Supporting Information for

$Tp'PtH_3$: A Stable Platinum(IV) Trihydride

Stefan Reinartz, Peter S. White, Maurice Brookhart* and Joseph L. Templeton*

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Chapel Hill, NC 27599-3290

Contents:

DISANG -- The NRCVAX Distance and Angle Program

The Space Group is P 1 NonCentrosymmetric
The Equivalent Positions are:
1) x y z

The Lattice is Primitive. There are no Centering Vectors

Pt(1)-Si(1)	2.325(3)	N(21)-N(22)	1.434(8)
Pt(1)-N(11)	2.169(3)	N(21)-C(25)	1.243(10)
Pt(1)-N(21)	2.299(10)	N(22)-C(23)	1.353(5)
Pt(1)-N(31)	2.161(3)	C(23)-C(24)	1.375(7)
Si(1)-C(41)	1.911(6)	C(23)-C(26)	1.496(7)
Si(1)-C(43)	1.828(14)	C(24)-C(25)	1.383(7)
Si(1)-C(45)	1.844(11)	C(25)-C(27)	1.507(7)
B(10)-N(12)	1.542(5)	N(31)-N(32)	1.373(4)
B(10)-N(22)	1.544(5)	N(31)-C(35)	1.346(4)
B(10)-N(32)	1.547(5)	N(32)-C(33)	1.360(4)
N(11)-N(12)	1.368(5)	C(33)-C(34)	1.373(5)
N(11)-C(15)	1.345(4)	C(33)-C(36)	1.491(6)
N(12)-C(13)	1.360(5)	C(34)-C(35)	1.397(6)
C(13)-C(14)	1.373(6)	C(35)-C(37)	1.486(6)
C(13)-C(16)	1.487(7)	C(41)-C(42)	1.499(8)
C(14)-C(15)	1.383(6)	C(43)-C(44)	1.060(17)
C(15)-C(17)	1.476(7)	C(45)-C(46)	1.238(24)

Si(1)-Pt(1)-N(11)	100.54(11)	Pt(1)-N(21)-C(25)	138.7(6)
Si(1)-Pt(1)-N(21)	171.15(18)	N(22)-N(21)-C(25)	107.2(7)
Si(1)-Pt(1)-N(31)	103.16(11)	B(10)-N(22)-N(21)	122.3(5)
N(11)-Pt(1)-N(21)	81.82(25)	B(10)-N(22)-C(23)	130.5(4)
N(11)-Pt(1)-N(31)	89.77(11)	N(21)-N(22)-C(23)	106.9(5)
N(21)-Pt(1)-N(31)	85.32(18)	N(22)-C(23)-C(24)	107.1(4)
Pt(1)-Si(1)-C(41)	118.34(20)	N(22)-C(23)-C(26)	122.5(4)
Pt(1)-Si(1)-C(43)	114.0(6)	C(24)-C(23)-C(26)	130.4(4)
Pt(1)-Si(1)-C(45)	109.0(4)	C(23)-C(24)-C(25)	106.2(4)
C(41)-Si(1)-C(43)	100.8(4)	N(21)-C(25)-C(24)	111.8(6)
C(41)-Si(1)-C(45)	106.2(5)	N(21)-C(25)-C(27)	118.5(6)
C(43)-Si(1)-C(45)	107.7(11)	C(24)-C(25)-C(27)	129.1(4)
N(12)-B(10)-N(22)	108.7(3)	Pt(1)-N(31)-N(32)	118.43(20)
N(12)-B(10)-N(32)	111.0(3)	Pt(1)-N(31)-C(35)	134.5(3)
N(22)-B(10)-N(32)	108.1(3)	N(32)-N(31)-C(35)	106.9(3)
Pt(1)-N(11)-N(12)	118.26(20)	B(10)-N(32)-N(31)	120.2(3)
Pt(1)-N(11)-C(15)	134.2(3)	B(10)-N(32)-C(33)	129.0(3)
N(12)-N(11)-C(15)	107.1(3)	N(31)-N(32)-C(33)	109.3(3)
B(10)-N(12)-N(11)	120.8(3)	N(32)-C(33)-C(34)	108.1(3)
B(10)-N(12)-C(13)	128.8(4)	N(32)-C(33)-C(36)	124.2(3)
N(11)-N(12)-C(13)	109.3(3)	C(34)-C(33)-C(36)	127.7(3)
N(12)-C(13)-C(14)	107.5(4)	C(33)-C(34)-C(35)	106.1(3)

