.40572500	-1.25688700
O	3.36098800	-0.99523400	-0.74082000
C	4.36224800	1.36728100	1.21914400
C	2.41478300	0.78470600	2.57697800
C	2.61317800	2.76452000	-0.88796700
C	3.14922200	1.13920100	-2.67238800
C	3.21271200	-2.40360900	-0.43691000
C	4.57329500	2.65661500	0.68340300
C	5.42123300	0.65990700	1.80041600
H	1.33266000	0.65554400	2.49234900
H	2.80948900	-0.03771100	3.19509300
H	2.61541100	1.74212200	3.07913900
C	3.45666400	3.40123400	0.05449200
C	1.58317000	3.48827200	-1.50498900
H	3.71740000	0.20556400	-2.76170700
H	2.23417600	1.06209800	-3.27913900
H	3.77305400	1.95847300	-3.05928800
C	3.53669900	-3.20025000	-1.70489600
C	4.11921500	-2.73698400	0.74359400
H	2.17169100	-2.60102700	-0.14295300
C	5.86352100	3.20904600	0.75875400
C	6.69737100	1.22381900	1.86447300
H	5.23130100	-0.33562700	2.20460700
C	3.22844900	4.75420500	0.35733300
C	1.38063500	4.83545200	-1.19940400
H	0.93357600	2.97167000	-2.21133800
C	3.56706600	-4.70185500	-1.36291000

H	4.55874000	-2.90003400	-2.00406300
C	2.58801300	-2.84071400	-2.87880800
C	4.14211400	-4.23692900	1.06122100
H	3.76977800	-2.16878900	1.62052400
H	5.14070300	-2.38923900	0.50750500
C	6.91697900	2.50365200	1.34424500
H	6.04035800	4.20056800	0.33514500
H	7.51885500	0.66276500	2.31654800
C	2.20195000	5.46977400	-0.26229000
H	3.86547200	5.24492800	1.09707400
H	0.56885000	5.38302400	-1.68372600
C	4.51530300	-5.02241700	-0.20373300
H	2.55170000	-5.03344600	-1.08528600
H	3.84886500	-5.27980500	-2.25719500
H	2.54009800	-1.74118200	-2.90663900
C	1.15044900	-3.34369000	-2.68818100
C	3.15181500	-3.30116100	-4.22857800
H	3.11407900	-4.53070600	1.34784300
C	5.07243900	-4.54469700	2.23537900
H	7.91320600	2.95069200	1.38640300
H	2.03945200	6.51986800	-0.00772200
H	5.55327800	-4.76813500	-0.48959200
H	4.50341100	-6.10539600	0.00695300
H	0.74465600	-3.06375400	-1.70353900
H	0.48945600	-2.90392600	-3.45107100
H	1.08344000	-4.43960700	-2.78233800
H	4.16344000	-2.89807100	-4.40014400
H	3.21332500	-4.40045000	-4.29109100
H	2.50924100	-2.96198900	-5.05729500
H	4.77526400	-3.98650800	3.13814700
H	5.06411100	-5.61877800	2.48223300
H	6.11212900	-4.26364200	1.99427700
P	-2.19285900	-0.82188200	0.18128600
N	-2.69412300	-1.89482800	1.38285200
N	-3.11120700	-1.38238400	-1.14520600
O	-2.94779900	0.49416100	0.74853500
C	-3.92729100	-1.68165300	2.06031600
C	-2.34142300	-3.29308300	1.13015800
C	-4.51599400	-1.21814600	-1.19641400
C	-2.40647300	-1.98665200	-2.27639400
C	-3.01586300	1.86483400	0.28114200
C	-5.16716200	-1.39107100	1.41671400
C	-3.83297100	-1.82502300	3.45631600
H	-2.30212800	-3.84449100	2.08081900
H	-3.07017400	-3.78656000	0.45927100
H	-1.34086400	-3.34431200	0.67826100
C	-5.02791800	-1.05660400	-2.50788400
C	-5.42086200	-1.15694700	-0.07047800
H	-2.94164900	-2.89129800	-2.60284800
H	-2.28037300	-1.30181800	-3.12876000
H	-1.40148100	-2.28124600	-1.95506800
C	-1.72110700	2.64160400	0.56023500
C	-3.47279200	1.95578100	-1.17184800

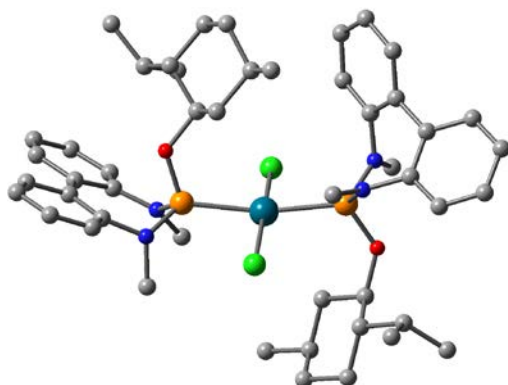
H	-3.81426800	2.28218900	0.91561500
C	-6.27061700	-1.32112500	2.31261900
C	-4.94132800	-1.74071700	4.28678400
H	-2.83731500	-2.01272300	3.86351500
C	-6.35955100	-0.79402400	-2.78370900
H	-4.33139000	-1.09502200	-3.34222400
C	-6.75924900	-0.82872400	-0.42164600
C	-1.94148500	4.10385500	0.12905800
H	-0.94458500	2.23099600	-0.10539000
C	-1.20396400	2.46485100	2.01082000
C	-3.64633000	3.41294900	-1.62441200
H	-4.42225300	1.41322700	-1.28447800
H	-2.72905600	1.46261400	-1.81691600
C	-6.17809000	-1.49150000	3.69017200
H	-7.27310200	-1.13874600	1.94075100
H	-4.84378700	-1.86340100	5.36789100
C	-7.23932000	-0.65525200	-1.71244300
H	-6.69225600	-0.67137000	-3.81721400
H	-7.49772900	-0.69810600	0.36081200
C	-2.36407100	4.20609200	-1.33964800
H	-2.71278600	4.57314600	0.76645300
H	-1.01500200	4.67402300	0.28394200
H	-0.94057100	1.39723400	2.10747100
C	-2.25052600	2.76496400	3.09185300
C	0.07997200	3.26920200	2.24939200
H	-4.45666900	3.86202000	-1.01748900
C	-4.05684600	3.48072400	-3.09658800
H	-7.08570500	-1.42392600	4.29506400
H	-8.29310600	-0.41506800	-1.86989500
H	-1.55329200	3.80924700	-1.97726700
H	-2.50330900	5.26343900	-1.62390600
H	-3.10803600	2.07744400	3.03418300
H	-1.80818600	2.65147100	4.09487000
H	-2.63072100	3.79761800	3.01622700
H	0.82985200	3.07819800	1.46597400
H	-0.11558000	4.35315300	2.26608500
H	0.52682900	3.00509300	3.21975900
H	-4.98550000	2.91589800	-3.27961200
H	-4.22014600	4.52149900	-3.42070400
H	-3.27044100	3.04724400	-3.73787600



t-TS_IXb-Xc (+22,9 vs. IXa)

C	1.41953400	-2.20749300	-3.91321200
C	1.62152300	-2.51021400	-2.54480600
C	0.66676500	-3.35911300	-1.86095300
C	-0.38444700	-3.83564000	-2.68991300
C	-0.55357200	-3.54201800	-4.03661100
C	0.36575200	-2.70490100	-4.66279500
H	2.10896700	-1.52245900	-4.39816200
H	-1.12838600	-4.50531500	-2.27630300
H	-1.39727300	-3.97196700	-4.58087500
H	0.26459900	-2.42957400	-5.71532300
C	0.61611200	-3.83362700	-0.40320800
C	-0.50768900	-4.60366800	0.01301800
C	1.56499300	-3.61270900	0.63585700
C	-0.66735300	-5.14581400	1.28179200
H	-1.31804300	-4.80966100	-0.67536400
C	1.40412800	-4.16864800	1.91878400
C	0.31070000	-4.94642800	2.25880400
H	-1.56827300	-5.72397700	1.50151000
H	2.16696300	-3.92680600	2.66105900
H	0.20403600	-5.35689400	3.26531000
P	2.55456300	-1.35501100	-0.35171700
C	4.00314100	-3.52401300	0.36685800
H	4.07944800	-4.27510700	1.16557700
H	4.08599900	-4.03440600	-0.61022800
H	4.83960400	-2.82088600	0.47043800
C	3.82939300	-1.38463900	-2.81469600
H	4.10252600	-2.13942800	-3.56710900
H	3.53897900	-0.44996100	-3.32289700
H	4.70999300	-1.17794100	-2.19851700
N	2.72958600	-2.80519200	0.49699200

N	2.76678200	-1.91622300	-1.96122600	C	-4.12678500	-1.32871900	1.78521500
Pd	0.53825300	-0.15538200	-0.11857700	C	-3.38554100	-1.45818400	-0.65347600
O	3.97728600	-0.61416800	-0.11900700	H	-2.11764100	-1.63409800	1.07909200
C	4.26939100	0.38422400	0.90214800	C	-3.88087200	4.94250500	-0.88146500
C	3.82208000	1.78095500	0.44882500	C	-5.51182000	3.28561100	-1.53933300
C	3.71132900	-0.02283400	2.26233500	H	-4.74477700	1.29338300	-1.85343300
H	5.36915100	0.35962900	0.95356100	C	-0.89182300	5.53350500	-1.13014700
C	4.15573700	2.79368600	1.56020900	C	1.12239000	5.21673300	0.15984100
H	2.72193200	1.74513400	0.35700600	H	1.16865300	3.46532100	1.41141900
C	4.37031000	2.15560000	-0.95300200	C	-4.49755200	-2.82154500	1.69214900
C	4.04585400	1.00027900	3.35637700	H	-5.01343500	-0.75877600	1.44771700
H	4.09569300	-1.02040500	2.52958600	C	-3.73660200	-0.81428200	3.20867700
H	2.61596100	-0.11272400	2.19880600	C	-3.81207100	-2.92769600	-0.74895500
C	3.56716900	2.38990600	2.91558700	H	-2.52460300	-1.29243600	-1.32057800
H	5.25131000	2.88928400	1.66071200	H	-4.20490200	-0.80539600	-1.00222600
H	3.78488500	3.78874900	1.27121400	C	-5.19860600	4.60322800	-1.18966300
H	4.01753000	1.35964800	-1.62529800	H	-3.63715200	5.96612900	-0.58757100
C	5.90224500	2.19234800	-1.03985100	H	-6.54224500	3.00429600	-1.76978500
C	3.76275800	3.46347200	-1.47177600	C	0.38703800	5.95961100	-0.76710400
H	5.14695800	1.04481000	3.46598300	H	-1.47158100	6.10988600	-1.85500600
C	3.44036700	0.57965700	4.69716400	H	2.12628300	5.53392800	0.44998000
H	2.46325200	2.37335400	2.85191100	C	-4.91565100	-3.22176700	0.27313200
H	3.82484000	3.14031900	3.68193500	H	-3.63397600	-3.43604700	2.00461400
H	6.36281900	1.23031000	-0.76482400	H	-5.31387400	-3.04869700	2.39300800
H	6.21839400	2.41945300	-2.07087600	H	-2.63389800	-0.77061900	3.24026100
H	6.33284800	2.97142700	-0.38886500	C	-4.18140600	-1.71988500	4.36528200
H	2.66529000	3.43508900	-1.42077400	C	-4.27470300	0.60760600	3.43352100
H	4.11409000	4.33807300	-0.89939700	H	-2.93607900	-3.53380800	-0.46314800
H	4.04685100	3.62753200	-2.52409200	C	-4.20806500	-3.30310700	-2.17717200
H	3.81885700	-0.40488100	5.01663800	H	-5.98187600	5.36385900	-1.14678700
H	3.67576500	1.30862800	5.48944000	H	0.80700600	6.86693300	-1.20738700
H	2.34268400	0.50425800	4.61805500	H	-5.82884100	-2.66581500	-0.01166300
Cl	1.20595800	0.97679900	-2.08982500	H	-5.17831300	-4.29310700	0.24292000
Cl	0.13513900	-0.97531100	2.06697000	H	-3.74435100	-2.72776100	4.30498200
P	-1.45771300	1.05456400	0.01274800	H	-3.86600600	-1.28214700	5.32648600
N	-2.13507900	1.68062900	-1.40026100	H	-5.27883700	-1.82740600	4.39965500
N	-1.27941300	2.46416000	0.96197500	H	-3.99731100	1.27702100	2.60850300
O	-2.67051400	0.34541400	0.84409900	H	-5.37689800	0.59409100	3.50131500
C	-3.17471600	2.66130200	-1.28786000	H	-3.88917500	1.03599700	4.37359300
C	-2.02275700	0.99348000	-2.69074000	H	-3.38481600	-3.10474700	-2.88235200
C	-0.70131100	3.61539500	0.34393400	H	-4.46962800	-4.37134900	-2.25155800
C	-1.00021600	2.26997900	2.39169200	H	-5.08407100	-2.71924500	-2.50815900
C	-3.00615700	-1.06106500	0.77042400				
C	-2.85072400	3.98560800	-0.92149600				
C	-4.50322500	2.32258500	-1.58428500				
H	-1.22962200	0.24000200	-2.64795600				
H	-2.96419000	0.49493200	-2.97137200				
H	-1.75329200	1.71841600	-3.47381700				
C	-1.45982800	4.37118800	-0.58259000				
C	0.58325100	4.05046500	0.70366700				
H	-1.69359700	1.52566200	2.79671000				
H	0.02343200	1.91097900	2.58769100				
H	-1.15780800	3.22721100	2.90847000				

