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Supporting Information

for

Thermodynamic Control of Oxidative Addition and Reductive Elimination Processes in *cis*-Bis(dimethoxyboryl)-bis(tricyclohexylphosphine)platinum(II)

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Supporting materials for *cis*-bis(boryl) platinum complexes

Table 1 Comparison of bond lengths [Å] and angles [°] in *cis*-bis(boryl) platinum(II) complexes. (2: *cis*-[$(Ph_3P)_2Pt(BCat')_2$]; **3**: *cis*-[$(Ph_3P)_2Pt(BCat)_2$]; **4**: *cis*-[$(Cy_3P)_2Pt(BCat)_2$]; **5**: *cis*-[$(Cy_3P)_2Pt(BCat')_2$], BCat' = Cat-**4**-*t*Bu; **6**: *cis*-[$\{(CyCH_2)_3P\}_2Pt(BCat)_2$]).[4c,d,8]

Complex	Pt1−B1[a]	Pt1−B2[a]	Pt1−P1[a]	Pt1−P2[a]	P1−Pt1−P2[b]	B1−Pt−B2[b]
1	2.093(5)	2.108(5)	2.372(1)	2.372(1)	109.58(4)	71.3(2)
2	2.04(1)	2.04(1)	2.344(3)	2.353(3)	104.3(1)	77.2(4)
3	2.040(6)	2.058(6)	2.354(2)	2.346(2)	107.14(4)	77.1(2)
4	2.039(5)	2.060(5)	2.384(1)	2.390(1)	109.11(4)	70.1(2)
5	2.044(3)	2.047(3)	2.397(1)	2.388(1)	110.29(4)	72.1(1)
6	2.045(4)	2.049(4)	2.3473(8)	2.3408(8)	102.56(3)	76.0(1)

[a] distances given in Å. [b] angles given in degrees [°].

Table 2 Comparison of $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ NMR signals of *cis*-bis(boryl) platinum(II) complexes at room temperature.

Complex	$^{31}P\{^1H\}$[a]	$^1J_{P-Pt}$[b]	$^{11}B\{^1H\}$[a]
1	33.7	1442	45.8
2	29.0	1621	50.1
3	28.7	1639	47.0
4	35.4	1675	49.7
5	35.6	1683	49.9
6	9.8	1567	49.4

[a] NMR shifts given in [ppm]. [b] $^1J_{P-Pt}$ coupling constants given in [Hz].

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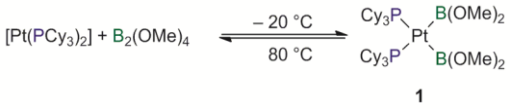
Experimental Section

General considerations

All syntheses were carried out under an argon atmosphere with standard Schlenk and glovebox techniques. $[Pt(PCy_3)_2]$[1] and $B_2(OMe)_4$ were prepared according to published procedures.[2] Pentane was dried by distillation over sodium under argon and stored over molecular sieves. C_6D_6 was degassed by three freeze-pump-thaw cycles and stored over molecular sieves. NMR spectra were recorded on a Bruker Avance 500 NMR spectrometer (500.1 MHz for ^1H, 160.4 MHz for ^{11}B, 126 MHz for $^{13}C\{^1H\}$, 202.3 MHz for $^{31}P\{^1H\}$) at 233 K, 298 K, and 353 K. Chemical shifts (δ) are given in ppm and are referenced against external Me_4Si (^1H, ^{13}C; *TMS*), $[BF_3{\cdot}Et_2O]$ (^{11}B) and 85% H_3PO_4 (^{31}P). Elemental analyses were acquired on an Elementar Vario MICRO cube instrument.

Synthesis of *cis*-$[(Cy_3P)_2Pt\{B(OMe)_2\}_2]$ (1)



1

Fig. 1 Synthesis of the *cis*-bis(boryl) platinum complex *cis*-$[(Cy_3P)_2Pt\{B(OMe)_2\}_2]$ (**1**).

To a solution of $[Pt(PCy_3)_2]$ (50.6 mg, 66.9 µmol) in pentane (1 mL) an excess of $B_2(OMe)_4$ (20.0 mg, 137 µmol, 2 eq.) was added at RT. The mixture was stored overnight at –25 °C resulting in formation of colourless single crystals of **1**, also suitable for X-ray diffraction. The solvent was removed, the crystals were washed with pentane (3 × 1 mL) and all volatiles were removed under vacuum, yielding 99.4% (60.0 mg, 66.5 µmol) of analytically pure **1**.

NMR at room temperature, 25 °C:

^1H NMR (500.1 MHz, C_7D_8, 298 K, TMS): δ = 3.92 (s, 12H; OC*H*$_3$), 2.42–1.14 (m; C*H* & CH_2; *Cy of* $[Pt(PCy_3)_2]$ *and* **1**); **$^{11}B\{^1H\}$ NMR** (160.4 MHz, C_7D_8, 298 K, $BF_3{\cdot}OEt_2$): δ = 45.8 ppm (br s, Pt*B*); **$^{13}C\{^1H\}$ NMR** (125.7 MHz, C_7D_8, 298 K, TMS): δ = 51.7 ppm (br s, 4C; O*C*H$_3$); **$^{31}P\{^1H\}$ NMR** (202.3 MHz, C_6D_8, 298 K, 85% H_3PO_4): δ = 62.14 (s, $^1J_{P\text{-}Pt}$ = 4180 Hz; $[Pt(PCy_3)_2]$), 33.7 ppm (s, $^1J_{P\text{-}Pt}$ = 1442 Hz).

NMR at 80 °C:

^1H NMR (500.1 MHz, C_7D_8, 353 K, TMS): δ = 3.87 (s, 6H; OC*H*$_3$), 3.44 (s, 6H; OC*H*$_3$); 2.29–2.15 (m, C*H*, *Cy of* $[Pt(PCy_3)_2]$ *and* **1**), 1.99–1.53 (m, CH_2, *Cy of* $[Pt(PCy_3)_2]$ *and* **1**), 1.41–1.10 ppm (m, CH_2, *Cy of* $[Pt(PCy_3)_2]$ *and* **1**).

NMR at low temperature, –40 °C:

^1H NMR (500.1 MHz, C_7D_8, 233 K, TMS): δ = 4.26 (s, 6H; OC*H*$_3$), 3.76 (s, 6H; OC*H*$_3$), 3.22–2.07 (m, 6H; C*H*, *Cy*), 2.01–1.03 ppm (m, 60H; C*H*$_2$, *Cy*); **$^{13}C\{^1H\}$ NMR** (125.7 MHz, C_7D_8, 233 K, TMS): δ = 53.6 (br s, 2C; O*C*H$_3$), 50.0 (br s, 2C; O*C*H$_3$), 39.2–37.5 (m, 6C; *C*H, *Cy*), 33.0–25.3 ppm (br m, 30C, *C*H$_2$, *Cy*); **$^{31}P\{^1H\}$ NMR** (202.3 MHz, C_6D_8, 298 K, 85% H_3PO_4): δ = 32.8 ppm (s, $^1J_{P\text{-}Pt}$ = 1460 Hz).

Free diborane(4), $B_2(OMe)_4$, at room temperature, 25 °C:

^1H NMR (500.1 MHz, C_7D_8, 298 K, TMS): δ = 3.54 ppm (s, 12H; OC*H*$_3$); **$^{11}B\{^1H\}$ NMR** (160.4 MHz, C_7D_8, 298 K, $F_3B{\cdot}OEt_2$): δ = 30.0 ppm (s, *B*OMe); **$^{13}C\{^1H\}$ NMR** (125.7 MHz, C_7D_8, 298 K, TMS): δ = 51.6 ppm (s, 4C; O*C*H$_3$).

Elemental analysis for calcd (%) for $C_{40}H_{78}B_2O_4P_2Pt$ (901.70 g·mol^{-1}): C 53.28, H 8.72; found: C53.30, H 8.76.

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Crystal structure determination

The crystal data of **1** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the ShelX software package (G. Sheldrick, *Acta Cryst*., **2008**, *A64*, 112–122) and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions.[3]

The displacement parameters of atoms C172 > C177, and C76 > C81 of the cyclohexyl groups were constrained to the same value.

The distances between C101 > C105, C111 > C115, and C121 > C125 of the three pentane solvent molecules were restrained during refinement to the same value with SADI restraint.

The Uii displacement parameters of all three pentane carbon atoms and of the cyclohexyl carbon atoms C76, and C172 > C176 were restrained with ISOR keyword to approximate isotropic behavior.

Crystal data for **1**: $C_{95}H_{192}B_4O_8P_4Pt_2$, M_r = 2019.79, colourless block, 0.11×0.24×0.32 mm^3, monoclinic space group $P2_1/n$, a = 11.8325(2) Å, b = 41.1461(9) Å, c = 21.8039(5) Å, β = 90.0190(10)°, V = 10615.5(4) Å^3, Z = 4, ρ_{calcd} = 1.264 g·cm^{-3}, μ = 2.741 mm^{-1}, F(000) = 4248, T = 100(2) K, R_1 = 0.0742, wR^2 = 0.1231, 20928 independent reflections [2θ≤52.04°] and 1064 parameters.