N(12)-C(13)-C(16)	124.3(4)	N(31)-C(35)-C(34)	109.5(3)
C(14)-C(13)-C(16)	128.3(4)	N(31)-C(35)-C(37)	123.2(3)
C(13)-C(14)-C(15)	106.8(3)	C(34)-C(35)-C(37)	127.2(3)
N(11)-C(15)-C(14)	109.3(4)	Si(1)-C(41)-C(42)	117.0(4)
N(11)-C(15)-C(17)	123.5(4)	Si(1)-C(43)-C(44)	149.6(21)
C(14)-C(15)-C(17)	127.1(3)	Si(1)-C(45)-C(46)	130.5(13)
Pt(1)-N(21)-N(22)	112.0(5)		

20-Dec-1999

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
Pt1	0.60202	0.56486	0.10964	2.034(4)
Si1	0.4554 (4)	0.5695 (4)	0.3043 (3)	3.81 (12)
B10	0.5062 (6)	0.8534 (6)	-0.1616 (4)	2.52 (17)
N11	0.3623 (4)	0.6555 (4)	0.0092 (3)	2.50 (14)
N12	0.3485 (4)	0.7848 (4)	-0.1036 (3)	2.59 (14)
C13	0.2015 (5)	0.8072 (6)	-0.1568 (4)	3.17 (19)
C14	0.1197 (5)	0.6923 (6)	-0.0756 (5)	3.47 (21)
C15	0.2239 (5)	0.5976 (6)	0.0256 (4)	3.01 (18)
C16	0.1465 (8)	0.9345 (8)	-0.2809 (6)	4.8 (3)
C17	0.2001 (7)	0.4470 (8)	0.1333 (5)	4.2 (3)
N21	0.7641 (13)	0.5092 (10)	-0.0717 (9)	2.94 (21)
N22	0.6922 (4)	0.6753 (5)	-0.1733 (3)	2.69 (15)
C23	0.8067 (6)	0.6321 (7)	-0.2729 (4)	3.31 (20)
C24	0.9508 (6)	0.4527 (7)	-0.2334 (4)	3.67 (22)
C25	0.9183 (7)	0.3950 (6)	-0.1081 (5)	3.02 (21)
C26	0.7712 (8)	0.7677 (9)	-0.3981 (5)	4.8 (3)
C27	1.0281 (6)	0.2081 (7)	-0.0183 (5)	3.68 (23)
N31	0.5956 (4)	0.8509 (4)	0.0341 (3)	2.35 (13)
N32	0.5359 (4)	0.9534 (4)	-0.0808 (3)	2.31 (13)
C33	0.5510 (5)	1.1244 (5)	-0.1136 (4)	2.56 (16)
C34	0.6201 (5)	1.1327 (5)	-0.0189 (4)	2.84 (17)
C35	0.6486 (5)	0.9590 (5)	0.0715 (4)	2.69 (16)
C36	0.5018 (7)	1.2716 (6)	-0.2337 (4)	3.73 (21)
C37	0.7315 (8)	0.8926 (7)	0.1897 (4)	4.1 (3)
C41	0.5889 (8)	0.5649 (8)	0.4233 (4)	4.1 (3)
C42	0.7824 (9)	0.4047 (10)	0.4445 (5)	5.5 (3)
C43	0.401 (3)	0.361 (4)	0.3837 (8)	23.5 (25)
C44	0.3392 (24)	0.2877 (16)	0.4608 (14)	14.7 (12)
C45	0.2322 (16)	0.789 (3)	0.2935 (10)	14.7 (10)
C46	0.1906 (25)	0.9412 (15)	0.3189 (22)	17.1 (15)
H1a	0.768	0.502	0.179	3.0
H1b	0.606	0.366	0.162	3.0
H10	0.474	0.942	-0.241	3.5
H14	0.011	0.680	-0.086	4.7
H16a	0.132	1.062	-0.287	5.9
H16b	0.029	0.942	-0.295	5.9
H16c	0.243	0.883	-0.341	5.9
H17a	0.303	0.324	0.132	5.6
H17b	0.083	0.442	0.132	5.6
H17c	0.199	0.478	0.206	5.6
H24	1.054	0.382	-0.283	4.8
H26a	0.653	0.791	-0.421	5.8
H26b	0.871	0.710	-0.454	5.8
H26c	0.769	0.888	-0.400	5.8
H27a	1.010	0.104	-0.028	4.4
H27b	0.985	0.220	0.063	4.4
H27c	1.160	0.181	-0.033	4.4
H34	0.645	1.237	-0.016	4.0
H36a	0.582	1.217	-0.298	4.7
H36b	0.519	1.382	-0.235	4.7
H36c	0.373	1.310	-0.245	4.7