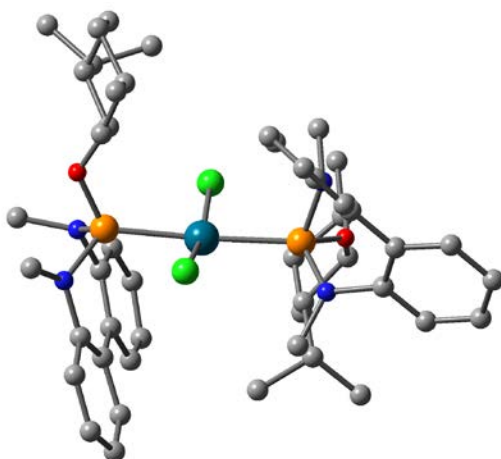


c-TS_IXb-Xb (+20,7 vs. IXa)

Pd	0.23194400	-0.65394400	-0.18800100
Cl	-0.28110100	0.27987700	-2.30785300
Cl	0.69994000	-1.89721400	1.77214300
P	2.47061200	0.06785200	-0.44615300
N	3.16688700	0.78015100	0.92014500
N	2.79191600	1.29128500	-1.58671200
O	3.48716800	-1.05620300	-1.05524700
C	4.43008000	1.45601000	0.82220600
C	2.65339600	0.65427100	2.28971900
C	2.46302300	2.64376700	-1.25352400
C	3.01102500	1.00465800	-3.00681600
C	3.39905600	-2.50135100	-1.16259600
C	4.50393100	2.73065000	0.21885500
C	5.56199600	0.90659700	1.43987200
H	1.56956900	0.51097800	2.28668800
H	3.10275400	-0.19267200	2.83231900
H	2.88398800	1.58494800	2.82794900
C	3.30363700	3.36563600	-0.37418200
C	1.36888500	3.28697200	-1.85289600
H	3.39875500	-0.01444400	-3.11690400
H	2.09001400	1.09548500	-3.60163000
H	3.76771800	1.70439100	-3.39634400
C	3.73167300	-3.18094200	0.17285600
C	2.06107400	-2.95612700	-1.74397300
H	4.19315100	-2.73475200	-1.89212200
C	5.73948000	3.40291200	0.22087700
C	6.77868300	1.59095800	1.43679700
H	5.47779900	-0.05926100	1.93818200
C	2.99862200	4.71042700	-0.09738600
C	1.09481100	4.62833900	-1.58123300
H	0.72218200	2.71516000	-2.51674800
C	3.63126600	-4.70762100	0.00440800
H	2.93667900	-2.87230100	0.87100700

C	5.07731000	-2.69463300	0.76460700
C	1.96569400	-4.48040500	-1.89113100
H	1.88649800	-2.45006300	-2.70718200
H	1.25278400	-2.63768100	-1.06463600
C	6.86937900	2.84138700	0.81723000
H	5.80862100	4.38046900	-0.26204500
H	7.65354500	1.14562600	1.91661300
C	1.90570200	5.34153500	-0.69300200
H	3.63184100	5.26271000	0.60090700
H	0.23305300	5.10985200	-2.04953400
C	2.26671800	-5.14044100	-0.53758600
H	4.41546400	-5.05811100	-0.68949800
H	3.83092000	-5.19694000	0.97114500
H	5.09314500	-1.60782500	0.60287100
C	6.31857800	-3.26708600	0.06812300
C	5.13857600	-2.92791000	2.27901600
H	2.74215500	-4.80930700	-2.60900100
C	0.59681700	-4.89279100	-2.43658600
H	7.81913900	3.38142700	0.80098900
H	1.68479500	6.38581900	-0.45974800
H	1.47771000	-4.85075400	0.18019700
H	2.22394000	-6.23846500	-0.63604400
H	6.27662300	-3.13725400	-1.02537300
H	7.22767300	-2.75589800	0.42425000
H	6.44423700	-4.34253400	0.27441500
H	4.28282700	-2.45624700	2.78898900
H	5.12330500	-4.00237000	2.52699500
H	6.06375800	-2.50740700	2.70708900
H	0.37578900	-4.39575800	-3.39502200
H	0.54104700	-5.98180100	-2.59494400
H	-0.20073500	-4.61901400	-1.72512100
P	-2.08930300	-0.90731100	0.15269000
N	-2.64165100	-1.88938400	1.40616300
N	-3.04713400	-1.46916300	-1.13857000
O	-2.75776500	0.50413000	0.59306700
C	-3.86277900	-1.57496100	2.06891400
C	-2.36244400	-3.31537100	1.22151600
C	-4.42888600	-1.16463900	-1.20099900
C	-2.41561900	-2.22159400	-2.22312500
C	-2.12452800	1.80222900	0.43276500
C	-5.08225900	-1.22446000	1.41405100
C	-3.77761200	-1.67640300	3.46970600
H	-2.37055500	-3.82468400	2.19603800
H	-3.10530200	-3.79883500	0.55895500
H	-1.35764900	-3.43812100	0.79254300
C	-4.91089900	-0.95691700	-2.51509600
C	-5.32958900	-1.02661200	-0.08019300
H	-3.03906900	-3.09290500	-2.47622100
H	-2.23568900	-1.61916100	-3.12579600
H	-1.43673500	-2.58573200	-1.88661800
C	-3.20887100	2.85847600	0.19577800
C	-1.28732300	2.11329900	1.66913900
H	-1.46788900	1.76369100	-0.44856700

C	-6.17273800	-1.03515900	2.30889700
C	-4.87470400	-1.48430400	4.29641400
H	-2.79720500	-1.91860600	3.88508000
C	-6.21889800	-0.60340500	-2.80241200
H	-4.20611900	-1.04159400	-3.33967900
C	-6.64431400	-0.62532900	-0.44270600
C	-2.49726200	4.21604200	0.02827000
H	-3.80993900	2.90470900	1.12381000
C	-4.18867900	2.49471700	-0.94764600
C	-0.57672600	3.46635600	1.53163500
H	-0.54873400	1.30933900	1.81961200
H	-1.94778100	2.11164500	2.55455600
C	-6.09045200	-1.16286600	3.69131300
H	-7.15770500	-0.78272300	1.93192100
H	-4.78341300	-1.57568200	5.38114700
C	-7.09975700	-0.42222000	-1.73848500
H	-6.53213700	-0.44781600	-3.83749000
H	-7.38366900	-0.45435300	0.33080900
C	-1.60675000	4.56426300	1.22681800
H	-1.87511500	4.18806200	-0.88266200
H	-3.24270400	5.01145800	-0.12628500
H	-4.58292500	1.49998700	-0.69413700
C	-3.52876200	2.37976500	-2.32749500
C	-5.38968200	3.44808800	-0.99178600
H	0.10326000	3.39298200	0.66494400
C	0.26601700	3.79623300	2.76345400
H	-6.98835100	-1.00274000	4.29323800
H	-8.13648200	-0.12158400	-1.90509800
H	-2.23998600	4.71491100	2.12128300
H	-1.08636100	5.52014200	1.04458700
H	-2.70946800	1.64617400	-2.33639900
H	-4.27021400	2.05041100	-3.07249100
H	-3.12286900	3.34697500	-2.66867200
H	-5.87223600	3.53564100	-0.00406300
H	-5.10163100	4.46194200	-1.31657100
H	-6.14692800	3.07868600	-1.70207200
H	1.01023700	3.00917800	2.95819900
H	0.80788600	4.74614400	2.62810100
H	-0.36731400	3.89064700	3.66229300

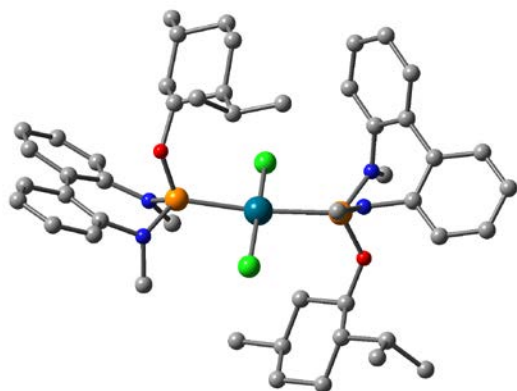


t-TS_IXb-Xb (+24,4 vs. IXa)

C	-1.71578800	-1.22582200	4.44979700
C	-1.91038700	-1.68589100	3.12433900
C	-1.15821300	-2.83359300	2.66076800
C	-0.22364700	-3.33650800	3.60615100
C	-0.04590100	-2.86845000	4.90020000
C	-0.82242900	-1.79974100	5.33911900
H	-2.26545900	-0.35061200	4.78267900
H	0.42912000	-4.15348100	3.32552800
H	0.69784100	-3.33743200	5.54802800
H	-0.71659300	-1.39172700	6.34721100
C	-1.21121500	-3.59162700	1.33049500
C	-0.40814100	-4.76054400	1.18859100
C	-1.97682500	-3.28697100	0.16819500
C	-0.32797200	-5.52434200	0.03097000
H	0.18320400	-5.12610300	2.01989900
C	-1.88086100	-4.05269000	-1.00809800
C	-1.06674400	-5.16939700	-1.10003600
H	0.31927100	-6.40460300	0.02050500
H	-2.46660800	-3.71443600	-1.86382200
H	-1.00174700	-5.74309300	-2.02695200
P	-2.42485500	-0.72743100	0.69406400
C	-4.32587500	-2.59295300	0.24385200
H	-4.55296300	-3.42642100	-0.43584800
H	-4.55554000	-2.90393700	1.27942500
H	-4.96734800	-1.74347900	-0.02496700
C	-3.72438900	0.01774700	3.01415400
H	-4.23264300	-0.48281200	3.85137600
H	-3.19849300	0.91232200	3.38840300
H	-4.48621700	0.34144800	2.29869300
N	-2.91526300	-2.21686900	0.08479300

N	-2.82665900	-0.93023900	2.35403200
Pd	-0.24643900	-0.07324500	0.20741700
O	-3.59697400	0.26468300	0.19345500
C	-3.40381400	1.50228000	-0.54721100
C	-4.43694300	1.51670300	-1.67991800
C	-3.56507300	2.65921900	0.43449300
H	-2.38384800	1.50401400	-0.96899100
C	-4.45024500	2.90336800	-2.34867600
H	-5.41413400	1.37945600	-1.18021200
C	-4.25452800	0.33857100	-2.67421100
C	-3.60272600	4.02992800	-0.25322600
H	-2.74719700	2.61239000	1.17077200
H	-4.51238400	2.50733400	0.98185300
C	-4.68163600	4.03473500	-1.34404600
H	-3.48430200	3.07610800	-2.85334400
H	-5.21918200	2.92255300	-3.13739100
H	-3.96939200	-0.53836900	-2.07085100
C	-3.13554700	0.56559700	-3.69941100
C	-5.57466400	-0.00388800	-3.37654200
H	-2.63142500	4.18067100	-0.75781400
C	-3.78897600	5.15494700	0.76548400
H	-5.67478600	3.92024600	-0.87092600
H	-4.68941300	5.00850400	-1.86262100
H	-2.18916600	0.85495300	-3.21970400
H	-2.93480600	-0.36389600	-4.25476100
H	-3.40949200	1.34004700	-4.43436500
H	-6.36284100	-0.26046200	-2.64961200
H	-5.94085400	0.84103000	-3.98407800
H	-5.44807800	-0.86397400	-4.05399200
H	-2.99520400	5.13690000	1.52927800
H	-3.77092600	6.14300200	0.27732700
H	-4.75690700	5.05484400	1.28559400
Cl	-0.39143500	1.31408800	2.12191900
Cl	-0.49500100	-1.06432900	-1.92062300
P	1.91956200	0.73522900	-0.33437600
N	2.90284000	1.20872900	0.94806500
N	1.75253500	2.21630200	-1.18641700
O	2.89479700	0.00005100	-1.41198800
C	4.04782000	2.02045400	0.66557800
C	2.79508800	0.67928900	2.30922900
C	1.48904500	3.39872000	-0.43510700
C	1.18484200	2.13045400	-2.53643100
C	3.20178400	-1.36159900	-1.81698700
C	3.87517600	3.39366100	0.39422200
C	5.33160900	1.45900900	0.69584100
H	1.97771200	-0.04644600	2.37082800
H	3.73054800	0.17896200	2.60741300
H	2.57788600	1.49181300	3.01932200
C	2.51813100	3.99145700	0.33885400
C	0.23449500	4.02176300	-0.50626600
H	1.73410900	1.37126800	-3.10759000
H	0.11684700	1.85146500	-2.54597100
H	1.30728800	3.10361600	-3.03245500