The unit cell contains 12 pentane molecules (3 per asymmetric unit) which have been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON.[4]

Crystal data for **1** (Squeezed): $C_{40}H_{78}B_2O_4P_2Pt$, M_r = 901.67, colourless block, 0.11×0.24×32 mm^3, monoclinic space group $P2_1/n$, a = 11.8325(2) Å, b = 41.1461(9) Å, c = 21.8039(5) Å, β = 90.0190(10)°, V = 10615.5(4) Å^3, Z = 4, ρ_{calcd} = 1.128 g·cm^{-3}, μ = 2.734 mm^{-1}, F(000) = 3744, T = 100(2) K, R_1 = 0.0664, wR^2 = 0.0779, 21788 independent reflections [2θ≤5288°] and 880 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-913240 (**1**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

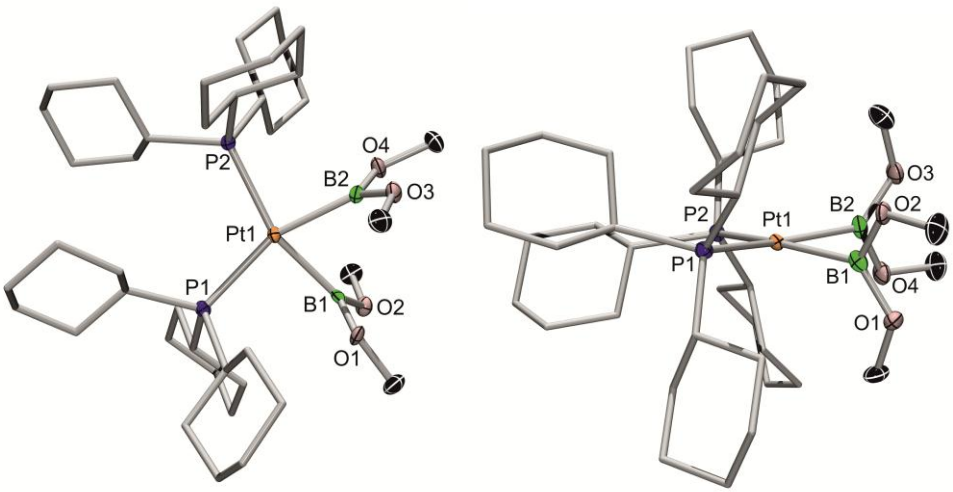

Fig. 2 Molecular structure of **1** in the crystal. Thermal ellipsoids are displayed at the 50% probability level. For clarity, the three solvent molecules pentane and the second molecule of **1** in the asymmetric unit have been omitted. Hydrogen atoms and thermal ellipsoids of the carbon atoms have been omitted. Selected bond lengths [Å] and bond angles [°]: Pt1–B1 2.093(5), Pt1–B2 2.108(5), Pt1–P1 2.3723(10), Pt1–P2 2.3724(10), B1···B2 2.451, B1–O1 1.384(5), B1–O2 1.383(5), B2–O3 1.369(5), B2–O4 1.36(6), B1–Pt1–B2 71.39(18), B1–Pt1–P1 89.76(12), P1–Pt1–P2 109.58(4), P2–Pt1–B1 159.52(12), P1–Pt1–B2 159.08(13), P2–Pt1–B2 90.35(13), O1–B1–O2 113.0(4), O3–B2–O4 113.9(4).

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Computational Results

Wiberg bond indices

Table 3 Calculated *Wiberg bond indices* (*WBIs*) for the free diboranes $B_2(OMe)_4$ and B_2Cat_2 and the diborane parts of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$.

WBIs[a]	B1–B2	B1–O1	B1–O2	B2–O3	B2–O4
$B_2(OMe)_4$[b]	0.9288	0.9565	0.9565	0.9565	0.9665
$[B_2(OMe)_4]^{\ddagger}$[c]	0.9690	0.9282	0.9498	0.9289	0.9479
$B_2(Cat)_2$[b]	0.9869	0.9260	0.9261	0.9260	0.9269
$[B_2(Cat)_2]^{\ddagger}$[c]	0.9704	0.9006	0.9012	0.8985	0.9016

[a] *WBI = Wiberg Bond Index*; [b] free optimized diboranes(4) at the ground state; [c] Single-Point calculations at the diborane part of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$ without geometry optimization.

Calculated B1−B2 bond distances

Table 4 Calculated B1−B2 bond distances for the free diboranes $B_2(OMe)_4$ and B_2Cat_2 and the diborane parts of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$.

	d (B1–B2)[a]
$B_2(OMe)_4$[b]	1.72751
$[B_2(OMe)_4]^{\ddagger}$[c]	1.73936
$B_2(Cat)_2$[b]	1.68422
$[B_2(Cat)_2]^{\ddagger}$[c]	1.89945

[a] [Å]; [b] free optimized diboranes(4) in the ground state; [c] Single-Point calculations at the diborane part of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$ without geometry optimization.

Natural Charges

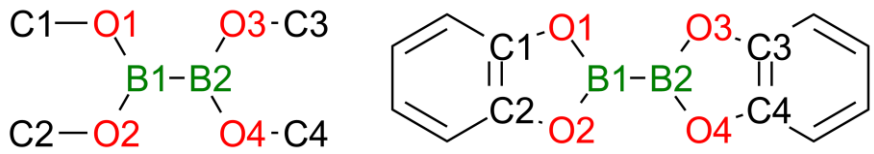


Fig. 3 Labeling of the calculated diboranes of Table 5.

Table 5 Calculated *Natural Charges* (*NC*) for the free diboranes $B_2(OMe)_4$ and B_2Cat_2 and the diborane parts of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$.

NC[a]	B1	B2	O1	C1	O2	C2	O3	C3	O4	C4
$B_2(OMe)_4$[b]	0.79517	0.79513	−0.68824	−0.35758	−0.68819	−0.35764	−0.68819	−0.35763	−0.68823	−0.35759
$[B_2(OMe)_4]^{\ddagger}$[c]	0.77704	0.77679	−0.69538	−0.35949	−0.69722	−0.35139	−0.69844	−0.35263	−0.69614	−0.35810
$B_2(Cat)_2$[b]	0.75740	0.75740	−0.61250	0.25143	−0.61249	0.25146	−0.61249	0.25145	−0.61250	0.25143
$[B_2(Cat)_2]^{\ddagger}$[c]	0.78414	0.78378	−0.62944	0.25706	−0.63020	0.25930	−0.63094	0.25939	−0.62891	0.25746

[a] *Natural Charges*; [b] free optimized diboranes(4) at the ground state; [c] Single-Point calculations at the diborane part of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$ without geometry optimization.

Calculated energy for the HOMO−LUMO-Gaps

Table 6 Calculated energy for the HOMO−LUMO gaps of the free diboranes $B_2(OMe)_4$ and B_2Cat_2 and the diborane parts of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$.

	E (HOMO)[a]	*E* (LUMO)[a]	*ΔE* (HOMO−LUMO)[a]	*ΔE* (HOMO−LUMO)[b]
$B_2(OMe)_4$[c]	−0.21528	−0.02081	0.19447	5.29
$[B_2(OMe)_4]^{\ddagger}$[d]	−0.21431	−0.03538	0.17893	4.86
$B_2(Cat)_2$[c]	−0.20237	−0.07377	0.12860	3.49
$[B_2(Cat)_2]^{\ddagger}$[d]	−0.20153	−0.06842	0.13311	3.62

[a] Energy in *atomic units* [a.u.]; [b] Energy in *eV*; [c] free optimized diboranes(4) at the ground state; [d] Single-point calculations at the diborane part of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$ without geometry optimization.

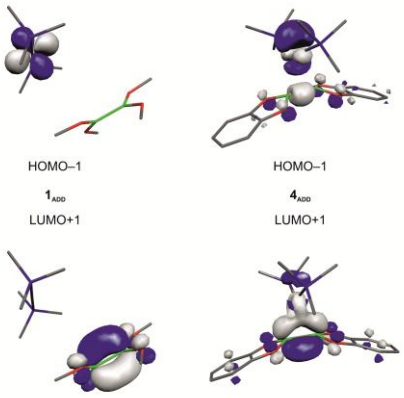
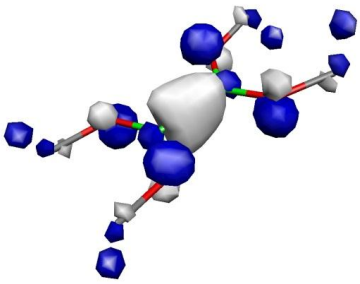
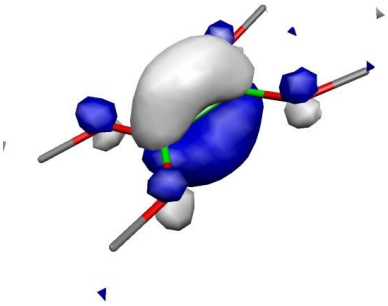
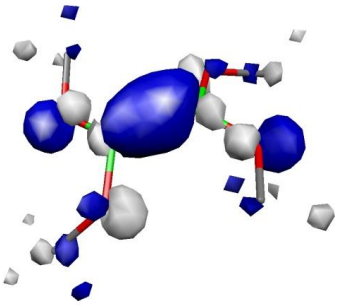
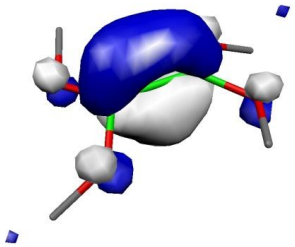
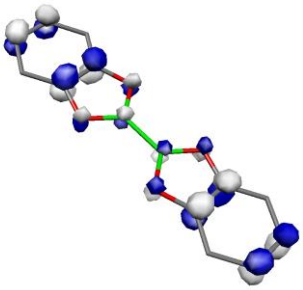
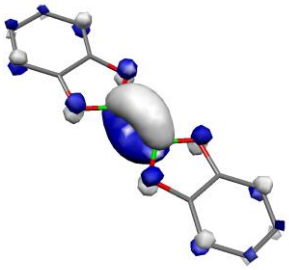
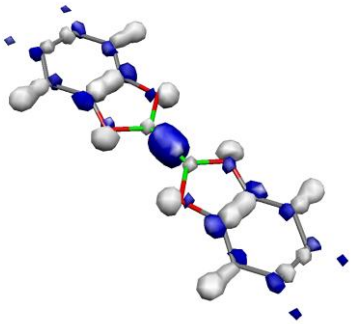


Fig. 4 Bonding interaction in $\mathbf{1'}_{ADD}$ and $\mathbf{4'}_{ADD}$.