H37a	0.638	0.955	0.247	5.5
H37b	0.836	0.925	0.178	5.5
H37c	0.774	0.755	0.221	5.5
H41a	0.601	0.684	0.404	5.1
H41b	0.514	0.555	0.499	5.1
H42a	0.775	0.283	0.468	6.2
H42b	0.833	0.413	0.508	6.2
H42c	0.863	0.415	0.371	6.2
H43a	0.387	0.321	0.315	32.0
H43b	0.535	0.265	0.404	32.2
H44a	0.354	0.331	0.530	25.6
H44b	0.327	0.168	0.484	16.6
H44c	0.189	0.438	0.436	32.2
H45a	0.146	0.738	0.341	12.5
H45b	0.204	0.832	0.210	12.0
H46a	0.222	0.917	0.399	17.8
H46b	0.059	1.026	0.311	17.8
H46c	0.263	0.991	0.262	17.5

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

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N(11)-Pt(1)-N(21)	81.82(25)	B(10)-N(22)-C(23)	130.5(4)
N(11)-Pt(1)-N(31)	89.77(11)	N(21)-N(22)-C(23)	106.9(5)
N(21)-Pt(1)-N(31)	85.32(18)	N(22)-C(23)-C(24)	107.1(4)
Pt(1)-Si(1)-C(41)	118.34(20)	N(22)-C(23)-C(26)	122.5(4)
Pt(1)-Si(1)-C(43)	114.0(6)	C(24)-C(23)-C(26)	130.4(4)
Pt(1)-Si(1)-C(45)	109.0(4)	C(23)-C(24)-C(25)	106.2(4)
C(41)-Si(1)-C(43)	100.8(4)	N(21)-C(25)-C(24)	111.8(6)
C(41)-Si(1)-C(45)	106.2(5)	N(21)-C(25)-C(27)	118.5(6)
C(43)-Si(1)-C(45)	107.7(11)	C(24)-C(25)-C(27)	129.1(4)
N(12)-B(10)-N(22)	108.7(3)	Pt(1)-N(31)-N(32)	118.43(20)
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B(10)-N(12)-N(11)	120.8(3)	N(32)-C(33)-C(34)	108.1(3)
B(10)-N(12)-C(13)	128.8(4)	N(32)-C(33)-C(36)	124.2(3)
N(11)-N(12)-C(13)	109.3(3)	C(34)-C(33)-C(36)	127.7(3)
N(12)-C(13)-C(14)	107.5(4)	C(33)-C(34)-C(35)	106.1(3)

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N(12)-C(13)-C(16)	124.3(4)	N(31)-C(35)-C(34)	109.5(3)
C(14)-C(13)-C(16)	128.3(4)	N(31)-C(35)-C(37)	123.2(3)
C(13)-C(14)-C(15)	106.8(3)	C(34)-C(35)-C(37)	127.2(3)
N(11)-C(15)-C(14)	109.3(4)	Si(1)-C(41)-C(42)	117.0(4)
N(11)-C(15)-C(17)	123.5(4)	Si(1)-C(43)-C(44)	149.6(21)
C(14)-C(15)-C(17)	127.1(3)	Si(1)-C(45)-C(46)	130.5(13)
Pt(1)-N(21)-N(22)	112.0(5)		