C	2.71511300	-2.43032100	-0.82552300
C	2.68357700	-1.52741500	-3.24587700
H	4.30556400	-1.38494700	-1.83282300
C	5.02053000	4.18146500	0.18128200
C	6.45681000	2.25601100	0.48056800
H	5.43808000	0.38960200	0.89061700
C	2.24342300	5.18676800	1.02366100
C	-0.01532100	5.21420600	0.17350900
H	-0.55554300	3.55334400	-1.09356100
C	2.85568900	-3.83587500	-1.43607400
H	1.63704300	-2.25737700	-0.68571000
C	3.40653300	-2.28510900	0.55665200
C	2.81786200	-2.95322300	-3.79683000
H	3.21287700	-0.80914600	-3.89430000
H	1.62133800	-3.24471700	-3.24496700
C	6.29920100	3.62334800	0.22687300
H	4.89752800	5.24464100	-0.03851100
H	7.45396800	1.80967300	0.50305200
C	0.99114500	5.79907100	0.94715300
H	3.03295200	5.63762100	1.62980200
H	-1.00076700	5.67986600	0.10905900
C	2.18757700	-3.94255700	-2.80701100
H	3.92289400	-4.09553900	-1.54523200
H	2.42185300	-4.57020500	-0.73870100
H	3.49618000	-1.20724800	0.74305000
C	4.83371100	-2.84553800	0.61710700
C	2.53719400	-2.85899100	1.67655500
H	3.89503900	-3.20040200	-3.87450600
C	2.20078400	-3.05857300	-5.19296800
H	7.17426100	4.25428400	0.05270600
H	0.80183200	6.72757100	1.49089700
H	1.10922200	-3.72445300	-2.71171500
H	2.27582900	-4.97262600	-3.19326600
H	5.46150800	-2.47490700	-0.20930900
H	5.31960600	-2.54636200	1.56013700
H	4.84294400	-3.94664800	0.57878700
H	1.53732100	-2.40058400	1.67495400
H	2.40041300	-3.94595800	1.56139900
H	2.98696000	-2.68072700	2.66634800
H	2.66990100	-2.35050800	-5.89571800
H	2.31583000	-4.07395800	-5.60630200
H	1.12210200	-2.82935200	-5.15711700

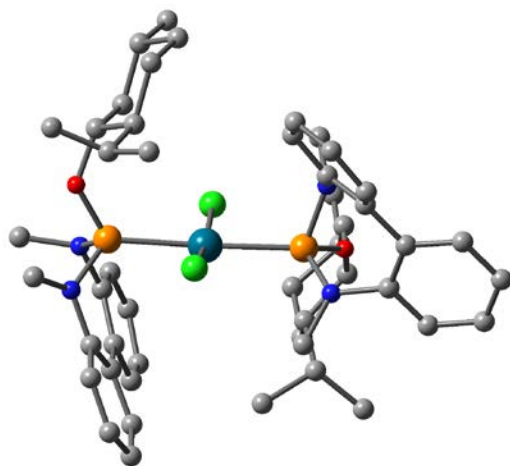


c-TS_IXc-Xd (+24,3 vs. IXa)

Pd	0.14124000	-0.46160300	-0.16684500
Cl	-0.27689600	0.71807700	-2.18949800
Cl	0.52452200	-1.88731300	1.68643500
P	2.44200600	0.03581000	-0.39792000
N	3.25769600	0.52031400	1.00302000
N	2.88815900	1.31344400	-1.42730800
O	3.29653400	-1.13916800	-1.14545400
C	4.59915300	1.02774200	0.92384000
C	2.75254000	0.35453600	2.37129000
C	2.75239200	2.65460000	-0.94696400
C	3.04988800	1.15335500	-2.87354800
C	3.05265600	-2.54877100	-1.38802700
C	4.83947900	2.32620700	0.42120500
C	5.65578400	0.28292200	1.46591800
H	1.66069700	0.32018900	2.37547400
H	3.12352800	-0.56828600	2.84511400
H	3.07788900	1.22075000	2.96507200
C	3.72350700	3.17303300	-0.06029900
C	1.71332400	3.47941300	-1.40272800
H	3.22853300	0.09763900	-3.10664900
H	2.16371000	1.48915300	-3.43220500
H	3.92936700	1.73156500	-3.20132000
C	3.33516500	-3.39196500	-0.13662900
C	1.66446200	-2.80728000	-1.97191800
H	3.80387600	-2.78943500	-2.15953800
C	6.15694800	2.81856800	0.43436900
C	6.95608900	0.79050300	1.47672300
H	5.44797400	-0.69688100	1.89535900
C	3.61460200	4.51214700	0.35440800
C	1.62986700	4.81031400	-0.99100400
H	0.96357300	3.05542400	-2.06975300
C	3.08596300	-4.87610400	-0.45934800
H	2.58340800	-3.08240400	0.60774700

C	4.72940100	-3.10256500	0.47005400
C	1.42204100	-4.29166800	-2.27825400
H	1.51959100	-2.18516300	-2.86987200
H	0.90772500	-2.48742300	-1.23639900
C	7.20947200	2.06039600	0.94880500
H	6.35132200	3.81388000	0.02788000
H	7.76875700	0.19238200	1.89598900
C	2.58061200	5.32849200	-0.10615200
H	4.35066200	4.91000600	1.05694300
H	0.81091200	5.43685200	-1.35149100
C	1.67995900	-5.12079300	-1.01150400
H	3.82360400	-5.22330700	-1.20398900
H	3.25125800	-5.48104400	0.44652000
H	4.85083700	-2.01222900	0.41716100
C	5.89943100	-3.71828100	-0.30799100
C	4.78566100	-3.49359000	1.95177900
H	2.15444400	-4.60966900	-3.04560000
C	0.01423100	-4.52000300	-2.83228800
H	8.22524900	2.46304100	0.94284800
H	2.51295600	6.36534500	0.23197700
H	0.93075700	-4.84302400	-0.24761600
H	1.53390700	-6.19292000	-1.22700700
H	5.85626100	-3.47463500	-1.38183900
H	6.85846400	-3.33491400	0.07662300
H	5.92250800	-4.81618100	-0.21276500
H	3.99035800	-2.99069600	2.52571500
H	4.66180900	-4.58049100	2.09170400
H	5.75516200	-3.21602500	2.39799800
H	-0.17711000	-3.89984700	-3.72292700
H	-0.13780300	-5.57505400	-3.11137300
H	-0.74656000	-4.26429300	-2.07587300
P	-2.19296000	-0.68507800	0.13278400
N	-2.73335100	-1.84437200	1.23185200
N	-3.15895100	-1.06567800	-1.22237700
O	-2.85979200	0.60842200	0.83976600
C	-3.94225000	-1.63466400	1.95252700
C	-2.45245900	-3.22683700	0.84218400
C	-4.55272800	-0.81358500	-1.22663700
C	-2.52705000	-1.64981400	-2.40691900
C	-2.84102200	2.02158400	0.51363600
C	-5.17282300	-1.21013200	1.36825100
C	-3.83479200	-1.92439300	3.32468700
H	-2.43638200	-3.86918800	1.73446100
H	-3.20679200	-3.61757700	0.13282500
H	-1.45719100	-3.28356700	0.37939600
C	-5.07016200	-0.48826800	-2.50461400
C	-5.43618500	-0.81643600	-0.08318200
H	-3.13276100	-2.49637600	-2.76479500
H	-2.37889400	-0.92752900	-3.22316600
H	-1.53504700	-2.03041800	-2.13860200
C	-1.47744900	2.67457500	0.78370800
C	-3.36310300	2.28690700	-0.89534200
H	-3.57050000	2.42917100	1.23185100

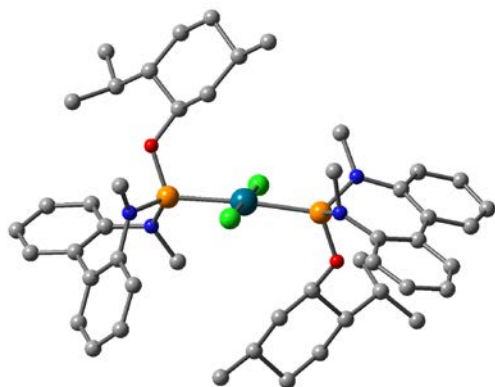
C	-6.25499800	-1.16349700	2.29100500
C	-4.92297600	-1.86046800	4.18311200
H	-2.84562000	-2.20865900	3.68946700
C	-6.38806900	-0.12575800	-2.72765000
H	-4.38584400	-0.47874200	-3.35011500
C	-6.75935200	-0.38375000	-0.37409700
C	-1.61537400	4.18496500	0.51273600
H	-0.77466100	2.28339400	0.03021000
C	-0.88669700	2.31654100	2.17114100
C	-3.45796000	3.79023300	-1.19303000
H	-4.35180400	1.81906000	-1.00603900
H	-2.68780800	1.81339200	-1.62556100
C	-6.15123600	-1.47793600	3.64214900
H	-7.24943500	-0.88181800	1.96197700
H	-4.81600100	-2.09779000	5.24404700
C	-7.24514800	-0.05276400	-1.63154700
H	-6.72658300	0.12236700	-3.73644800
H	-7.48035400	-0.29753300	0.43050300
C	-2.10962800	4.46545100	-0.90981100
H	-2.31532000	4.63610900	1.23911100
H	-0.64342600	4.67411600	0.66634200
H	-0.72362500	1.22507900	2.15835100
C	-1.82443800	2.61364200	3.34814600
C	0.48591400	2.96926100	2.37932500
H	-4.20115000	4.22656000	-0.49743100
C	-3.94066800	4.03380000	-2.62411300
H	-7.04291600	-1.41682600	4.27093600
H	-8.28627500	0.25757700	-1.74435100
H	-1.36571800	4.08505500	-1.63306500
H	-2.18898900	5.55324600	-1.07870400
H	-2.75589500	2.03015200	3.28775000
H	-1.33707900	2.35191200	4.30131700
H	-2.09068700	3.68277600	3.39877000
H	1.15943900	2.77358300	1.53032000
H	0.40584300	4.06170000	2.49643100
H	0.96542300	2.57869300	3.28970900
H	-4.91520400	3.55183500	-2.80539100
H	-4.04720400	5.11055900	-2.83422600
H	-3.22215200	3.61794500	-3.35102900



t-TS_IXc-Xd (+26,1 vs. IXa)

C	2.41149000	-1.11442400	-4.05395700
C	2.49434200	-1.59705000	-2.72600400
C	1.75051800	-2.77585400	-2.35129500
C	0.94322600	-3.30860200	-3.39327600
C	0.87845500	-2.82554800	-4.69259000
C	1.63888900	-1.71051300	-5.03671400
H	2.95056700	-0.20605200	-4.30909900
H	0.30363500	-4.15862600	-3.19146800
H	0.22895100	-3.31789400	-5.41970800
H	1.61075200	-1.28804100	-6.04399300
C	1.70155300	-3.53286400	-1.02162900
C	0.97349300	-4.75760600	-0.98525000
C	2.28518500	-3.17999800	0.23172300
C	0.78628800	-5.53083000	0.15324800
H	0.53691600	-5.16065100	-1.89184600
C	2.07672900	-3.95835100	1.38589000
C	1.33413900	-5.12720000	1.37283200
H	0.20930100	-6.45573000	0.07857000
H	2.51629300	-3.58739200	2.31267600
H	1.18167600	-5.70579000	2.28645700
P	2.71370500	-0.59764300	-0.26551600
C	4.58270000	-2.39750000	0.48657600
H	4.74069000	-3.22635000	1.19073200
H	4.96179500	-2.69999900	-0.50733400
H	5.15665100	-1.52990900	0.83632100
C	4.37188400	0.00053200	-2.42459000
H	4.93125700	-0.58458900	-3.16970700
C	3.98954900	0.91662500	-2.90564100
H	5.06163400	0.29930300	-1.62944700
N	3.15194300	-2.06430200	0.44751100