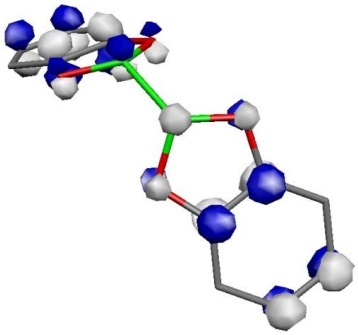
Bonding interaction in HOMO and LUMO orbitals

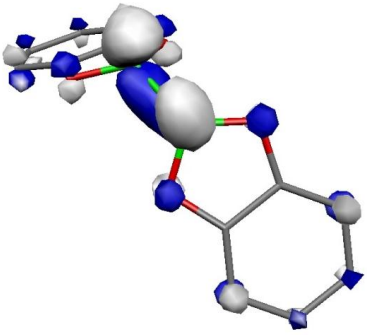
Table 6 Rendered HOMO−1, HOMO−5 (selected) and LUMO+1 orbitals of the free diboranes $B_2(OMe)_4$ and B_2Cat_2 and the diborane parts of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$.

	HOMO	LUMO	HOMO −1
$B_2(OMe)_4$[a]			
$[B_2(OMe)_4]^{\ddagger}$[b]			
$B_2(Cat)_2$[a]			

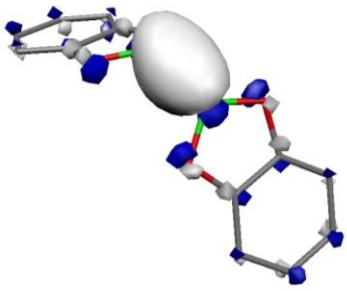


HOMO −5



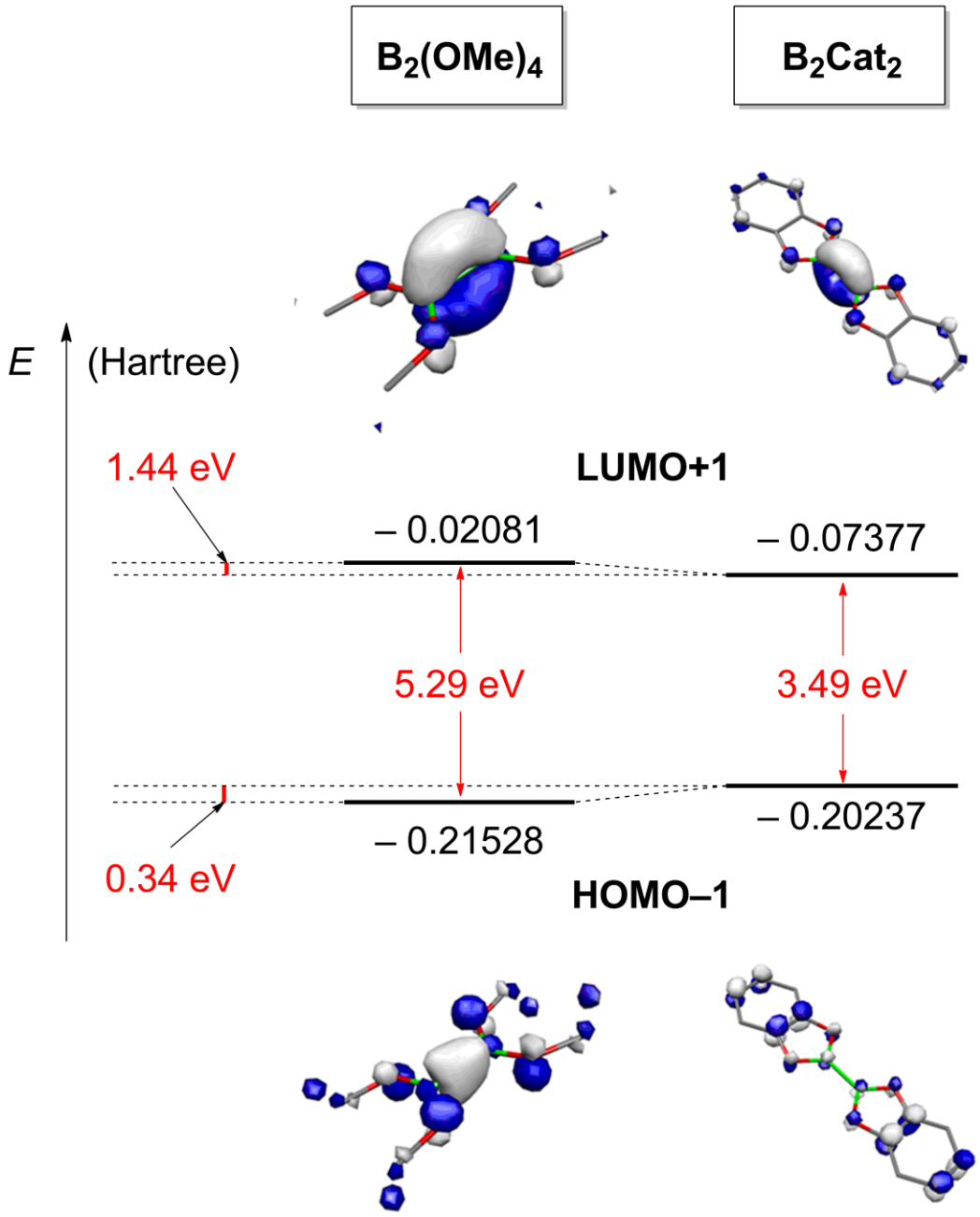


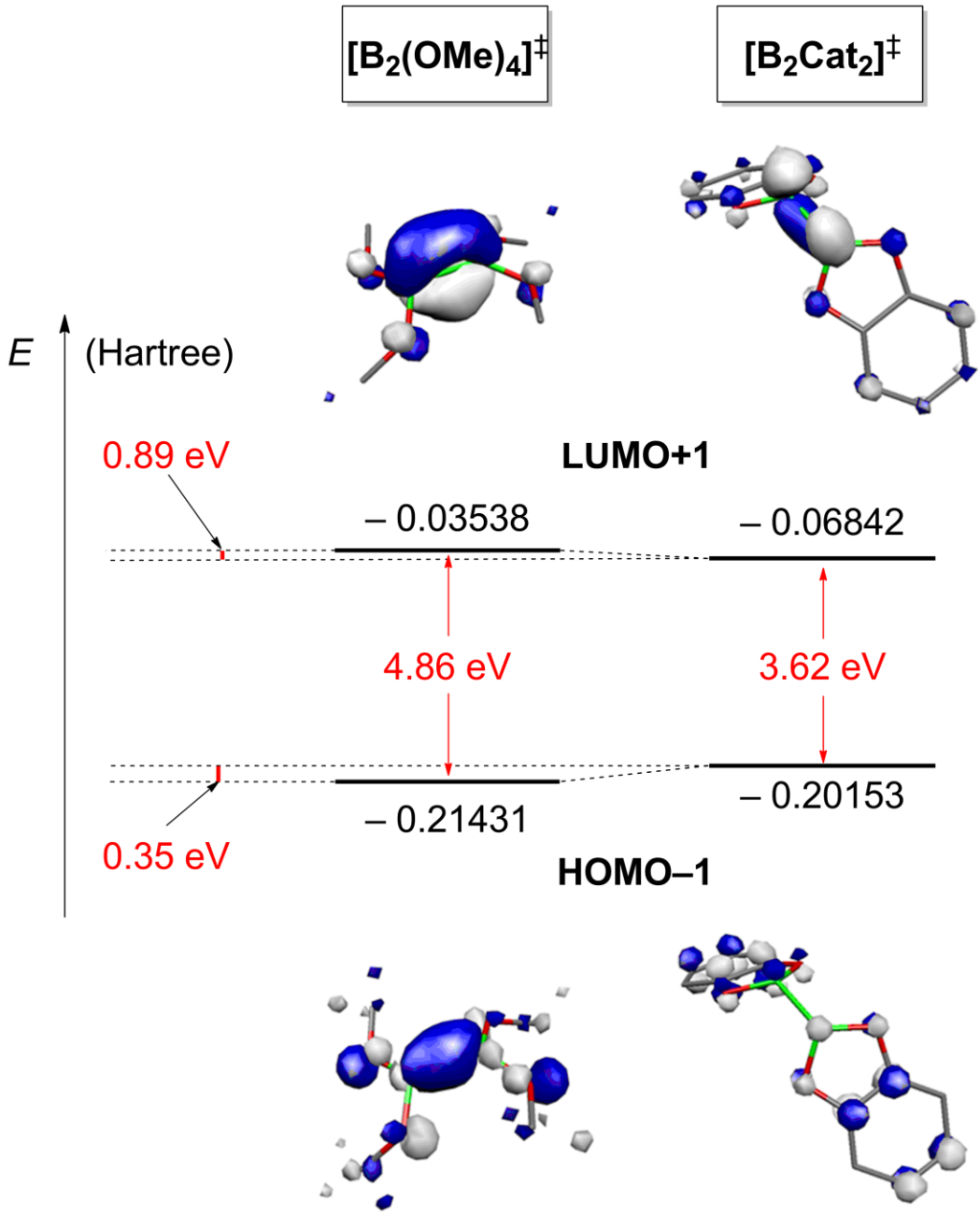
$[B_2(Cat)_2]^{‡b}$ **HOMO −1**



HOMO −5

[a] free optimized diboranes(4) at the ground state; [b] Single-point calculations at the diborane part of the transition states $\mathbf{1}_{TS}$ and $\mathbf{4}_{TS}$ without geometry optimization.