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N11	0.3623 (4)	0.6555 (4)	0.0092 (3)	2.50 (14)
N12	0.3485 (4)	0.7848 (4)	-0.1036 (3)	2.59 (14)
C13	0.2015 (5)	0.8072 (6)	-0.1568 (4)	3.17 (19)
C14	0.1197 (5)	0.6923 (6)	-0.0756 (5)	3.47 (21)
C15	0.2239 (5)	0.5976 (6)	0.0256 (4)	3.01 (18)
C16	0.1465 (8)	0.9345 (8)	-0.2809 (6)	4.8 (3)
C17	0.2001 (7)	0.4470 (8)	0.1333 (5)	4.2 (3)
N21	0.7641 (13)	0.5092 (10)	-0.0717 (9)	2.94 (21)
N22	0.6922 (4)	0.6753 (5)	-0.1733 (3)	2.69 (15)
C23	0.8067 (6)	0.6321 (7)	-0.2729 (4)	3.31 (20)
C24	0.9508 (6)	0.4527 (7)	-0.2334 (4)	3.67 (22)
C25	0.9183 (7)	0.3950 (6)	-0.1081 (5)	3.02 (21)
C26	0.7712 (8)	0.7677 (9)	-0.3981 (5)	4.8 (3)
C27	1.0281 (6)	0.2081 (7)	-0.0183 (5)	3.68 (23)
N31	0.5956 (4)	0.8509 (4)	0.0341 (3)	2.35 (13)
N32	0.5359 (4)	0.9534 (4)	-0.0808 (3)	2.31 (13)
C33	0.5510 (5)	1.1244 (5)	-0.1136 (4)	2.56 (16)
C34	0.6201 (5)	1.1327 (5)	-0.0189 (4)	2.84 (17)
C35	0.6486 (5)	0.9590 (5)	0.0715 (4)	2.69 (16)
C36	0.5018 (7)	1.2716 (6)	-0.2337 (4)	3.73 (21)
C37	0.7315 (8)	0.8926 (7)	0.1897 (4)	4.1 (3)
C41	0.5889 (8)	0.5649 (8)	0.4233 (4)	4.1 (3)
C42	0.7824 (9)	0.4047 (10)	0.4445 (5)	5.5 (3)
C43	0.401 (3)	0.361 (4)	0.3837 (8)	23.5 (25)
C44	0.3392 (24)	0.2877 (16)	0.4608 (14)	14.7 (12)
C45	0.2322 (16)	0.789 (3)	0.2935 (10)	14.7 (10)
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H1a	0.768	0.502	0.179	3.0
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H17c	0.199	0.478	0.206	5.6
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H26a	0.653	0.791	-0.421	5.8
H26b	0.871	0.710	-0.454	5.8
H26c	0.769	0.888	-0.400	5.8
H27a	1.010	0.104	-0.028	4.4
H27b	0.985	0.220	0.063	4.4
H27c	1.160	0.181	-0.033	4.4
H34	0.645	1.237	-0.016	4.0
H36a	0.582	1.217	-0.298	4.7
H36b	0.519	1.382	-0.235	4.7
H36c	0.373	1.310	-0.245	4.7

H37a	0.638	0.955	0.247	5.5
H37b	0.836	0.925	0.178	5.5
H37c	0.774	0.755	0.221	5.5
H41a	0.601	0.684	0.404	5.1
H41b	0.514	0.555	0.499	5.1
H42a	0.775	0.283	0.468	6.2
H42b	0.833	0.413	0.508	6.2
H42c	0.863	0.415	0.371	6.2
H43a	0.387	0.321	0.315	32.0
H43b	0.535	0.265	0.404	32.2
H44a	0.354	0.331	0.530	25.6
H44b	0.327	0.168	0.484	16.6
H44c	0.189	0.438	0.436	32.2
H45a	0.146	0.738	0.341	12.5
H45b	0.204	0.832	0.210	12.0
H46a	0.222	0.917	0.399	17.8
H46b	0.059	1.026	0.311	17.8
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