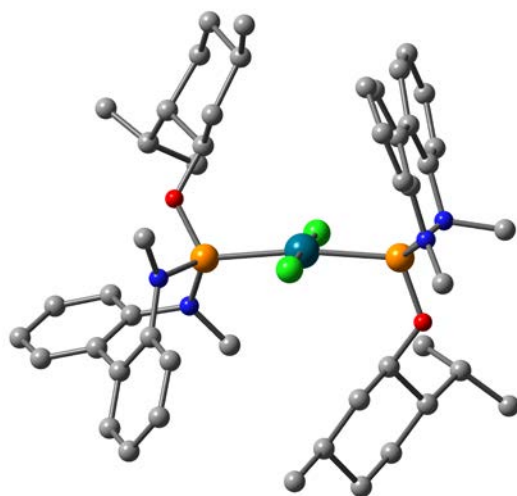
N	3.31351400	-0.83633900	-1.85939200	C	-2.59877300	-2.62701600	0.50389500
Pd	0.43094300	-0.06611700	-0.07500000	C	-2.98064700	-1.72640600	2.89782400
O	3.83826800	0.43001400	0.27902000	H	-4.35114000	-1.61614000	1.23857000
C	3.74961200	1.47874100	1.28123300	C	-5.19362300	3.67857500	-0.80024500
C	3.02629800	2.72162000	0.74512800	C	-6.33064100	1.61718600	-1.35909700
C	3.16570800	0.96335400	2.58963000	H	-5.05196500	-0.10224000	-1.64986900
H	4.80901000	1.73029600	1.44783600	C	-2.49853600	5.05192600	-1.17876000
C	3.04360100	3.79972900	1.84601000	C	-0.44627800	5.37257500	0.04465700
H	1.97418100	2.42972900	0.57881500	H	0.13842500	3.75084400	1.33138000
C	3.57315200	3.19114100	-0.62748900	C	-2.79270000	-4.03681900	1.08944600
C	3.18007700	2.04073200	3.68314000	H	-1.51746300	-2.42360200	0.52858300
H	3.72699700	0.07103700	2.91165800	C	-3.07580900	-2.49830200	-0.96680700
H	2.12758300	0.64034500	2.42437800	C	-3.16274900	-3.15715300	3.42168000
C	2.46166400	3.29730300	3.17148200	H	-3.63047500	-1.02569000	3.44847600
H	4.08107300	4.13862100	2.01468600	H	-1.94180000	-1.41535000	3.07251300
H	2.48345900	4.68333000	1.50421600	C	-6.37615400	2.98175100	-1.05174600
H	3.41439000	2.34257600	-1.30683300	H	-5.23245300	4.73847000	-0.53825400
C	5.07280400	3.51483400	-0.63061600	H	-7.25282800	1.06059800	-1.54293100
C	2.75771300	4.35254700	-1.20522600	C	-1.38736300	5.84063800	-0.87524900
H	4.23387300	2.31606100	3.88359300	H	-3.24155100	5.41461500	-1.89312300
C	2.56214500	1.51267900	4.97938700	H	0.43075700	5.97387700	0.29376200
H	1.39175000	3.05568600	3.03756500	C	-2.35044100	-4.12504900	2.55033800
H	2.50626500	4.09462100	3.93248100	H	-3.85514300	-4.32978500	1.02806600
H	5.68823700	2.65279600	-0.32882300	H	-2.23127500	-4.75717200	0.47289600
H	5.39644100	3.80543400	-1.64322100	H	-3.16099700	-1.42282100	-1.16566400
H	5.31415800	4.35485200	0.04198800	C	-4.46127400	-3.09507200	-1.24574900
H	1.68711200	4.10565700	-1.22761900	C	-2.02718900	-3.04263200	-1.93570400
H	2.89000100	5.28206200	-0.62675300	H	-4.23041400	-3.43566000	3.32178200
H	3.07490700	4.56477600	-2.23930000	C	-2.78095800	-3.24886400	4.90047900
H	3.10911400	0.63265500	5.35463200	H	-7.33583500	3.50142600	-0.99637000
H	2.56961600	2.28118900	5.76926300	H	-1.26006100	6.81491400	-1.35277000
H	1.51549500	1.20657600	4.81249100	H	-1.27798000	-3.87312700	2.62960100
Cl	0.76328900	1.36268700	-1.93208000	H	-2.46823600	-5.15782800	2.92105900
Cl	0.30941500	-1.14839400	2.02036200	H	-5.21791500	-2.74616200	-0.52453200
P	-1.84117900	0.59679800	0.13018800	H	-4.80514600	-2.80271900	-2.25144100
N	-2.64677300	0.99860600	-1.29291500	H	-4.44737300	-4.19625900	-1.21240100
N	-1.91329100	2.07523200	1.00229200	H	-1.05990800	-2.54372100	-1.78120100
O	-2.91849500	-0.20365500	1.05099700	H	-1.86741600	-4.12346200	-1.79235800
C	-3.90903500	1.66572800	-1.18152600	H	-2.32325900	-2.88293100	-2.98476700
C	-2.28385700	0.48952700	-2.61806100	H	-3.37911900	-2.55623500	5.51509600
C	-1.72074900	3.31386300	0.32949000	H	-2.93359500	-4.26820500	5.29126100
C	-1.52447400	1.99842200	2.41514500	H	-1.71798400	-2.98916900	5.04215100
C	-3.26007200	-1.57107300	1.40235800				
C	-3.94228600	3.03721900	-0.85727400				
C	-5.09950400	0.96367100	-1.41871600				
H	-1.41023400	-0.16659900	-2.54758100				
H	-3.11659900	-0.08415600	-3.05503500				
H	-2.02701900	1.32197200	-3.29056000				
C	-2.69541900	3.79477000	-0.58300900				
C	-0.61060900	4.11810400	0.63208700				
H	-2.07729700	1.18164200	2.89616100				
H	-0.44742000	1.80713600	2.55961300				
H	-1.79090100	2.94353900	2.90823700				



c-TS_Xa-IXa (+20,7 vs. IXa)

Pd	0.14172100	0.30332200	-0.50210900
Cl	0.16587700	1.08136500	1.74399100
Cl	0.10842100	-0.47516900	-2.73148200
P	2.45330000	-0.06739000	-0.40504200
N	2.93363400	-0.92157300	0.96265900
N	3.28961900	-0.90084200	-1.62780700
O	3.30544100	1.32283100	-0.48340700
C	4.32299800	-1.22974700	1.14565500
C	2.01629100	-1.71725200	1.78290900
C	3.29781400	-2.33112800	-1.57020400
C	3.57515200	-0.28028500	-2.92482100
C	2.80276200	2.63301100	-0.12078700
C	4.92235000	-2.24793700	0.37184700
C	5.04659800	-0.58072600	2.15000000
H	2.20999700	-2.79321900	1.63471800
H	0.98019400	-1.50543200	1.50329900
H	2.13953500	-1.47116000	2.84878000
C	4.12227000	-2.99695600	-0.62958500
C	2.53430600	-3.08074400	-2.47836600
H	3.69592400	0.80075000	-2.78462100
H	2.77556100	-0.44972100	-3.66116200
H	4.52322200	-0.68620500	-3.31093700
C	3.98881800	3.57590000	0.14032900
C	1.88944200	3.17040400	-1.21960000
H	2.22602100	2.53106000	0.81310900
C	6.26779500	-2.56877400	0.62033300
C	6.38084600	-0.91704500	2.38833000
H	4.54558500	0.18763700	2.74122500
C	4.15774200	-4.40292000	-0.64209000
C	2.58830500	-4.47546200	-2.47627800
H	1.87716000	-2.55359900	-3.16982100
C	3.39753300	4.94314600	0.54478100
H	4.50714800	3.72298900	-0.82607900

C	5.01910300	2.97314500	1.14364500	C	-6.64479200	-0.27676400	-1.58839900
C	1.29813900	4.53239300	-0.84059100	C	-5.76845700	-1.36429100	-3.55869100
H	2.46832000	3.25409600	-2.15689700	H	-3.65291100	-1.03583600	-3.85161000
H	1.07839300	2.44867100	-1.41417700	C	-5.67981400	2.66229900	2.50541200
C	6.99311900	-1.90863900	1.61518600	H	-3.59822500	3.07453700	2.31523000
H	6.74894500	-3.34249100	0.01732800	C	-6.57027500	1.24343300	0.78821400
H	6.94248700	-0.40007400	3.16993300	C	-2.70491800	-3.33772800	2.90166300
C	3.40458600	-5.14071000	-1.55639500	H	-4.11574700	-2.73811300	1.39508200
H	4.77948800	-4.92000900	0.09262600	C	-4.07121600	-1.12226400	2.80891000
H	1.97955100	-5.04193600	-3.18516000	C	-1.00150000	-3.89016900	1.10436400
C	2.43642200	5.50589800	-0.50907800	H	-0.88334900	-2.36589800	-0.44678300
H	2.86654400	4.83956700	1.50847800	H	-2.41315300	-3.25898500	-0.42437300
H	4.20949100	5.66503500	0.71298300	C	-6.83877300	-1.07280100	-2.71177600
H	4.46152100	2.28032400	1.79855500	H	-7.53280600	-0.11060900	-0.98866700
C	5.70045200	4.00239000	2.05689100	H	-5.89278000	-2.00082600	-4.43774600
C	6.09300600	2.16307400	0.40124700	C	-6.75678300	1.96856500	1.95763500
H	0.70483200	4.38600500	0.08202600	H	-5.77970200	3.23727600	3.42905200
C	0.36890200	5.06628500	-1.93153600	H	-7.45143900	0.72400600	0.43057200
H	8.04018900	-2.17004200	1.78672400	C	-2.05374100	-4.45010000	2.07056400
H	3.44533100	-6.23244500	-1.54137100	H	-1.93864600	-2.88030200	3.55235100
H	2.99945000	5.71965000	-1.43688300	H	-3.46495500	-3.76770900	3.57177000
H	2.02243900	6.46901300	-0.16507000	H	-4.51041500	-0.46511800	2.04481500
H	4.98757800	4.54284700	2.69717700	C	-3.13780200	-0.25380600	3.66339000
H	6.41963900	3.49524900	2.72043500	C	-5.23560200	-1.66562500	3.64649400
H	6.26514600	4.74876800	1.47274300	H	-0.22394800	-3.40312100	1.71996000
H	5.64662600	1.38401900	-0.22918600	C	-0.32098600	-4.96953800	0.26194100
H	6.69198600	2.82999700	-0.24352400	H	-7.83621400	-1.47017900	-2.91510500
H	6.77977600	1.67301200	1.10841300	H	-7.74042100	1.98233700	2.43225900
H	-0.44918300	4.35908200	-2.14495100	H	-2.83062700	-4.97908100	1.48753300
H	-0.08243000	6.02783200	-1.63805400	H	-1.59374400	-5.20055200	2.73599900
H	0.92259400	5.22675900	-2.87216800	H	-2.35715100	0.23754600	3.06278600
P	-2.21457300	0.50486500	-0.53003400	H	-3.71492600	0.54377800	4.15724500
N	-3.00723700	0.50405900	-2.01640500	H	-2.63964200	-0.84059400	4.45338900
N	-2.91106600	1.87345200	0.20740800	H	-5.89811100	-2.31059600	3.04536800
O	-2.94464500	-0.76095100	0.17172800	H	-4.88546800	-2.25495000	4.51030400
C	-4.33633300	0.00469900	-2.11815000	H	-5.84427000	-0.83576600	4.04025100
C	-2.65929300	1.62226700	-2.89354800	H	0.46065700	-4.53772900	-0.38407500
C	-4.24914100	1.84831700	0.66964900	H	0.15171300	-5.73478500	0.89909900
C	-2.09899500	3.07565000	0.39850000	H	-1.05218100	-5.47846900	-0.38930300
C	-2.28954600	-1.70853400	1.05577600				
C	-5.40156800	0.30836300	-1.21629900				
C	-4.53127100	-0.82673700	-3.23743200				
H	-2.88693100	1.36273900	-3.93741700				
H	-3.21037200	2.54509600	-2.62865500				
H	-1.57837000	1.81515400	-2.82999400				
C	-4.45590400	2.58086500	1.86219900				
C	-5.35290600	1.14551800	0.06047300				
H	-2.68908400	3.96404700	0.12636200				
H	-1.71241000	3.18533100	1.42261100				
H	-1.22700200	3.02861000	-0.26495700				
C	-3.34860400	-2.24719100	2.02361500				
C	-1.63933300	-2.80875900	0.22239700				
H	-1.51381500	-1.17618400	1.62874200				