B2(OMe)4
B2Cat2
E
(Hartree)
1.44 eV
LUMO+1
– 0.02081
– 0.07377
5.29 eV
3.49 eV
– 0.21528
– 0.20237
0.34 eV
HOMO–1


[B2(OMe)4]‡
[B2Cat2]‡
E (Hartree)
0.89 eV
LUMO+1
– 0.03538
– 0.06842
4.86 eV
3.62 eV
– 0.21431
– 0.20153
0.35 eV
HOMO–1

Computational Details

The geometries of $B_2(OMe)_4$, $B_2(Cat)_2$, $[Pt(PCy_3)_2]$, *cis*-$[(Cy_3P)_2Pt\{B(OMe)_2\}_2]$ (**1**$_{cal}$), and *cis*-$[(Cy_3P)_2Pt\{Bcat\}_2]$ (**4**$_{cal}$) were optimized without symmetry restraints using Turbomole 5.10.[5] Subsequent final optimizations were conducted with the Gaussian09 program package.[6a] Frequency calculations were used to verify that the final geometries represent energy minima. The computations were performed using DFT methods, applying the Perdew–Burke–Ernzerhof (PBE) exchange correlation functional using 6-31G(d,p) basis sets for H, B, C, O, P Stuttgart relativistic, small core ECP basis sets for Pt.[7] The transition state **1**$_{TS}$ was localized applying the *Synchronous-Guided Quasi-Newton* method embedded within the Gaussian09 software package (QST2 option) or direct methods,[8] while the nature of the transition state was further verified by frequency calculations. The pre-configured adducts **1**$_{ADD}$ und **4**$_{ADD}$ were calculated by the *intrinsic reaction coordinate* method in Gaussian09 by starting from the corresponding transition state, and a subsequent final optimization and frequency analysis was also conducted within the Gaussian09 program package.[9] The NBO analysis and the calculation of the *Wiberg bond indices* (WBI) were performed on *single-point* calculations of **1'**$_{ADD}$ and **4'**$_{ADD}$ using the NBO program (version 5.0) embedded within the Gaussian03 software package.[6] Calculations of the *WBIs* were performed on *single-point* calculations of the free diboranes and the diborane parts of the transition states **1**$_{TS}$ and **4**$_{TS}$ using the NBO program (version 3.1) embedded within the Gaussian 09 software package.[6b]

For the calculation of the energy values of the Gibbs free energy (ΔG_{Total}, 1 atm, 298 K) the values of the SCF energy *E* were corrected by the correlation energy ΔG_{corr} (thermal and entropic correction of the Gibbs free energy values), the dispersion energy ΔE_{Disp} derived from the XYZ-Viewer on the PBE0 level of theory,[10] and the solvation energy ΔE_{solv} for toluene.

Absolute energies of all calculated species:

Table 6 Calculated SCF energy *E*, thermal correction to Gibbs free energy ΔG_{Corr}, solvation energy ΔE_{Solv} and dispersion energy ΔE_{Disp} (PBE / H, C, B, O, P 6-31G(d,p); Pt Stutt, Stutt-ECP; T = 298.15 K).

No.	Compound[a]	*E* (SCF)[b]	ΔG_{Corr}[b]	ΔE_{Solv}[c]	ΔE_{Disp}[c]
	$B_2(OMe)_4$	−509.74935285	0.131921	−5.537556	−10.022765
	B_2Cat_2	−811.91260541	0.141070	−6.902501	−10.083750
	$[Pt(PCy_3)_2]$	−2211.56270310	0.862423	−2.013973	−85.635090
1$_{ADD}$	$[(Cy_3P)_2Pt + B_2(OMe)_4]$	−2721.33336024	1.015602	−2.466978	−104.451736
4$_{ADD}$	*cis*-$[(Cy_3P)_2Pt\cdots(BCat)_2]$	−3023.49867160	1.030818	−2.911412	−114.699986
1$_{OPT}$	*cis*-$[(Cy_3P)_2Pt\{B(OMe)_2\}_2]$	−2721.31777232	1.023651	−1.978732	−118.159872
4$_{OPT}$	*cis*-$[(Cy_3P)_2Pt(BCat)_2]$	−3023.50822196	1.034153	−3.918540	−119.835057
1$_{TS}$	$[(Cy_3P)_2Pt\{B(OMe)_2\}_2]$	−2721.31522994	1.026336	−1.600237	−118.986974
4$_{TS}$	$[(Cy_3P)_2Pt(BCat)_2]$	−3023.49336086	1.032530	−3.009034	−115.059012

[a] Me = Methyl; Cy = cyclohexyl; Cat = catecholato = $[1,2\text{-}O_2C_6H_4]^{2-}$. [b] Energy in Hartree. [c] Solvent toluene; Energy in kcal·mol^{-1}.

Cartesian coordinates for 1_{OPT} and 1_{TS}

	1_{OPT}				1_{TS}		
Pt	-0.07593800	0.96559200	-0.22908500	Pt	-0.08136700	0.34070400	-0.12286600
P	0.48450400	-0.72333000	-1.87051900	P	0.49462800	-0.77960400	-2.06539700
P	-0.43817200	0.06501400	1.98110300	P	-0.52383400	0.04926400	2.13520200
B	0.22082000	2.91834300	0.45327000	B	-0.27473500	3.08292600	0.22686500
B	-0.59771600	2.41413900	-1.64937500	B	-0.27236400	2.66526900	-1.46160200
O	-0.81134800	3.81779800	0.75505100	O	-1.51163600	3.50684600	0.72911900
C	5.12817300	-0.14717100	-1.90371600	C	5.13501300	-1.19934200	-1.80389400
C	4.65042800	-1.44731600	-2.60044800	C	4.43679200	-2.41124400	-2.47765300
C	3.16240500	-1.36273300	-3.02824600	C	3.04522600	-2.03420200	-3.04575900
C	-0.01137400	-5.38106400	-1.49281900	C	-1.06997700	-5.20421900	-1.74535500
C	2.37035000	-0.54997200	-1.98226100	C	2.37415200	-1.01867300	-2.09208400
C	-1.30797700	-4.58345000	-1.77602300	C	-2.14020000	-4.12824600	-2.05211400
C	2.82278600	0.93403600	-2.04828200	C	3.13008000	0.33267900	-2.17117100
C	4.32671800	1.06132200	-2.40997700	C	4.64806900	0.12337500	-2.41627900
C	-0.63018900	4.99662400	1.54060900	C	-1.59935500	4.48132100	1.76824800
C	0.18012000	1.21101800	3.36074500	C	-0.03702400	1.35696100	3.42742200
C	1.70390500	1.47219100	3.32195100	C	1.49224100	1.49804500	3.58289000
C	-0.27966100	0.93227600	4.80684200	C	-0.69521800	1.32062900	4.82556900
C	2.07307900	2.65090300	4.24092100	C	1.84557900	2.78496500	4.34920400
C	0.08983800	2.10982700	5.73158600	C	-0.34505900	2.59745400	5.61828500
C	-0.92490600	-2.36279000	3.63643200	C	0.02704800	-2.06873400	4.11616400
C	1.59545300	2.41727600	5.68378400	C	1.17346900	2.80774000	5.73178500
C	-0.04740000	-1.72990800	2.53198700	C	0.26214100	-1.59743500	2.66521200
C	1.44786600	-1.90570400	2.87762600	C	1.76233500	-1.69652000	2.30752200
C	-0.54764000	-3.83893900	3.87444300	C	0.55017200	-3.50474000	4.31928400
C	1.82439800	-3.37768400	3.12691900	C	2.28973200	-3.12799900	2.51445900
C	0.94058600	-4.00121600	4.21808000	C	2.03747500	-3.62053600	3.94908700
C	-2.31852000	0.13089300	2.20669400	C	-2.35434900	-0.23445700	2.52939300
C	-2.88492200	1.56578400	2.14946800	C	-3.18407200	1.04780700	2.30079700
C	-3.00449900	-0.75059100	1.13821900	C	-2.95431300	-1.39417000	1.70816400
C	-4.41811800	1.57115900	2.29454600	C	-4.67156100	0.82832900	2.63166900
C	-4.53714700	-0.73763700	1.27659500	C	-4.44167200	-1.61822000	2.03675100
C	-5.09110600	0.69414300	1.22808900	C	-5.26388400	-0.33782500	1.82624400
C	-0.20401900	-0.32337500	-3.59893300	C	0.00021200	-0.09970800	-3.77308600
C	0.21531000	-1.20607700	-4.79510500	C	0.80887500	-0.55159000	-5.00673600
C	-1.74692900	-0.19391800	-3.59243500	C	-1.50995300	-0.26416200	-4.05297900
C	-0.28162500	-0.60042700	-6.12434600	C	0.36691100	0.20691300	-6.27642800
C	0.30154300	-2.61528800	-1.79763900	C	-0.12882700	-2.57263900	-2.07052600
C	1.27627900	-3.29387900	-0.80022500	C	0.64899600	-3.45655100	-1.05443300
C	-1.13728900	-3.07174800	-1.48244800	C	-1.63165300	-2.69949600	-1.74380100
C	0.79196700	-4.70504600	-0.37290600	C	-0.14385300	-4.71874400	-0.62208700
O	1.56602200	3.27713400	0.61815100	O	0.82074100	3.50561600	0.96924600
C	2.09177800	4.55810300	0.27596100	C	2.16349800	3.26570800	0.55356800
O	0.33524500	3.18890400	-2.35344600	O	0.90787200	3.01706400	-2.13601200
O	-1.97464100	2.54550900	-1.87268400	O	-1.39785200	2.55842400	-2.27196900
C	0.02142900	3.94027300	-3.52701100	C	0.91297400	3.47405800	-3.48750800
C	-2.64442400	3.78705900	-2.07808600	C	-2.68838300	2.26729200	-1.73922500
C	-2.25657200	0.42292700	-4.90709300	C	-1.94037700	0.53329900	-5.29603500
C	-1.80446900	-0.39536600	-6.12696500	C	-1.14268400	0.09473000	-6.53321300
H	4.99088400	-0.23133300	-0.80942000	H	4.91598800	-1.19121000	-0.71971700
H	6.21041100	-0.00231600	-2.06510900	H	6.23116100	-1.29205400	-1.89144900
H	5.26952300	-1.65050100	-3.49288500	H	5.06445200	-2.80505200	-3.29715600
H	4.79359900	-2.30778800	-1.92150800	H	4.33117900	-3.23200100	-1.74486300
H	2.75864300	-2.37756700	-3.18212200	H	2.43901800	-2.94115700	-3.20222100
H	3.09412100	-0.85056300	-4.00479300	H	3.17396500	-1.58233300	-4.04256000
H	-0.25038000	-6.42612500	-1.23075700	H	-1.54756300	-6.16297800	-1.47948500
H	0.61338900	-5.42864300	-2.40423900	H	-0.46194400	-5.40412700	-2.64753600
H	2.65957800	-0.93675500	-0.98455000	H	2.52123700	-1.40977200	-1.06613800
H	-1.60930400	-4.72754500	-2.82922500	H	-2.44601300	-4.19811500	-3.11196900
H	-2.13641800	-4.97891600	-1.16107200	H	-3.05043600	-4.31918300	-1.45499500
H	2.21717800	1.49165800	-2.78277000	H	2.71268900	0.96987700	-2.97050000
H	2.60723400	1.41239800	-1.07768200	H	2.95658900	0.88284800	-1.23189600