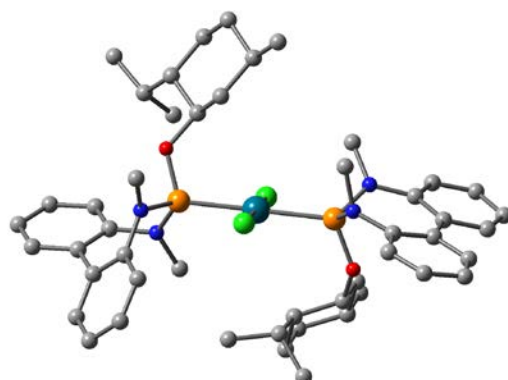


t-TS_Xa-IXa (+17,7 vs. IXa)

C	3.92105800	0.01550200	3.46892400
C	3.76117100	0.02175400	2.06103000
C	3.81502300	1.29049400	1.35906400
C	3.86871400	2.42472700	2.21121400
C	3.98583800	2.39805400	3.59349800
C	4.05101300	1.16362700	4.23340200
H	3.89672900	-0.93468200	3.99320000
H	3.81313700	3.41324400	1.77388300
H	4.02740800	3.33549800	4.15222200
H	4.16101600	1.08678700	5.31779600
C	3.86435000	1.61357900	-0.13665000
C	4.09576900	2.96320100	-0.53232400
C	3.72836700	0.71676700	-1.23227300
C	4.14427100	3.39344400	-1.85325100
H	4.28004300	3.73192200	0.21012400
C	3.76417200	1.15498500	-2.56720100
C	3.96815700	2.48469200	-2.89955000
H	4.32932900	4.45060700	-2.05897200
H	3.60864700	0.39957100	-3.33908600
H	3.98897100	2.80628700	-3.94313300
P	2.49597200	-1.21957300	0.08690500
C	4.83260900	-1.45785000	-1.24582000
H	5.23480800	-1.27906600	-2.25366600
H	5.59357800	-1.16943800	-0.49911400
H	4.62526200	-2.53070900	-1.14239100
C	3.63643900	-2.45831100	2.27710100
H	4.63651600	-2.49869100	2.73404500

H	2.86992100	-2.52139500	3.06795600
H	3.52648700	-3.32677000	1.62127200
N	3.58895500	-0.69293600	-1.07785500
N	3.50999700	-1.24164700	1.47432900
Pd	0.40415200	-0.15135300	0.24486200
O	2.35494800	-2.80854300	-0.22215800
C	1.10277200	-3.40132900	-0.66948800
C	1.40633200	-4.45349000	-1.74034400
C	0.37335300	-3.98015400	0.53758400
H	0.48876200	-2.60533600	-1.12006100
C	0.07762800	-5.12496800	-2.14158100
H	2.03517700	-5.21910700	-1.24754700
C	2.22338600	-3.89704200	-2.93460200
C	-0.94291700	-4.66106200	0.13846600
H	0.18740000	-3.17761800	1.26780100
H	1.03917400	-4.71586700	1.02394600
C	-0.66936900	-5.71688800	-0.94181900
H	-0.57190700	-4.37907200	-2.63176100
H	0.27070100	-5.90802600	-2.89117600
H	3.07203000	-3.35437300	-2.49024200
C	1.45566200	-2.89468500	-3.80693800
C	2.81089000	-5.02790800	-3.78916200
H	-1.59549100	-3.88601700	-0.30601800
C	-1.66277000	-5.24095000	1.35597200
H	-0.06805500	-6.53218400	-0.49772600
H	-1.61815500	-6.17174700	-1.27388500
H	1.04035000	-2.05912700	-3.22443900
H	2.12916300	-2.45687500	-4.56167000
H	0.62871100	-3.37962100	-4.35139300
H	3.39370400	-5.73670200	-3.17790100
H	2.02306600	-5.60001400	-4.30671100
H	3.48079500	-4.62214900	-4.56447000
H	-1.87653000	-4.45845400	2.09981700
H	-2.62199100	-5.70234400	1.07005400
H	-1.04638300	-6.01655000	1.84224400
Cl	0.40010400	-0.71221500	2.54303300
Cl	0.45021900	0.36989200	-2.05661300
P	-1.81661100	0.60989100	0.34368400
N	-2.81349900	-0.14514000	-0.77844200
N	-2.75248800	0.44404000	1.76024300
O	-1.98346400	2.22162200	0.15386200
C	-4.20138000	0.21034000	-0.82383400
C	-2.43533400	-1.28918600	-1.60904000
C	-3.42264800	-0.79082000	2.01283700
C	-2.48125600	1.31322000	2.91107900
C	-0.92002400	3.14473500	-0.19242700
C	-5.07899100	-0.28475200	0.16355100
C	-4.68438700	0.97994000	-1.88801200
H	-3.08399800	-2.15005900	-1.37550100
H	-1.39647300	-1.57158100	-1.41721400
H	-2.52670900	-1.04751400	-2.67961700
C	-4.57245900	-1.14507600	1.26191200
C	-3.00028200	-1.61912800	3.06489900

H	-2.39880800	2.35096800	2.56447500
H	-1.55720400	1.04050000	3.44466200
H	-3.33124700	1.24891700	3.60533100
C	-1.53585800	4.34686800	-0.91930800
C	-0.18960000	3.57749200	1.07691100
H	-0.21549400	2.63558800	-0.86762200
C	-6.44520400	0.03141800	0.05758200
C	-6.04456100	1.28309800	-1.97763300
H	-3.97836700	1.32976200	-2.64255100
C	-5.25244600	-2.33117200	1.59214200
C	-3.70069000	-2.78274400	3.38521900
H	-2.09860700	-1.34808300	3.61358100
C	-0.38013700	5.29289500	-1.29632400
H	-2.16300000	4.87319700	-0.17431000
C	-2.48404500	3.96218400	-2.07981100
C	0.91965900	4.60137500	0.79405900
H	-0.92927300	4.01676600	1.77019700
H	0.23783200	2.69195700	1.57744300
C	-6.92468000	0.80950700	-0.99830300
H	-7.13462200	-0.32994500	0.82427100
H	-6.41464100	1.89118200	-2.80654900
C	-4.82937000	-3.14509200	2.64370400
H	-6.12862800	-2.61531300	1.00437900
H	-3.35266600	-3.41552100	4.20530600
C	0.38267600	5.76499400	-0.05421300
H	0.31423100	4.77330600	-1.97997100
H	-0.76842900	6.16400500	-1.84614500
H	-3.24493000	3.31007700	-1.62329700
C	-1.81123600	3.16412300	-3.20250300
C	-3.22081200	5.18564300	-2.64068100
H	1.69788700	4.08371700	0.20388200
C	1.54582200	5.10522300	2.09675900
H	-7.98934400	1.04922800	-1.05521900
H	-5.37498100	-4.06215000	2.87831200
H	-0.29632700	6.37425800	0.57136100
H	1.21665900	6.42704400	-0.34414900
H	-1.37148200	2.22495700	-2.83803600
H	-2.54638300	2.90843300	-3.98406600
H	-1.01026300	3.74414500	-3.69041900
H	-3.69225800	5.77829100	-1.83909900
H	-2.54401200	5.85367300	-3.19880700
H	-4.01525200	4.87212800	-3.37492000
H	1.87054000	4.27192200	2.73695700
H	2.42016300	5.74733000	1.89971000
H	0.81611900	5.70130400	2.67114200

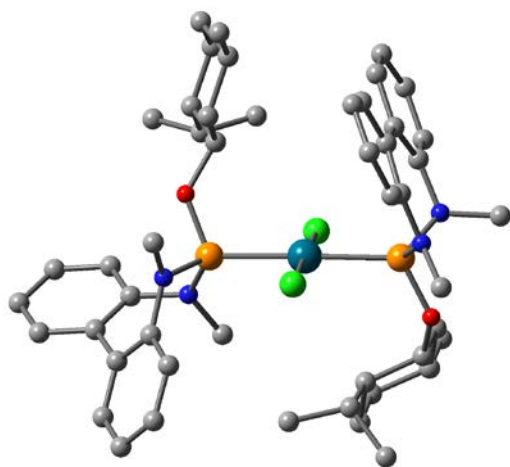


c-TS_Xb-IXb (+18,5 vs. IXa)

Pd	0.02844500	0.06481000	-0.38827800
Cl	0.18956600	1.12437200	1.74497900
Cl	-0.07533400	-1.01558200	-2.48534900
P	2.36533200	-0.07690300	-0.42435100
N	3.06316400	-0.75743900	0.94331600
N	3.20684700	-0.90459200	-1.64955900
O	3.03107500	1.39469600	-0.66852600
C	4.49277900	-0.85991900	1.01025700
C	2.34080500	-1.42212400	2.02934100
C	3.42294500	-2.31148100	-1.51031400
C	3.31379000	-0.34604600	-3.00111400
C	2.35184400	2.67224300	-0.57605400
C	5.15633000	-1.86540800	0.27605800
C	5.20688100	-0.01054500	1.86238300
H	2.64541400	-2.48023000	2.08672100
H	1.26350500	-1.37919200	1.85386600
H	2.54677500	-0.93252600	2.99384200
C	4.39095900	-2.79206600	-0.59358400
C	2.73604300	-3.21658800	-2.33280400
H	2.43677400	-0.57362600	-3.62592000
H	4.21809100	-0.75302500	-3.47814900
H	3.42318200	0.74297600	-2.93141300
C	3.41435800	3.75043100	-0.33210300
C	1.54740200	2.93794300	-1.84530900
H	1.66272700	2.64348100	0.28025900
C	6.55090500	-1.98021400	0.41438000
C	6.59184000	-0.13831000	1.98693300
H	4.65916300	0.74541500	2.42596500
C	4.62815500	-4.17646400	-0.52880300
C	2.99457000	-4.58578300	-2.25981500
H	1.97352400	-2.83268500	-3.01011900
C	2.71284600	5.12183600	-0.27838400
H	4.07170600	3.74830700	-1.22257300
C	4.31882300	3.43628500	0.88587900

C	0.83812200	4.29701600	-1.78267200
H	2.22628700	2.91318100	-2.71643100
H	0.81175900	2.12896300	-1.99089000
C	7.26390500	-1.12522800	1.25747100
H	7.07962900	-2.74401400	-0.16073300
H	7.14428700	0.53378500	2.64796200
C	3.94179800	-5.07000200	-1.35247400
H	5.36127900	-4.55176500	0.18923300
H	2.44172700	-5.27598100	-2.90178700
C	1.87451400	5.40126600	-1.53157300
H	2.05603700	5.16268700	0.60819400
H	3.46252500	5.91714000	-0.14745600
H	4.76552200	2.45329900	0.66845100
C	3.55369200	3.30521000	2.21016400
C	5.47397800	4.43700900	1.01638000
H	0.16029800	4.27889400	-0.90813700
C	-0.00701000	4.54842800	-3.03165300
H	8.34854600	-1.22768800	1.34255700
H	4.14148500	-6.14183900	-1.28026100
H	2.53955800	5.47124500	-2.41255500
H	1.37041800	6.37842800	-1.44003100
H	2.78839300	2.51478600	2.17408200
H	4.24849300	3.05955100	3.03021200
H	3.05165800	4.24695500	2.48674200
H	6.01235600	4.55963100	0.06190300
H	5.12281700	5.43261800	1.33444300
H	6.20107600	4.09215900	1.76950000
H	-0.76735400	3.76102700	-3.16213500
H	-0.52860800	5.51746300	-2.97394300
H	0.62357900	4.55837300	-3.93694100
P	-2.34808000	0.19057100	-0.38970200
N	-3.12518500	0.09225700	-1.88165800
N	-3.05474800	1.60277900	0.25218700
O	-3.10344900	-1.04943200	0.33371200
C	-4.45490100	-0.40903500	-1.96478700
C	-2.75974100	1.13911200	-2.83505500
C	-4.39922100	1.61494100	0.69444900
C	-2.25961400	2.83045100	0.32000000
C	-2.78408500	-1.69494900	1.59180400
C	-5.53023900	-0.04752700	-1.09610000
C	-4.63927400	-1.31104000	-3.02979900
H	-2.96768900	0.80183400	-3.86060600
H	-3.31330700	2.08037900	-2.65246000
H	-1.68052400	1.33789600	-2.76712600
C	-4.62041000	2.44195000	1.82147900
C	-5.49503500	0.86908200	0.12576200
H	-2.86495500	3.67857400	-0.03465500
H	-1.87192500	3.04663200	1.32654700
H	-1.38824000	2.73245400	-0.33966500
C	-1.44663000	-2.44765100	1.52196400
C	-2.85919700	-0.69942700	2.74710200
H	-3.60157200	-2.42576100	1.69953900
C	-6.77082500	-0.65089900	-1.44595600