H	4.73008800	2.00079700	-1.99352500	H	5.21476600	0.97725600	-2.00642400
H	4.45258600	1.13587900	-3.50707500	H	4.85848800	0.11184400	-3.50225800
H	-0.32893600	5.86177300	0.92236400	H	-0.72443700	5.15248100	1.77523100
H	0.12652700	4.85269000	2.33289500	H	-1.67189800	4.00206100	2.76278100
H	-1.59588300	5.23333900	2.01769900	H	-2.51780500	5.06941100	1.60439900
H	-0.29910900	2.15887500	3.04018500	H	-0.37872200	2.27815900	2.92056000
H	2.02603000	1.67885700	2.28879400	H	1.98204500	1.48622200	2.59547900
H	2.25064800	0.57708000	3.66723200	H	1.88464800	0.63147300	4.14872300
H	0.21406800	0.01646400	5.18363100	H	-0.34106500	0.43829400	5.38903500
H	-1.36767400	0.74877400	4.85303400	H	-1.79196700	1.22857600	4.75622000
H	1.60805000	3.57511000	3.84424200	H	1.50891200	3.65334600	3.75171700
H	3.16502000	2.81804500	4.21919600	H	2.94199900	2.87448400	4.45539800
H	-0.47631500	3.00701000	5.41231100	H	-0.79466500	3.47104000	5.10635600
H	-0.22760300	1.89158600	6.76730100	H	-0.80468200	2.55324700	6.62223400
H	-0.80359900	-1.80473400	4.58243400	H	0.56115800	-1.39547300	4.81248400
H	-1.99375700	-2.30410200	3.37114400	H	-1.04271200	-2.01940300	4.38501100
H	1.82875700	3.29161800	6.31776800	H	1.39089900	3.75652600	6.25423100
H	2.15202500	1.56130900	6.11393400	H	1.60423800	2.00016300	6.35610900
H	-0.23974000	-2.29712900	1.59917500	H	-0.26273600	-2.30762400	1.99353300
H	2.07987200	-1.47151000	2.08110800	H	1.90690700	-1.35745500	1.26497400
H	1.67098500	-1.33781600	3.79899800	H	2.34743100	-1.00949800	2.94409000
H	-0.77498400	-4.42172900	2.95974400	H	-0.03875800	-4.19672600	3.68554000
H	-1.17941700	-4.26029500	4.67709200	H	0.38578200	-3.82064600	5.36519800
H	1.70864400	-3.95516600	2.19106800	H	1.78460000	-3.81185900	1.80466700
H	2.89100800	-3.44586700	3.40740600	H	3.36820100	-3.16991400	2.27701900
H	1.19124700	-5.06801700	4.35689600	H	2.38352800	-4.66288800	4.06738900
H	1.14671900	-3.50102300	5.18482100	H	2.63446900	-3.00895500	4.65382700
H	-2.54562500	-0.28654400	3.20779900	H	-2.41649100	-0.50409300	3.60307800
H	-2.59105400	2.02962700	1.19112700	H	-3.07320600	1.36013600	1.24694800
H	-2.44375300	2.18922700	2.94703400	H	-2.79145600	1.88344500	2.90453400
H	-2.63567500	-1.79081600	1.19482800	H	-2.39483300	-2.33093600	1.88059100
H	-2.71001600	-0.36518000	0.14254900	H	-2.83895700	-1.14914100	0.63549300
H	-4.79195800	2.60918900	2.23342300	H	-5.23684600	1.75782100	2.43938800
H	-4.69670400	1.19623400	3.29995800	H	-4.77948700	0.61376900	3.71359500
H	-4.98905000	-1.35627100	0.48031500	H	-4.84064400	-2.44149300	1.41708500
H	-4.82387600	-1.20618700	2.23937300	H	-4.53850500	-1.94400500	3.09135400
H	-4.89390700	1.12489200	0.22721400	H	-5.25709400	-0.07557200	0.75009800
H	-6.18767900	0.68977000	1.36380100	H	-6.31991700	-0.50524400	2.10391700
H	0.20825900	0.69419500	-3.76111000	H	0.17559800	0.98033800	-3.62923500
H	1.30617700	-1.34238000	-4.84000600	H	1.88385100	-0.37221000	-4.85120900
H	-0.22635800	-2.21517400	-4.68076700	H	0.68572100	-1.64103200	-5.16449400
H	-2.19363100	-1.20127600	-3.49059900	H	-1.73395300	-1.33351000	-4.23193000
H	-2.08485000	0.40587000	-2.73304100	H	-2.09763200	0.05256200	-3.17637900
H	0.02194500	-1.24702500	-6.96752300	H	0.93820700	-0.16194200	-7.14743000
H	0.21909000	0.37511800	-6.28209300	H	0.63199100	1.27595200	-6.15831200
H	0.55217400	-2.96941200	-2.81601100	H	0.04598900	-2.95135600	-3.09830500
H	2.27589500	-3.37577300	-1.26047300	H	1.61661300	-3.76540400	-1.48368800
H	1.40134500	-2.66016200	0.09661500	H	0.87574400	-2.84932400	-0.16041200
H	-1.88677400	-2.49542100	-2.04625000	H	-2.24596300	-1.96101300	-2.27704700
H	-1.34242400	-2.85948300	-0.41765100	H	-1.75087200	-2.46518100	-0.67256100
H	0.14834200	-4.62978600	0.52409900	H	-0.75563500	-4.49434900	0.27231500
H	1.65705000	-5.32311300	-0.07557700	H	0.56052400	-5.51240600	-0.31773900
H	2.11716700	5.24480600	1.14298500	H	2.32024800	2.19113900	0.34718600
H	1.51662700	5.03064200	-0.53970300	H	2.82926800	3.58122800	1.37404200
H	3.12694000	4.41314800	-0.07631900	H	2.40370700	3.83291800	-0.35974900
H	-0.71189400	3.41867600	-4.16822600	H	-0.10489100	3.55450000	-3.90266400
H	-0.37802700	4.94108300	-3.28219200	H	1.40067200	4.46467800	-3.52164400
H	0.95464200	4.07300000	-4.09939800	H	1.50497500	2.78476600	-4.11792300
H	-2.70979300	4.05930200	-3.14837100	H	-2.65937600	1.33017200	-1.15027200
H	-2.15399200	4.60897700	-1.52715400	H	-3.38174700	2.14422500	-2.58814300
H	-3.67140300	3.68144600	-1.68988100	H	-3.04180900	3.08193800	-1.08697600
H	-1.86959600	1.45768400	-4.99240600	H	-1.77627600	1.61046200	-5.10264400
H	-3.35820600	0.50393900	-4.88310600	H	-3.02385700	0.40249100	-5.46960600
H	-2.12610100	0.09088000	-7.06560400	H	-1.42749400	0.69494300	-7.41582200
H	-2.30142100	-1.38514600	-6.10039900	H	-1.39553600	-0.95691800	-6.77313100