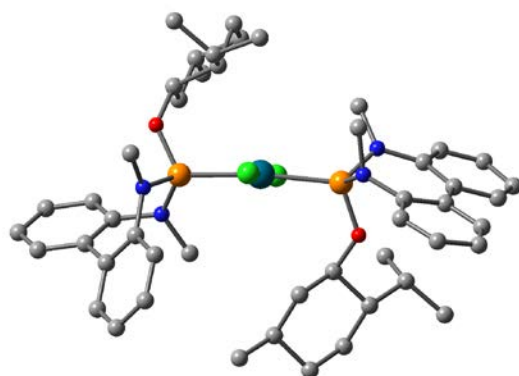
C	-5.87448100	-1.86460900	-3.33149700
H	-3.75372500	-1.56362400	-3.61671500
C	-5.85430300	2.58009100	2.43545900
H	-3.76700300	2.96983900	2.24400100
C	-6.72285300	1.02578200	0.82630900
C	-1.16421000	-3.09761900	2.88756900
H	-0.67541800	-1.67177400	1.37780500
C	-1.33913800	-3.40175100	0.30613800
C	-2.54345200	-1.34798400	4.10168300
H	-3.86056700	-0.24220200	2.75989800
H	-2.13372600	0.10967500	2.56719100
C	-6.95422700	-1.51635600	-2.51892100
H	-7.66538400	-0.44407100	-0.86881700
H	-5.98986900	-2.55644100	-4.16902300
C	-6.92467600	1.84500400	1.92917000
H	-5.96794500	3.23154500	3.30523000
H	-7.60060500	0.48204300	0.49682300
C	-1.19171100	-2.07176700	4.02528800
H	-1.91358900	-3.88350600	3.08929300
H	-0.18552900	-3.60123800	2.85832800
H	-1.58705400	-2.79618400	-0.57997600
C	-2.32468400	-4.57628800	0.34808400
C	0.09848600	-3.89490300	0.10165900
H	-3.32007100	-2.11054200	4.30694100
C	-2.58029600	-0.30857000	5.22377400
H	-7.95055600	-1.92294600	-2.70904400
H	-7.91582600	1.90055800	2.38492500
H	-0.39800800	-1.32040800	3.86097200
H	-0.97240700	-2.56421100	4.98795200
H	-3.36973100	-4.23846300	0.43147100
H	-2.24779100	-5.17217100	-0.57560600
H	-2.11849300	-5.25390700	1.19318800
H	0.80562500	-3.05517400	0.03367200
H	0.43090700	-4.55758700	0.91764000
H	0.18651100	-4.46063600	-0.83845500
H	-3.56073700	0.19258700	5.27383300
H	-2.38194500	-0.76958400	6.20504500
H	-1.81552600	0.46856000	5.05474000



t-TS_Xb-IXb (+17,6 vs. IXa)

C	-3.66404300	-0.09135900	-3.56982500
C	-3.57656100	-0.11006100	-2.15485400
C	-3.62879300	1.15386400	-1.43869000
C	-3.68516500	2.29789100	-2.28026100
C	-3.75321900	2.29007200	-3.66588800
C	-3.76331400	1.06476600	-4.32524900
H	-3.61029900	-1.03289400	-4.10641000
H	-3.68652300	3.28473400	-1.83589200
H	-3.80256800	3.23506400	-4.21101700
H	-3.81856200	1.00106100	-5.41464200
C	-3.65636300	1.46478400	0.06224900
C	-3.73253800	2.82382500	0.48422300
C	-3.63804300	0.54185400	1.14363300
C	-3.76573300	3.23334500	1.81190500
H	-3.79139600	3.62705500	-0.24002100
C	-3.66546900	0.95573100	2.48679100
C	-3.73033300	2.29256800	2.84351100
H	-3.82120300	4.30181900	2.03377000
H	-3.61169000	0.17374600	3.24575400
H	-3.73989000	2.59599500	3.89243400
P	-2.48869500	-1.46847300	-0.14239300
C	-4.90456800	-1.54883100	1.07854900
H	-5.33987000	-1.33168500	2.06517900
H	-5.61218200	-1.22166600	0.29581600
H	-4.76167500	-2.63378700	0.99381100
C	-3.56726400	-2.59002700	-2.42609000
H	-4.54204200	-2.56120400	-2.93556000
H	-2.76412300	-2.68185500	-3.17647400
H	-3.54322600	-3.47666800	-1.78645000
N	-3.60994100	-0.86837100	0.96001000

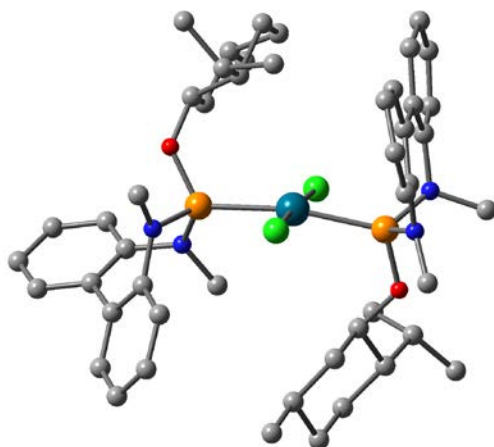
N	-3.41393000	-1.39988200	-1.58791600	C	0.90715100	4.04383000	1.16360000
Pd	-0.36770900	-0.44021400	-0.23236600	C	0.13541200	3.59268800	-1.22891900
O	-2.50292200	-3.07339500	-0.11514600	H	-0.30946400	2.36925700	0.50833800
C	-1.70988000	-3.80642700	1.09423200	C	6.41960600	0.63631400	-0.06864200
C	-0.21542000	-3.80097200	0.74320200	C	5.83552100	1.91137500	1.90699500
C	-1.98911600	-3.30377200	2.50974200	H	3.78407400	1.69234800	2.57869100
H	-2.10037000	-4.83168400	0.99332400	C	5.55348700	-1.90286700	-1.56246700
C	0.55583200	-4.58906000	1.81683200	C	4.07617800	-2.55376900	-3.35832000
H	0.10603300	-2.74851400	0.82929900	H	2.30005700	-1.33878600	-3.58797700
C	0.08190300	-4.22902500	-0.71392500	C	-0.16611800	5.14471100	1.23431700
C	-1.20138700	-4.08263500	3.57265300	H	1.83041800	4.50535200	0.76719900
H	-3.07069100	-3.36759200	2.70978700	C	1.25200000	3.41500800	2.54265000
H	-1.70913500	-2.24086700	2.57339000	C	-0.92123600	4.69756300	-1.12893600
C	0.29329400	-4.05161400	3.22646100	H	1.05029500	4.01892600	-1.67733100
H	0.26680600	-5.65427700	1.77602100	H	-0.20985700	2.78686500	-1.89789600
H	1.63304200	-4.55017900	1.59374800	C	6.77888900	1.52219400	0.94965200
H	-0.55221400	-3.59629600	-1.35366800	H	7.15317100	0.35022500	-0.82615000
C	-0.26627400	-5.69118600	-1.01935300	H	6.10900000	2.61058800	2.70089500
C	1.52979200	-3.91138100	-1.10234400	C	5.23972300	-2.76698500	-2.61288700
H	-1.53085900	-5.13969600	3.54261100	H	6.45974200	-2.06805700	-0.97468000
C	-1.47993100	-3.52908300	4.97154300	H	3.81347100	-3.22856700	-4.17677800
H	0.64883700	-3.00756900	3.29539700	C	-0.45708600	5.76745800	-0.13265500
H	0.86550600	-4.63317500	3.96899500	H	-1.10410000	4.71793800	1.62694100
H	-1.31884900	-5.92541900	-0.79295900	H	0.15114100	5.91693100	1.95404300
H	-0.10679900	-5.90579900	-2.08836900	H	1.65908400	2.41342900	2.33359900
H	0.36548600	-6.39106200	-0.44774300	C	0.03612900	3.22159900	3.45909800
H	1.77053800	-2.85588100	-0.90961100	C	2.34645500	4.22015900	3.25446900
H	2.25494800	-4.53640500	-0.55568900	H	-1.83390200	4.24290300	-0.71120400
H	1.69218600	-4.08265100	-2.17713600	C	-1.25466000	5.27451600	-2.50479200
H	-2.55346700	-3.57701300	5.21697600	H	7.79699400	1.91731900	0.99032800
H	-0.92955200	-4.09300700	5.74203300	H	5.89981600	-3.60625200	-2.84489800
H	-1.16751500	-2.47306100	5.03763700	H	0.45132400	6.26098000	-0.52627500
Cl	-0.29696700	-0.98824000	-2.53296600	H	-1.22692600	6.55237800	-0.03751200
Cl	-0.40365000	0.04291700	2.08283100	H	-0.78668500	2.70164100	2.94832600
P	1.75399200	0.54350100	-0.31326800	H	0.31436800	2.60805000	4.33103800
N	2.85802400	-0.05079200	0.80447000	H	-0.34281500	4.18459500	3.83930500
N	2.70556700	0.51474500	-1.73102000	H	3.26845700	4.26351200	2.65193300
O	1.68770500	2.15333100	-0.08854100	H	2.02051000	5.25716400	3.44535300
C	4.17539300	0.51605800	0.82350200	H	2.60080800	3.77049000	4.22866500
C	2.68172400	-1.25499600	1.61534700	H	-1.59438500	4.48592700	-3.19479000
C	3.53863500	-0.61563200	-1.98796800	H	-2.04951600	6.03525500	-2.43738300
C	2.32943300	1.35592700	-2.87271000	H	-0.36807600	5.75396300	-2.95398100
C	0.51657800	2.98801200	0.12079500				
C	5.11405600	0.12140200	-0.15280500				
C	4.53536200	1.40539000	1.84172900				
H	3.40806600	-2.02793700	1.31170400				
H	1.67255600	-1.65445800	1.48745000				
H	2.82250200	-1.02708700	2.68355600				
C	4.72486500	-0.81499900	-1.23595300				
C	3.23113500	-1.49004300	-3.04148600				
H	2.26804200	2.40224100	-2.54850700				
H	1.36903500	1.05960900	-3.32341700				
H	3.11724600	1.28015800	-3.63449100				



c-TS_Xc-IXb (+19,2 vs. IXa)

Pd	-0.29805600	0.39375900	0.49299600
Cl	-0.09276600	1.11558500	-1.77057000
Cl	-0.41514500	-0.30625700	2.74093800
P	-2.64191100	0.14551000	0.32381600
N	-3.13671100	-0.65087400	-1.07698800
N	-3.49839600	-0.72712300	1.50962600
O	-3.50977100	1.51887000	0.45030200
C	-4.53748100	-0.91513600	-1.24931500
C	-2.25239300	-1.46422700	-1.91483600
C	-3.52249000	-2.15292700	1.40188600
C	-3.86224700	-0.15179100	2.80726800
C	-3.20899300	2.87294700	0.03402300
C	-5.14196800	-1.97018300	-0.53064800
C	-5.27349200	-0.17624300	-2.18060000
H	-2.48553600	-2.53533500	-1.79009700
H	-1.20836500	-1.29755500	-1.63552300
H	-2.36982900	-1.19124300	-2.97506400
C	-4.34893700	-2.77473600	0.43247500
C	-2.79081000	-2.94340400	2.30127300
H	-4.04658000	0.92219400	2.68611000
H	-3.08105500	-0.29135700	3.56937100
H	-4.79693500	-0.62211800	3.15057600
C	-1.95413100	3.44277400	0.71389300
C	-3.17722000	2.97349400	-1.48851100
H	-4.08459700	3.43427500	0.39874500
C	-6.49713700	-2.25182100	-0.77277900
C	-6.62146000	-0.46719500	-2.40585100
H	-4.77013000	0.62038100	-2.73058400
C	-4.41277600	-4.17894500	0.40240800
C	-2.87725900	-4.33613000	2.26090500
H	-2.13974000	-2.44738000	3.02128700
C	-1.73869600	4.88553000	0.22296100
H	-1.10065800	2.85490700	0.33417000
C	-1.96167000	3.27077000	2.25411700