Cartesian coordinates for 4_{OPT} and 4_{TS}

	4_{OPT}				4_{TS}		
Pt	0.40008200	-0.35977000	0.10601300	Pt	0.03411700	0.01677600	-0.13865500
P	-2.02316100	-0.36139900	0.45321400	P	-2.31557400	-0.30173600	0.16461000
P	0.92349200	2.02880600	-0.02902300	P	1.09067500	2.06359300	0.46457000
C	-4.26232200	-4.47677300	1.67398700	C	-3.60765300	-3.38779900	3.65017600
C	-2.86006700	-4.48913700	1.04752400	C	-2.16191100	-3.32159400	3.13452000
C	-2.57223400	-3.17578500	0.29695900	C	-2.07821900	-2.65777900	1.74874600
C	-4.01007700	2.51913300	3.76595000	C	-4.88812100	3.62661800	1.34384200
C	-2.71504800	-1.95150800	1.23282000	C	-2.73148800	-1.25818400	1.75109600
C	-2.55016300	2.05964100	3.89809300	C	-3.40716400	3.48820300	1.73082800
C	-4.14639500	-1.93173600	1.81971700	C	-4.19445100	-1.35045700	2.24289700
C	-4.44938700	-3.24449800	2.57137900	C	-4.25785500	-1.99555100	3.64233200
C	1.02053500	2.70486600	1.73959400	C	0.81637400	2.50578800	2.28714400
C	1.70796400	4.06758300	1.98595000	C	1.76279100	3.52233400	2.96394800
C	1.61295200	1.63968100	2.69743600	C	0.70747300	1.22926800	3.15463300
C	1.55247200	4.50102400	3.45746000	C	1.27252700	3.86093400	4.38645100
C	1.48223200	2.06984600	4.16898300	C	0.22484500	1.55995700	4.57746600
C	3.79028500	1.92298700	-0.12759400	C	3.66755900	1.03762400	0.99683300
C	2.11997900	3.44594400	4.41976600	C	1.13260300	2.60022600	5.25418500
C	2.55778700	2.43293900	-0.91217300	C	2.94896900	2.08704500	0.11517400
C	2.81838900	3.88771600	-1.36946000	C	3.72353300	3.42337100	0.10260900
C	5.06710300	1.99319500	-0.98540800	C	5.12582900	0.83599800	0.54966700
C	4.09799700	3.97188100	-2.22720400	C	5.17972300	3.19998000	-0.35551800
C	5.32494900	3.42268500	-1.48433500	C	5.89984700	2.16303600	0.52013500
C	-0.40772000	3.06771400	-0.90897200	C	0.30559600	3.48866400	-0.50678200
C	-0.38973200	2.79386200	-2.43176000	C	0.62537500	3.34437600	-2.01219300
C	-0.54255600	4.57428300	-0.59421300	C	0.49118200	4.94305900	-0.02219400
C	-1.59629700	3.43906800	-3.13889600	C	-0.19589400	4.33390800	-2.85794400
C	-1.75589400	5.18785600	-1.32112200	C	-0.33746000	5.91650800	-0.88498800
C	-1.69524000	4.94193000	-2.83592600	C	-0.00304400	5.78147100	-2.37868800
C	-2.84909900	-0.11899500	-1.23602700	C	-3.18572900	-1.06965900	-1.34423700
C	-4.34857700	-0.46097300	-1.39287000	C	-4.55216500	-1.74941400	-1.10061300
C	-2.03110200	-0.82473700	-2.34768100	C	-2.27648400	-2.01384900	-2.15526100
C	-4.85829700	-0.06337200	-2.79269400	C	-5.22275400	-2.13906000	-2.43299100
C	-2.65198400	1.06422400	1.54764100	C	-3.22190800	1.37069900	0.32203900
C	-4.10821200	1.56097200	1.40724300	C	-4.71791000	1.49211500	-0.04512300
C	-2.26171600	0.82368400	3.02565200	C	-2.95851600	2.01643000	1.69724100
C	-4.36227600	2.79454800	2.29657500	C	-5.16590200	2.96810300	-0.01642600
C	-2.54380000	-0.44972100	-3.74914100	C	-2.93862000	-2.41320900	-3.48588700
C	-4.04465700	-0.74386300	-3.90443600	C	-4.31895800	-3.05361200	-3.27331100
C	3.92162700	-1.45399200	-1.95640100	C	1.88577900	-0.57042500	-3.81322300
C	4.34317000	-1.81414100	-0.66561600	C	3.08770500	-0.46078100	-3.09142600
O	3.34418000	-1.52017000	0.23860900	O	2.81995500	-0.53808200	-1.74510600
O	2.65120500	-0.92203300	-1.89116100	O	0.84067700	-0.73269500	-2.93922900
C	4.73645900	-1.63387200	-3.07147300	C	1.85883000	-0.51894400	-5.20577200
C	6.00880200	-2.19675200	-2.84375300	C	3.09619300	-0.35448500	-5.85837200
C	0.83082800	-4.24157000	1.71816000	C	1.77471100	-3.58336000	0.98153700
C	0.97087200	-4.58658200	0.36358500	C	0.91958100	-4.16904000	0.03031900
O	0.60260500	-2.88585400	1.82389000	O	1.79732700	-2.22337100	0.79905400
O	0.83793000	-3.45352500	-0.41136600	O	0.37480000	-3.18642000	-0.75994700
C	1.19985500	-5.89865300	-0.04154400	C	0.71131700	-5.54627400	-0.02242900
C	1.28636300	-6.87069600	0.97547900	C	1.39815200	-6.32777500	0.92678900
C	1.14645600	-6.52630100	2.33118900	C	2.25239200	-5.74197800	1.87911400
C	0.91400100	-5.19439000	2.73056700	C	2.45763100	-4.34952000	1.92482000
C	6.42989200	-2.55676100	-1.55178100	C	4.29853300	-0.24706700	-5.13633400
C	5.59760900	-2.36988500	-0.42970300	C	4.31656600	-0.29935700	-3.72870700
B	0.61287000	-2.36807500	0.49187400	B	0.88586900	-1.93601900	-0.27740100
B	2.26443400	-0.96365000	-0.51589200	B	1.39527300	-0.68339500	-1.61132900
H	-5.02248400	-4.45781300	0.86817000	H	-4.19602800	-4.06565300	3.00105200
H	-4.43878600	-5.40232600	2.25025200	H	-3.63753100	-3.82159300	4.66555300
H	-2.74996500	-5.34272300	0.35582400	H	-1.71517200	-4.33033400	3.08983900
H	-2.09951200	-4.63040100	1.83823600	H	-1.54784200	-2.73797600	3.84845300
H	-3.29409500	-3.08291100	-0.53625800	H	-2.58338200	-3.30125200	1.00271400

H	-1.57194100	-3.21058000	-0.16225100	H	-1.02705000	-2.57627400	1.43226500
H	-4.68035100	1.73099000	4.16149400	H	-5.51175500	3.13847500	2.11820200
H	-4.18805300	3.41950700	4.38014300	H	-5.18625200	4.68987200	1.32533400
H	-2.00586800	-2.10577500	2.07162200	H	-2.17711400	-0.65067600	2.49758900
H	-2.30502700	1.83717200	4.95199600	H	-3.22715600	3.91609300	2.73372800
H	-1.88376700	2.89004000	3.59107200	H	-2.78901600	4.07527800	1.02243300
H	-4.28657400	-1.08582800	2.51031900	H	-4.66922900	-0.35573000	2.27324600
H	-4.88376600	-1.80169600	1.00686400	H	-4.78946800	-1.96324300	1.54480600
H	-3.77033800	-3.32249500	3.44287800	H	-3.73339300	-1.34325200	4.36831200
H	-5.47688400	-3.21027600	2.97625400	H	-5.30897800	-2.05584600	3.97722200
H	-0.05263900	2.81919000	2.00412300	H	-0.19203000	2.96993300	2.25815900
H	1.31188500	4.85046400	1.32045200	H	1.85080600	4.44598100	2.36919300
H	2.78588500	3.97791200	1.75938800	H	2.77827400	3.09108200	3.03149700
H	2.68147600	1.48851500	2.45818200	H	1.69631500	0.73680700	3.20668000
H	1.12576400	0.66266300	2.51827000	H	0.03413800	0.50308000	2.66199600
H	0.47790700	4.65896300	3.67817300	H	0.29037300	4.36957100	4.31911200
H	2.04951500	5.47529000	3.61332600	H	1.96516000	4.58039500	4.85880100
H	0.41019700	2.11253000	4.44407100	H	-0.80853100	1.95779600	4.52677300
H	1.94224600	1.30623700	4.82094200	H	0.17709800	0.63740600	5.18332000
H	3.93629600	2.55214100	0.77063500	H	3.66327900	1.37441200	2.05144700
H	3.63126200	0.89572700	0.23604000	H	3.12343100	0.07827600	0.95942600
H	1.96724900	3.75890700	5.46803000	H	0.74349700	2.86245500	6.25414900
H	3.21476300	3.37242500	4.26962800	H	2.13506600	2.15702400	5.41271700
H	2.47352400	1.80108000	-1.82000900	H	2.97193700	1.68634900	-0.91653200
H	1.97255900	4.28373700	-1.95259000	H	3.24066900	4.14804900	-0.57420100
H	2.92980700	4.54470400	-0.48770100	H	3.72918500	3.88067200	1.10780900
H	4.96286700	1.31005400	-1.84915600	H	5.12377300	0.38299600	-0.45915200
H	5.92733500	1.62362500	-0.40009500	H	5.62388400	0.11171900	1.21883000
H	3.94445900	3.38923200	-3.15652800	H	5.17599200	2.84816100	-1.40584900
H	4.26725900	5.01874700	-2.53746100	H	5.72426000	4.16140500	-0.34758700
H	6.21480000	3.45163200	-2.13794100	H	6.93048500	2.00286200	0.15581700
H	5.54847800	4.07734400	-0.61890500	H	5.98972000	2.55835800	1.55142300
H	-1.33336600	2.59245400	-0.52753700	H	-0.77076700	3.24880900	-0.38498000
H	-0.37452900	1.70421100	-2.61194200	H	0.42862500	2.30562000	-2.33441200
H	0.53656800	3.19569500	-2.88073200	H	1.70243300	3.53402100	-2.18380200
H	0.36921700	5.11985400	-0.89438000	H	1.55527500	5.23526800	-0.07024700
H	-0.65901300	4.72499600	0.49289600	H	0.18255300	5.03889600	1.03332400
H	-2.52816900	2.94336100	-2.80151600	H	-1.26894300	4.06723500	-2.78626700
H	-1.52727100	3.26431600	-4.22746700	H	0.08125500	4.23668300	-3.92247500
H	-2.68575200	4.73876700	-0.91835900	H	-1.41495800	5.70475200	-0.73468400
H	-1.81182500	6.26927200	-1.10333200	H	-0.17211200	6.95328300	-0.54133600
H	-2.57959800	5.37813900	-3.33311100	H	-0.62481500	6.47242000	-2.97524800
H	-0.81075700	5.46006200	-3.25557800	H	1.04977100	6.08306500	-2.54477900
H	-2.73667200	0.97497900	-1.39499500	H	-3.36039000	-0.17172400	-1.97574500
H	-4.96093500	0.02723900	-0.61871800	H	-5.23134800	-1.10834100	-0.51694300
H	-4.48909600	-1.54960200	-1.26457100	H	-4.38984400	-2.66805800	-0.50560800
H	-2.10596700	-1.91966000	-2.21628000	H	-2.05982900	-2.92000700	-1.56171300
H	-0.95747600	-0.58316900	-2.23258800	H	-1.30438000	-1.53521800	-2.34538000
H	-4.78658800	1.03673400	-2.90655400	H	-5.44818400	-1.21819000	-3.00664000
H	-5.92950200	-0.31741100	-2.88500800	H	-6.19332600	-2.62769500	-2.23232700
H	-2.01058300	1.89682400	1.19629900	H	-2.66138300	1.96579700	-0.42960800
H	-4.31832100	1.82396500	0.35624500	H	-4.91420600	1.07450000	-1.04673700
H	-4.82205500	0.76542500	1.68406300	H	-5.33600000	0.91586300	0.66817300
H	-2.82665200	-0.03359500	3.43426100	H	-3.51149600	1.46156600	2.47887400
H	-1.19362000	0.54867600	3.08714700	H	-1.88783700	1.92855500	1.94700500
H	-3.74669400	3.63992300	1.92924600	H	-4.62315600	3.52320900	-0.80685100
H	-5.41612400	3.11119600	2.20081400	H	-6.23948500	3.03733400	-0.26719300
H	-2.36616000	0.62886200	-3.92796200	H	-3.05087200	-1.51061100	-4.11937700
H	-1.96227100	-0.99351200	-4.51456700	H	-2.27343500	-3.10062100	-4.03778900
H	-4.40280900	-0.41909000	-4.89761000	H	-4.79753600	-3.28354100	-4.24214500
H	-4.20811600	-1.83800700	-3.85326300	H	-4.19393200	-4.01982600	-2.74637100
H	4.39791100	-1.35399700	-4.07244300	H	0.91959300	-0.60744000	-5.75759600
H	6.67975100	-2.35812800	-3.69263600	H	3.12065500	-0.31221000	-6.95119800
H	1.31041200	-6.15395800	-1.09848500	H	0.04628600	-5.99072100	-0.76726900
H	1.46838900	-7.91401800	0.70155700	H	1.26393700	-7.41339900	0.92139500
H	1.22167700	-7.30612400	3.09475800	H	2.77104400	-6.38088300	2.59987600

H	0.80754700	-4.91545500	3.78211200	H	3.12054900	-3.88504200	2.65924300
H	7.42310000	-2.99342000	-1.41193200	H	5.24099800	-0.12168800	-5.67722800
H	5.91280300	-2.64909500	0.57887100	H	5.24606600	-0.22112100	-3.15874300

Cartesian coordinates for 1_{ADD} and 4_{ADD}

1_{ADD}				4_{OPT}			
Pt	0.376764	-0.680513	0.152649	Pt	-0.035004	0.099543	-0.084121
P	1.069559	-1.147583	-1.970216	P	-2.332698	-0.467990	-0.185985
P	-0.379042	-0.265355	2.266840	P	1.383930	1.793668	0.701625
B	-1.299097	4.689650	-1.283677	C	-3.795958	-2.679480	3.841448
B	0.378054	4.329559	-1.050476	C	-2.330687	-2.730474	3.380178
O	-1.935482	4.074205	-2.347769	C	-2.191987	-2.403967	1.882652
C	5.426183	0.416663	-2.674836	C	-4.889269	3.637911	-0.107533
C	4.961130	-0.639826	-3.708958	C	-2.837837	-1.040090	1.547156
C	3.419879	-0.823854	-3.713661	C	-3.446371	3.586008	0.418889
C	1.055781	-5.804441	-2.403972	C	-4.321397	-1.025111	1.979688
C	2.849694	-0.618092	-2.297402	C	-4.442286	-1.330600	3.486458
C	-0.308189	-5.101859	-2.618010	C	1.037188	2.062958	2.545166
C	3.065163	0.850651	-1.838171	C	1.981354	2.978428	3.357381
C	4.338283	1.478250	-2.458084	C	0.848377	0.715128	3.281276
C	-3.340312	4.271516	-2.559262	C	1.434345	3.199954	4.782011
C	0.728586	0.929458	3.228172	C	0.310139	0.927998	4.706573
C	2.138240	0.340697	3.452925	C	3.927607	0.674436	1.322223
C	0.189894	1.568916	4.525667	C	1.214483	1.869260	5.519187
C	3.109755	1.412660	3.978494	C	3.252553	1.725349	0.410077
C	1.164917	2.644539	5.045331	C	4.063785	3.040407	0.426143
C	-1.034194	-1.721123	4.747484	C	5.378002	0.413984	0.878197
C	2.577137	2.075756	5.259511	C	5.521518	2.781596	-0.008321
C	-0.648306	-1.848927	3.260343	C	6.201341	1.711210	0.859348
C	0.505910	-2.860221	3.079623	C	0.718883	3.365860	-0.133653
C	-1.416296	-3.095129	5.333137	C	1.047835	3.363395	-1.643222
C	0.126588	-4.231773	3.665986	C	0.990429	4.742162	0.514872
C	-0.287276	-4.121968	5.143545	C	0.332998	4.507296	-2.383016
C	-2.068555	0.576077	2.314639	C	0.269213	5.868327	-0.253809
C	-1.994107	1.944159	1.598479	C	0.636819	5.871229	-1.745344
C	-3.151452	-0.308152	1.655920	C	-3.126163	-1.587327	-1.503679
C	-3.362472	2.647201	1.551013	C	-4.552652	-2.111534	-1.214346
C	-4.518193	0.399018	1.604036	C	-2.235031	-2.769953	-1.936671
C	-4.428758	1.758081	0.893732	C	-5.150706	-2.797413	-2.458789
C	0.069721	-0.311083	-3.345407	C	-3.186558	1.213184	-0.476656
C	0.054593	-1.007248	-4.723704	C	-4.644633	1.255816	-0.984179
C	-1.373367	-0.004641	-2.882845	C	-3.019031	2.143952	0.744777
C	-0.693317	-0.150815	-5.764657	C	-5.066913	2.702189	-1.312816
C	1.092363	-2.985406	-2.369067	C	-2.820384	-3.474447	-3.174095
C	2.159735	-3.704904	-1.492551	C	-4.261984	-3.952049	-2.944374
C	-0.291874	-3.627374	-2.143723	C	0.726481	-0.114731	-4.065504
C	1.798470	-5.184198	-1.212350	C	1.949824	0.443294	-3.647704
O	-2.090182	5.497959	-0.495949	O	2.195670	0.091964	-2.346104
C	-1.600213	6.232533	0.626405	O	0.172998	-0.834238	-3.039045
O	0.821726	4.249148	0.256597	C	0.231550	0.084555	-5.353372
O	1.311675	4.085041	-2.035123	C	1.014051	0.869888	-6.222896
C	2.176787	3.882493	0.553310	C	2.378016	-3.117899	0.798477
C	1.037875	4.201474	-3.430073	C	1.180019	-3.776028	0.465250
C	-2.132378	0.836710	-3.923460	O	2.430841	-1.910624	0.151842
C	-2.125696	0.170511	-5.309159	O	0.453546	-2.997671	-0.398136
H	5.642415	-0.072533	-1.706520	C	0.863918	-5.031611	0.982459
H	6.373317	0.879343	-3.001993	C	1.804824	-5.615729	1.853459
H	5.290156	-0.346992	-4.722256	C	3.003288	-4.958578	2.184798
H	5.449208	-1.607214	-3.493639	C	3.313534	-3.688171	1.660504
H	3.168641	-1.821050	-4.114907	C	2.235902	1.427545	-5.806111
H	2.958310	-0.087780	-4.397543	C	2.728381	1.223687	-4.501672
H	0.910953	-6.889117	-2.259852	B	1.194735	-1.775781	-0.576909
H	1.683626	-5.696529	-3.308662	B	1.053876	-0.680778	-1.904775
H	3.417088	-1.273712	-1.609295	H	-4.361957	-3.492448	3.345674