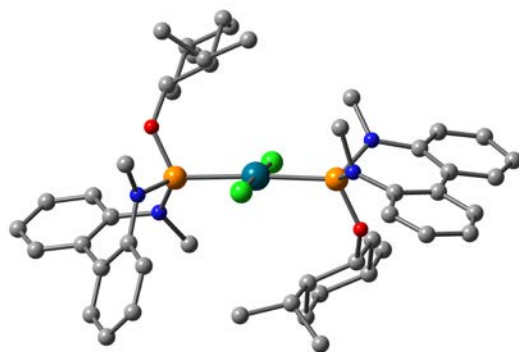
C	-2.91409300	4.40567400	-1.97543900	C	5.39485900	-1.93910200	3.55412600
H	-2.38738200	2.31106300	-1.87360400	H	3.30109700	-1.47358900	3.81964800
H	-4.13856500	2.60742600	-1.88168900	C	5.75004600	2.42132700	-2.26099200
C	-7.23263900	-1.50729200	-1.69820200	H	3.70379000	2.98217600	-2.08884600
H	-6.98025100	-3.05646900	-0.21335200	C	6.49443800	0.85942300	-0.60105600
H	-7.19218900	0.11706700	-3.13166700	C	2.45756600	-3.39347200	-2.94143300
C	-3.69039100	-4.95745800	1.30814900	H	3.79943600	-2.92930800	-1.32849900
H	-5.03630400	-4.66189500	-0.35380300	C	3.98342100	-1.29679100	-2.71113100
H	-2.29497000	-4.93579500	2.96470600	C	0.59231200	-3.83113600	-1.27997000
C	-1.64858900	4.95753700	-1.30466600	H	0.47760900	-2.32142000	0.28478600
H	-2.56629300	5.52927300	0.57176000	H	1.93014400	-3.33418200	0.36112100
H	-0.81840000	5.29224100	0.66929600	C	6.50993300	-1.66298800	2.76168600
H	-2.01995300	2.18769500	2.44233900	H	7.32494700	-0.62942600	1.13525400
C	-3.16084600	3.92107200	2.95478100	H	5.44709200	-2.64271000	4.38813400
C	-0.64287400	3.73681500	2.88218200	C	6.76052700	-1.62340600	-1.72941400
H	-3.76403200	5.03853700	-1.65295900	H	5.91094200	3.02884400	-3.15470500
C	-2.82697300	4.45796200	-3.50198200	H	7.32370000	0.25238600	-0.25773900
H	-8.28779600	-1.73824100	-1.86409600	C	1.66434100	-4.46081400	-2.17868300
H	-3.75353800	-6.04723100	1.26176100	H	1.77761500	-2.86825100	-3.63532700
H	-0.78001100	4.36559200	-1.64640800	H	3.22770700	-3.87328800	-3.56447000
H	-1.47483500	5.99811900	-1.62768000	H	4.42029900	-1.06894900	-1.90622300
H	-4.12027900	3.51058100	2.60329900	C	3.18427600	-0.34090800	-3.60707000
H	-3.10976200	3.74569400	4.04145500	C	5.15501900	-1.92117800	-3.47925400
H	-3.18304200	5.01241100	2.79884900	H	-0.09761000	-3.27556900	-1.94069500
H	0.22073700	3.31296800	2.34812400	C	-0.22879300	-4.86464400	-0.50951100
H	-0.54195000	4.83417900	2.87038200	H	7.47179800	-2.13989000	2.96545400
H	-0.57574300	3.40855500	3.93133200	H	7.75170600	1.58350200	-2.18648800
H	-3.74940700	4.07752600	-3.97050400	H	2.35364500	-5.05650100	-1.55149400
H	-2.66410300	5.48776100	-3.85938900	H	1.19571600	-5.16462600	-2.88762600
H	-1.98807800	3.83858400	-3.86222600	H	2.41288200	0.20727000	-3.04520900
P	2.06383400	0.39665200	0.59806300	H	3.85749400	0.41053700	-4.04885700
N	2.82753900	0.24531200	2.09308100	H	2.68897600	-0.87226900	-4.43706000
N	2.88239200	1.74694600	-0.04557700	H	5.71900900	-2.62885400	-2.84878200
O	2.71124100	-0.88355400	-0.15489400	H	4.81935000	-2.46501900	-4.37795000
C	4.10830900	-0.37264800	2.17961400	H	5.85551000	-1.13823900	-3.81173000
C	2.58626600	1.34927700	3.02329600	H	-1.01626500	-4.38279600	0.09093800
C	4.22334300	1.63598900	-0.48972500	H	-0.71482600	-5.57963900	-1.19328300
C	2.15784600	3.00381900	-0.23824300	H	0.41232000	-5.44067700	0.17970500
C	2.04050300	-1.76022500	-1.09714900				
C	5.21738600	-0.08883400	1.32652100				
C	4.20909400	-1.29152400	3.24104600				
H	2.81309800	1.02391800	4.04859400				
H	3.20650400	2.23517500	2.78676200				
H	1.52449200	1.62801800	2.99452100				
C	4.51044500	2.40366100	-1.64323500				
C	5.25860400	0.82036800	0.10043300				
H	2.80286500	3.84560700	0.05550900				
H	1.79963700	3.15101100	-1.26805800				
H	1.27273400	3.01231600	0.40945900				
C	3.11987600	-2.37003900	-1.99935300				
C	1.24614200	-2.81529900	-0.33359600				
H	1.35276100	-1.15728200	-1.70916400				
C	6.40715100	-0.77915900	1.69308200				



t-TS_Xc-IXb (+20,2 vs. IXa)

C	3.80231000	1.72161200	-3.33185200
C	3.64369300	1.37857500	-1.96622500
C	4.14623200	0.09738200	-1.50648800
C	4.67764100	-0.71936700	-2.53898700
C	4.72420100	-0.40917900	-3.88512500
C	4.34452500	0.87018900	-4.28084500
H	3.44085800	2.68647300	-3.67347200
H	5.02562300	-1.71470900	-2.29461600
H	5.10619200	-1.14017200	-4.60097000
H	4.42842500	1.19562900	-5.32054000
C	4.29639000	-0.47916400	-0.09616100
C	4.93533800	-1.74420100	0.05556100
C	3.83654200	0.07425700	1.13079300
C	5.18583000	-2.35055200	1.28217200
H	5.34709800	-2.26097600	-0.80439100
C	4.01701700	-0.58023600	2.36141100
C	4.68466100	-1.79050900	2.45978400
H	5.73845700	-3.29302200	1.30487700
H	3.59272100	-0.09837400	3.24369600
H	4.81147800	-2.28550300	3.42509200
P	1.99444400	1.69822200	0.11261900
C	4.06586800	2.44618200	1.66989900
H	4.54983800	2.16355000	2.61570100
H	4.84821600	2.67877700	0.92481600
H	3.46348200	3.34638100	1.84678300
C	2.67904500	3.66022400	-1.71905600
H	3.61531800	4.10327200	-2.08970200
H	1.93719700	3.65116000	-2.53627900
H	2.30017600	4.29694900	-0.91507600
N	3.19873100	1.34491400	1.22656500

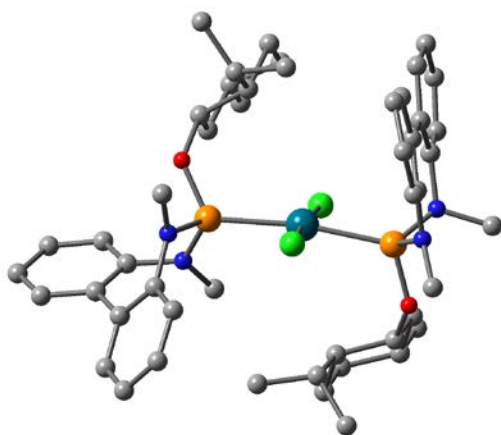
N	2.94830100	2.32817000	-1.17997800	C	0.90448100	-3.48254800	-0.12624100
Pd	0.32550400	0.06392700	-0.20484700	C	-0.72714200	-3.66034100	1.86023600
O	1.35087300	3.06451200	0.71189000	H	-0.83163200	-4.74870400	0.01223600
C	-0.07682200	3.27984100	0.87703600	C	-6.28339000	-1.76288200	-0.20862100
C	-0.28535000	4.26031800	2.03476900	C	-5.63467800	-3.10287300	1.70228100
C	-0.66514300	3.78848700	-0.43544300	H	-3.62057400	-2.75342900	2.43526400
H	-0.53761400	2.31511600	1.13730300	C	-5.62389800	0.93327800	-1.49696800
C	-1.79614900	4.54192100	2.15525900	C	-4.20119600	1.84098400	-3.22265600
H	0.21009400	5.20045900	1.72710900	H	-2.31822400	0.81452300	-3.51247000
C	0.38074100	3.80605500	3.36021200	C	1.88109100	-4.35625900	0.67920700
C	-2.16222900	4.10494100	-0.32185800	H	1.13937100	-2.43574800	0.13377300
H	-0.49436700	3.03914900	-1.22496600	C	1.04264800	-3.61643700	-1.66422400
H	-0.12021600	4.70377600	-0.72689600	C	0.29288900	-4.50039800	2.64324200
C	-2.40139300	5.06749100	0.85052000	H	-0.63221200	-2.61056500	2.17167900
H	-2.31660700	3.61059400	2.43714000	H	-1.75242100	-3.98528000	2.09890200
H	-1.97505600	5.25642200	2.97420100	C	-6.58804400	-2.73499400	0.74681700
H	1.37357600	3.41467200	3.08508300	H	-7.02558200	-1.48820600	-0.96187700
C	-0.36895500	2.67710700	4.08006500	H	-5.86805700	-3.86356300	2.45115600
C	0.60526800	4.99598300	4.30261800	C	-5.38458100	1.89430700	-2.48021800
H	-2.68815200	3.15666000	-0.09957000	H	-6.54601900	0.97246300	-0.91203500
C	-2.70796900	4.65571700	-1.63952600	H	-4.00075500	2.58818000	-3.99395700
H	-1.94944500	6.04622100	0.60297700	C	1.71624900	-4.15045000	2.18653200
H	-3.48297000	5.24453700	0.97751400	H	1.71651000	-5.42228600	0.44129900
H	-0.54942300	1.81397300	3.42390300	H	2.91270200	-4.11854800	0.37711500
H	0.22572100	2.31098500	4.93250600	H	0.20745800	-3.04764400	-2.09719500
H	-1.33640400	3.02234000	4.47986500	C	0.92901400	-5.05563500	-2.18348900
H	1.20665500	5.78506500	3.82193000	C	2.31924500	-2.94517400	-2.16758600
H	-0.34973600	5.44817500	4.61905500	H	0.11883300	-5.56765800	2.40215800
H	1.13444400	4.67830400	5.21565000	C	0.10824600	-4.31141600	4.15040600
H	-2.50930100	3.96274200	-2.47033100	H	-7.57186300	-3.21075300	0.74169700
H	-3.79711900	4.81301400	-1.58695500	H	-6.11815400	2.68295700	-2.66378300
H	-2.23522400	5.62303300	-1.88197900	H	1.92792800	-3.09638700	2.43699200
Cl	0.26739800	0.61668000	-2.49852300	H	2.44964000	-4.76469100	2.73683200
Cl	0.51153300	-0.37966400	2.11490500	H	0.01608700	-5.56055600	-1.82907700
P	-1.64180100	-1.26696400	-0.37321200	H	0.90057900	-5.06215700	-3.28509600
N	-2.80110800	-0.85495600	0.78001000	H	1.79249200	-5.66753500	-1.87512700
N	-2.57192400	-1.20590000	-1.80671800	H	2.34913400	-1.89221600	-1.85935900
O	-1.49227500	-2.89047500	-0.33359200	H	3.22414400	-3.43879700	-1.77831400
C	-4.06976400	-1.52380600	0.73444400	H	2.37540900	-2.96816100	-3.26761300
C	-2.77877500	0.35654400	1.59935700	H	-0.91274600	-4.57967400	4.46854200
C	-3.49516200	-0.13240900	-1.98278000	H	0.81651800	-4.93317300	4.72202500
C	-2.13709300	-1.92941500	-3.00763600	H	0.28105500	-3.25839900	4.43013900
C	-0.53394300	-3.74170500	0.34776300				
C	-5.02234100	-1.14177800	-0.23355800				
C	-4.37782800	-2.49351900	1.69402000				
H	-3.52528400	1.08635100	1.24013700				
H	-1.78809700	0.81546400	1.56543600				
H	-2.99706800	0.10903400	2.64974000				
C	-4.70246900	-0.09713100	-1.23820700				
C	-3.26049300	0.84308600	-2.96521900				
H	-1.93783100	-2.97706600	-2.74666500				
H	-1.23652200	-1.49252200	-3.46685500				
H	-2.95634300	-1.90918800	-3.73998900				



c-TS_Xd-IXc (+22,3 vs. IXa)

Pd	0.13814900	0.16294300	-0.44923200
Cl	0.09405800	1.43313600	1.57135000
Cl	0.13952200	-1.14390100	-2.41068700
P	2.50452000	0.09488600	-0.42136600
N	3.17388000	-0.39539700	1.04214300
N	3.35291100	-0.90735500	-1.51163100
O	3.23865400	1.47621100	-0.88471300
C	4.60105700	-0.50666000	1.14229000
C	2.43848800	-0.88689800	2.20838800
C	3.55858000	-2.28262200	-1.18515000
C	3.51017600	-0.53304100	-2.92219200
C	2.92211800	2.87500600	-0.70711900
C	5.25564200	-1.61720200	0.56981600
C	5.31968900	0.44165400	1.87888200
H	2.73082700	-1.92797900	2.42261400
H	1.36293500	-0.85667600	2.02376400
H	2.64740100	-0.26407500	3.09240300
C	4.49394300	-2.64400500	-0.18293700
C	2.91174500	-3.28643900	-1.92180100
H	3.71086500	0.54227300	-2.99169900
H	2.62135700	-0.76848400	-3.52681700
H	4.37897500	-1.07138900	-3.32900000
C	1.59038200	3.27467300	-1.36007800
C	3.03763500	3.27500700	0.76113600
H	3.73561500	3.37422000	-1.25881200
C	6.64562000	-1.73560400	0.74920300
C	6.69930400	0.30765800	2.04765500
H	4.77898800	1.27818800	2.32442500
C	4.72331400	-4.00937900	0.06393300
C	3.16919500	-4.63485500	-1.67421700
H	2.18158600	-2.99276500	-2.67521500
C	1.36419600	4.78072500	-1.13596900
H	0.79732500	2.75224400	-0.80061300
C	1.47375400	2.81161500	-2.83572800

C	2.76444000	4.76945500	0.98233900	C	-5.54049900	-2.67113600	-3.09105500
H	2.32018700	2.68462000	1.35003600	H	-3.45237600	-2.21930400	-3.41524700
H	4.04929500	3.01713900	1.11131900	C	-5.99314800	2.49990300	2.01258700
C	7.36258500	-0.78441300	1.47761600	H	-3.95109000	3.05316900	1.77055700
H	7.16822300	-2.58131100	0.29616800	C	-6.69710400	0.67525600	0.62413500
H	7.25468300	1.05479900	2.61969700	C	-0.96323600	-2.68091600	3.25787100
C	4.07188800	-5.00059800	-0.67128100	H	-0.50137800	-1.41028100	1.60738400
H	5.42828800	-4.29079500	0.84987000	C	-1.00281500	-3.29700400	0.72657500
H	2.64771200	-5.40063900	-2.25374700	C	-2.51978100	-0.91087000	4.19819400
C	1.41847900	5.14922800	0.35023300	H	-3.84604100	-0.07229400	2.68455600
H	2.12640300	5.36206200	-1.68584300	H	-2.14252200	0.39093600	2.51941200
H	0.38878000	5.07232400	-1.55408100	C	-6.65894900	-2.31111100	-2.33811200
H	1.51743500	1.71079300	-2.81582200	H	-7.48749000	-1.08617700	-0.85812500
C	2.61250800	3.29643900	-3.74197300	H	-5.58103600	-3.48195900	-3.82203300
C	0.11258000	3.18000800	-3.43965600	C	-6.98642600	1.60987300	1.60929400
H	3.55231400	5.34319500	0.45593300	H	-6.17438400	3.24672000	2.78927400
C	2.82462900	5.12384000	2.46940900	H	-7.51713100	0.01370200	0.37058900
H	8.44322500	-0.89420900	1.59739200	C	-1.11862300	-1.53492300	4.26296400
H	4.26694800	-6.05455800	-0.45911700	H	-1.66403000	-3.49283000	3.52183000
H	0.61277500	4.61562400	0.88639300	H	0.04891800	-3.10823900	3.32870300
H	1.23203000	6.22874500	0.48186400	H	-1.22889500	-2.81166500	-0.23628000
H	3.59711600	2.94009800	-3.40247400	C	-1.93213500	-4.51063600	0.85475300
H	2.46763200	2.92560000	-4.76945500	C	0.46472900	-3.73227000	0.65400100
H	2.65160200	4.39727900	-3.79254000	H	-3.24972000	-1.70195500	4.45942600
H	-0.71242500	2.91441100	-2.76207900	C	-2.68613800	0.24284500	5.18915200
H	0.03530600	4.25847400	-3.65278400	H	-7.61207100	-2.82889200	-2.47071000
H	-0.04978600	2.64358800	-4.38786600	H	-7.98356300	1.63303500	2.05462100
H	3.80264000	4.86217000	2.90556800	H	-0.37188200	-0.75050300	4.04221800
H	2.65732500	6.20098900	2.63233800	H	-0.91258200	-1.89427600	5.28561100
H	2.04987200	4.57332200	3.02967800	H	-2.99529600	-4.22405900	0.83218000
P	-2.24974000	0.09164800	-0.47428100	H	-1.76563000	-5.20801400	0.01800400
N	-3.00338700	-0.28013800	-1.93505200	H	-1.75006300	-5.06927000	1.78789100
N	-3.08811900	1.50893100	-0.02562300	H	1.13199000	-2.86948200	0.51277400
O	-2.90969900	-1.10107500	0.40248700	H	0.78592800	-4.26857600	1.56198100
C	-4.27816800	-0.91292500	-1.94371400	H	0.63023500	-4.40447300	-0.20087700
C	-2.72258600	0.64198100	-3.03326300	H	-3.70053300	0.67108200	5.13879000
C	-4.43469600	1.45320700	0.41158200	H	-2.50619600	-0.08814000	6.22495700
C	-2.40214100	2.80113200	-0.07263700	H	-1.97020300	1.05160400	4.96382600
C	-2.61010200	-1.56062600	1.74200200				
C	-5.39260800	-0.53416200	-1.13476700				
C	-4.36487100	-1.96957100	-2.86988700				
H	-2.93387300	0.15259900	-3.99464500				
H	-3.32824500	1.56663100	-2.96716400				
H	-1.65707600	0.90551300	-3.02733500				
C	-4.74547400	2.39698700	1.42002100				
C	-5.45242500	0.54034400	-0.05062400				
H	-3.06692600	3.55127800	-0.52726700				
H	-2.06337100	3.15418300	0.91247300				
H	-1.50688200	2.71336700	-0.69918700				
C	-1.22414700	-2.21635200	1.81458500				
C	-2.81402600	-0.44638900	2.76518200				
H	-3.37932300	-2.33241700	1.90575500				
C	-6.56937000	-1.29023900	-1.39803500				



t-TS_Xd-IXc (+24,3 vs. IXa)

C	-3.71104900	-1.06823000	-3.66831800
C	-3.62130600	-0.85253600	-2.27075200
C	-3.95823300	0.45702900	-1.74456100
C	-4.26490000	1.41947500	-2.74214800
C	-4.24099500	1.21673400	-4.10918700
C	-4.03029300	-0.07581500	-4.58084200
H	-3.47445100	-2.05205000	-4.06129000
H	-4.47503900	2.43801100	-2.44224900
H	-4.44152100	2.04836000	-4.78807500
H	-4.07226600	-0.30922900	-5.64745900
C	-4.14022000	0.94907300	-0.30624500
C	-4.58697500	2.28642700	-0.09771400
C	-3.88031400	0.24362100	0.90120600
C	-4.84705000	2.83692200	1.15300500
H	-4.83728000	2.92213300	-0.93993900
C	-4.06439900	0.82997400	2.16518900
C	-4.54319000	2.12179700	2.31397600
H	-5.24738500	3.85196400	1.21285400
H	-3.79831800	0.22504600	3.03346800
H	-4.67591400	2.56125700	3.30502700
P	-2.22965200	-1.59921200	-0.10209900
C	-4.55774900	-2.06572600	1.17451000
H	-5.00760300	-1.86011200	2.15705400
H	-5.33912900	-1.98143200	0.39888200
H	-4.17519700	-3.09322000	1.17561100
C	-2.99922400	-3.25400900	-2.17795000
H	-3.94827700	-3.53509300	-2.65765800
H	-2.19575800	-3.25000300	-2.93388800
H	-2.76278300	-4.01079700	-1.42655500
N	-3.45716900	-1.11657500	0.93804600
N	-3.15225200	-1.95471600	-1.51664500

Pd	-0.31544700	-0.21382600	-0.22129600	C	1.24590700	3.23694100	2.01822300
O	-1.91645400	-3.12627300	0.34508100	H	1.54811100	4.44885100	0.27222000
C	-1.09152500	-3.64953900	1.42139700	C	6.49954300	0.87177500	-0.34747900
C	0.39934300	-3.41102200	1.15833200	C	6.08254000	2.17438100	1.64708600
C	-1.55819800	-3.13689500	2.78209300	H	4.07707800	2.03512400	2.44420400
H	-1.29441100	-4.73109500	1.36523700	C	5.52419900	-1.63360800	-1.76703600
C	1.21423800	-3.99901300	2.32407700	C	3.99898700	-2.23240700	-3.53705200
H	0.53686700	-2.31805400	1.18950600	H	2.23063900	-1.00311700	-3.69814700
C	0.85791400	-3.86537400	-0.24938500	C	-1.21280100	4.46389500	0.94851000
C	-0.72668200	-3.71875400	3.93429400	H	-0.79518100	2.51951500	0.17353900
H	-2.62172300	-3.38847200	2.91821900	C	-0.47048800	3.88226300	-1.46797900
H	-1.47713200	-2.04005400	2.79957600	C	0.37493100	4.15273300	2.89155000
C	0.76225100	-3.44979700	3.68025200	H	0.97611300	2.19413500	2.23611500
H	1.11861000	-5.09956100	2.32763400	H	2.30978000	3.36647200	2.27319900
H	2.28146900	-3.78060900	2.17049800	C	6.95316400	1.74966500	0.63754000
H	0.23887100	-3.30501400	-0.96799000	H	7.17557200	0.55357100	-1.14441700
C	0.64472800	-5.35859400	-0.52760800	H	6.42656100	2.86574700	2.42015900
C	2.30939300	-3.45731100	-0.52137000	C	5.17667700	-2.47527300	-2.82364500
H	-0.87082300	-4.81696800	3.94429800	H	6.44691000	-1.81403500	-1.21032100
C	-1.19197800	-3.15942800	5.28014700	H	3.71216100	-2.88224900	-4.36763800
H	0.93279700	-2.35835800	3.71137700	C	-1.08706200	4.08522900	2.42563000
H	1.36923100	-3.88914200	4.48996100	H	-0.87747900	5.50810900	0.82048200
H	-0.41312700	-5.65279500	-0.43943900	H	-2.26823700	4.42949100	0.63481900
H	0.96643900	-5.60412500	-1.55252600	H	0.33105600	3.31145800	-1.95637200
H	1.23076100	-5.99162800	0.15938500	C	-0.23149000	5.36378900	-1.78809600
H	2.46936100	-2.38680200	-0.32456200	C	-1.78185100	3.38936000	-2.07428600
H	3.02297200	-4.02770600	0.09523600	H	0.72129400	5.19558400	2.75020300
H	2.57263800	-3.63136400	-1.57416500	C	0.52586000	3.79194200	4.37096700
H	-2.25724600	-3.37799500	5.46022900	H	7.98515400	2.10815600	0.61338600
H	-0.61162600	-3.58726300	6.11367900	H	5.82270600	-3.31570300	-3.08856400
H	-1.06545200	-2.06375800	5.30769400	H	-1.46922400	3.06136500	2.57796700
Cl	-0.19876400	-0.81127100	-2.49966200	H	-1.70766500	4.75702700	3.04340900
Cl	-0.62441600	0.30992700	2.07259800	H	0.69013400	5.75071200	-1.32385200
P	1.81591500	0.90554300	-0.34069100	H	-0.13701700	5.50834700	-2.87650500
N	2.97057100	0.31514300	0.74107600	H	-1.06878200	5.99368200	-1.44585900
N	2.69396600	0.80948000	-1.80613000	H	-1.89681600	2.30777100	-1.92007800
O	1.84805200	2.54036500	-0.25290900	H	-2.65159300	3.88899800	-1.61867300
C	4.30658200	0.83375600	0.67192100	H	-1.82088000	3.57692200	-3.15941900
C	2.68785000	-0.52156900	1.90656900	H	1.57682700	3.85950900	4.69750500
C	3.50492800	-0.32526800	-2.10396100	H	-0.07197500	4.46205500	5.01005900
C	2.27776700	1.65633600	-2.93331100	H	0.18385500	2.75880500	4.55126500
C	1.07104700	3.48613700	0.52176300				
C	5.17473500	0.39646100	-0.34921900				
C	4.76468800	1.71607800	1.65962200				
H	3.39422400	-1.36605000	1.93276200				
H	1.67067900	-0.91274000	1.85322300				
H	2.77239400	0.04547200	2.84801600				
C	4.71563100	-0.54247500	-1.40056400				
C	3.16852800	-1.17365200	-3.17158800				
H	2.33237700	2.71324000	-2.64097400				
H	1.25891300	1.42542600	-3.28330400				
H	2.97679200	1.49419900	-3.76417800				
C	-0.38677900	3.53581800	0.04175100				