H	-0.584927	-5.149871	-3.686760	H	-3.866784	-2.865803	4.927868
H	-1.100498	-5.643238	-2.070368	H	-1.890285	-3.721609	3.588405
H	2.192611	1.479651	-2.089329	H	-1.739484	-1.996440	3.962971
H	3.121220	0.855284	-0.735674	H	-2.684939	-3.198324	1.289004
H	4.703788	2.295926	-1.813039	H	-1.131034	-2.402532	1.583926
H	4.095057	1.945804	-3.431221	H	-5.581950	3.328321	0.699491
H	-3.592262	5.343628	-2.622537	H	-5.165466	4.672332	-0.378461
H	-3.930616	3.828233	-1.738661	H	-2.312910	-0.280508	2.163341
H	-3.604571	3.771840	-3.503757	H	-3.337597	4.222837	1.315394
H	0.840798	1.741641	2.481175	H	-2.764867	4.002873	-0.349065
H	2.507558	-0.100923	2.509339	H	-4.793495	-0.053008	1.758263
H	2.081251	-0.481060	4.192594	H	-4.888272	-1.786722	1.418114
H	0.060815	0.795631	5.304306	H	-3.945662	-0.524511	4.062002
H	-0.803970	2.020184	4.361376	H	-5.505728	-1.320235	3.785636
H	3.248941	2.186339	3.197972	H	0.040059	2.553308	2.510385
H	4.104285	0.966725	4.159490	H	2.131793	3.949101	2.858739
H	1.213116	3.471667	4.309750	H	2.977337	2.505240	3.429877
H	0.778247	3.081833	5.983467	H	1.817464	0.183885	3.329300
H	-0.173504	-1.320565	5.315742	H	0.171152	0.068046	2.692528
H	-1.865451	-1.006516	4.884187	H	0.472860	3.747085	4.719851
H	3.264786	2.871160	5.598610	H	2.125737	3.846957	5.351026
H	2.544853	1.322081	6.070823	H	-0.707843	1.362748	4.648248
H	-1.518241	-2.282432	2.724872	H	0.206894	-0.045447	5.218866
H	0.754830	-2.933880	2.004782	H	3.939140	1.040888	2.366093
H	1.414577	-2.488487	3.589497	H	3.355726	-0.264760	1.301434
H	-2.331377	-3.460946	4.827377	H	0.785000	2.050610	6.520520
H	-1.669499	-2.992803	6.403823	H	2.194302	1.379151	5.681070
H	-0.715969	-4.653357	3.082820	H	3.279899	1.322763	-0.622159
H	0.969222	-4.937567	3.554420	H	3.618229	3.789570	-0.248257
H	-0.596385	-5.108141	5.533914	H	4.058784	3.479631	1.441009
H	0.590208	-3.808271	5.742670	H	5.367378	-0.035594	-0.132945
H	-2.347248	0.741235	3.375488	H	5.846264	-0.329880	1.548147
H	-1.623967	1.771008	0.568576	H	5.524296	2.447466	-1.064306
H	-1.253664	2.605515	2.080773	H	6.092654	3.726979	0.023350
H	-3.258571	-1.263959	2.198371	H	7.226187	1.517357	0.495442
H	-2.815425	-0.562436	0.631342	H	6.302163	2.093267	1.894471
H	-3.266416	3.603549	1.006749	H	-0.372478	3.188412	-0.052290
H	-3.684142	2.896895	2.581963	H	0.760038	2.391701	-2.077448
H	-5.255413	-0.253888	1.103009	H	2.138865	3.463837	-1.796201
H	-4.888260	0.554727	2.636882	H	2.073205	4.957806	0.534638
H	-4.160259	1.594935	-0.168920	H	0.646344	4.746085	1.563304
H	-5.412163	2.261896	0.898915	H	-0.760740	4.329999	-2.354719
H	0.586876	0.664797	-3.463907	H	0.624281	4.496614	-3.448039
H	1.077180	-1.217737	-5.078263	H	-0.825588	5.732475	-0.151597
H	-0.456281	-1.985216	-4.635348	H	0.507407	6.842789	0.208992
H	-1.912738	-0.957428	-2.716165	H	0.094717	6.676134	-2.272824
H	-1.342069	0.501976	-1.901625	H	1.716294	6.094458	-1.855651
H	-0.704180	-0.669350	-6.740415	H	-3.180259	-0.893685	-2.370170
H	-0.138292	0.795867	-5.918208	H	-5.227277	-1.313789	-0.868100
H	1.361015	-3.099035	-3.436992	H	-4.494501	-2.856096	-0.398088
H	3.139272	-3.653573	-2.001321	H	-2.148834	-3.492265	-1.104548
H	2.265760	-3.167690	-0.530360	H	-1.219586	-2.421888	-2.157906
H	-1.085731	-3.061502	-2.660159	H	-5.257457	-2.048407	-3.268261
H	-0.526129	-3.551307	-1.065994	H	-6.169650	-3.159191	-2.230952
H	1.155958	-5.249018	-0.314310	H	-2.549839	1.625084	-1.287082
H	2.714731	-5.752706	-0.976417	H	-4.766523	0.630508	-1.884324
H	-0.522839	6.073216	0.788918	H	-5.327906	0.849053	-0.215222
H	-2.147819	5.909738	1.528552	H	-3.637916	1.772441	1.583518
H	-1.800616	7.305561	0.463808	H	-1.968278	2.112198	1.088405
H	2.882179	4.292823	-0.187877	H	-4.451652	3.073232	-2.155861
H	2.417715	4.276907	1.553790	H	-6.115032	2.713863	-1.661272
H	2.274975	2.783236	0.565603	H	-2.800364	-2.769313	-4.028732
H	1.260129	3.236645	-3.919010	H	-2.172269	-4.322840	-3.456758
H	1.703005	4.968870	-3.863018	H	-4.677799	-4.398617	-3.865308
H	-0.013047	4.465169	-3.627789	H	-4.262237	-4.752397	-2.178635
H	-1.665363	1.838348	-3.985129	H	-0.717283	-0.357590	-5.668623

H	-3.171221	1.000761	-3.582901
H	-2.629401	0.814231	-6.052686
H	-2.707923	-0.770903	-5.263287

H	0.662944	1.046191	-7.243830
H	-0.067893	-5.536498	0.714565
H	1.597921	-6.602546	2.277820
H	3.712330	-5.443155	2.862375
H	4.244768	-3.171953	1.908409
H	2.819460	2.030090	-6.508331
H	3.678928	1.649689	-4.169662

Cartesian coordinates for $[B_2(OMe)_4]_{OPT}$ and $[B_2Cat_2]_{OPT}$

$[B_2(OMe)_4]_{OPT}$

B	0.01777100	-0.02910100	0.01362900
B	0.01355800	1.69839900	0.01808200
O	-0.93223800	2.29977000	0.82264400
O	0.95636500	2.30841700	-0.78334700
O	-0.88242600	-0.63892600	0.86287300
O	0.92079000	-0.63050700	-0.83862600
C	1.22339700	-2.01320400	-0.98504100
C	-1.17967300	-2.02330200	1.00344000
C	1.12722300	3.69272400	-1.06463400
C	-1.10841100	3.68218600	1.11035400
H	2.21208500	-2.08802900	-1.46773600
H	1.27123500	-2.54860500	-0.02127800
H	0.48895000	-2.52180000	-1.63608000
H	-2.16841200	-2.10401000	1.48509500
H	-1.22466600	-2.55509300	0.03753800
H	-0.44367200	-2.53160100	1.65297200
H	1.71119700	3.77323300	-1.99663200
H	0.17139200	4.22413200	-1.21217300
H	1.69475300	4.20146800	-0.26398400
H	-1.69273600	3.75613900	2.04266900
H	-1.67781700	4.19244300	0.31201200
H	-0.15459600	4.21646500	1.26043300

$[B_2Cat_2]_{OPT}$

B	-0.31257200	0.16571800	1.71061300
B	0.72949700	1.48228000	1.57883600
O	0.32411100	2.82390600	1.63016700
O	2.11731700	1.38196700	1.40312000
O	-1.70040900	0.26609200	1.88618000
O	0.09276200	-1.17592400	1.65934800
C	-1.06726200	-1.91317600	1.80616100
C	-2.15593400	-1.03759700	1.94384600
C	2.57278600	2.68567800	1.34545100
C	1.48410100	3.56120900	1.48333600
C	3.87626600	3.14714500	1.18030900
C	4.04605200	4.54389300	1.15873500
C	2.95418500	5.42194300	1.29700600
C	1.64085900	4.94478100	1.46339800
C	-1.22407900	-3.29674200	1.82609100
C	-2.53744100	-3.77384700	1.99235900
C	-3.62928800	-2.89575200	2.13048900
C	-3.45945000	-1.49901100	2.10886000
H	4.71558500	2.45627700	1.07400200
H	5.05117700	4.95533400	1.03142100
H	3.12888700	6.50118100	1.27483500
H	0.78612100	5.61617400	1.57161500
H	-0.36936000	-3.96817100	1.71795500
H	-2.71218700	-4.85307800	2.01455000
H	-4.63443900	-3.30715000	2.25773800
H	-4.29875500	-0.80810600	2.21504000

Cartesian coordinates for $1'_{ADD}$ and $4'_{ADD}$

$1'_{ADD}$				$4'_{ADD}$			
				Pt	-0.035004	0.099543	-0.084121
				P	-2.332698	-0.467990	-0.185985
Pt	0.376764	-0.680513	0.152648	P	1.383930	1.793668	0.701625
P	1.069559	-1.147583	-1.970216	C	0.726481	-0.114731	-4.065504
P	-0.379042	-0.265355	2.266839	C	1.949824	0.443294	-3.647704
B	-1.299096	4.689649	-1.283674	O	2.195670	0.091964	-2.346104
B	0.378056	4.329558	-1.050474	O	0.172998	-0.834238	-3.039045
O	-1.935481	4.074204	-2.347766	C	0.231550	0.084555	-5.353372
C	-3.340311	4.271515	-2.559258	C	1.014051	0.869888	-6.222896
O	-2.090181	5.497956	-0.495944	C	2.378016	-3.117899	0.798477
C	-1.600211	6.232530	0.626410	C	1.180019	-3.776028	0.465250
O	0.821728	4.249147	0.256599	O	2.430841	-1.910624	0.151842
O	1.311676	4.085040	-2.035121	O	0.453546	-2.997671	-0.398136
C	2.176789	3.882492	0.553311	C	0.863918	-5.031611	0.982459
C	1.037875	4.201473	-3.430071	C	1.804824	-5.615729	1.853459
H	-3.592262	5.343627	-2.622532	C	3.003288	-4.958578	2.184798
H	-3.930615	3.828231	-1.738657	C	3.313534	-3.688171	1.660504
H	-3.604570	3.771840	-3.503754	C	2.235902	1.427545	-5.806111
H	-0.522837	6.073213	0.788923	C	2.728381	1.223687	-4.501672
H	-2.147817	5.909733	1.528557	B	1.194735	-1.775781	-0.576909
H	-1.800614	7.305557	0.463815	B	1.053876	-0.680778	-1.904775
H	2.882181	4.292822	-0.187876	H	-0.717283	-0.357590	-5.668623
H	2.417718	4.276905	1.553791	H	0.662944	1.046191	-7.243830
H	2.274978	2.783235	0.565603	H	-0.067893	-5.536498	0.714565
H	1.260129	3.236645	-3.919008	H	1.597921	-6.602546	2.277820
H	1.703005	4.968869	-3.863016	H	3.712330	-5.443155	2.862375
H	-0.013047	4.465169	-3.627787	H	4.244768	-3.171953	1.908409
C	1.092232	-2.974908	-2.366789	H	2.819460	2.030090	-6.508331
H	1.432117	-3.117689	-3.371274	H	3.678928	1.649689	-4.169662
H	1.752611	-3.478183	-1.691871	C	0.729544	3.340658	-0.120264
H	0.104941	-3.374432	-2.264136	H	-0.282715	3.505636	0.184720
C	0.082848	-0.322065	-3.327353	H	1.329752	4.178478	0.167325
H	0.496876	-0.583373	-4.278773	H	0.767159	3.223035	-1.183113
H	-0.934432	-0.650215	-3.278794	C	3.230372	1.726160	0.413538
H	0.121513	0.739749	-3.201036	H	3.435044	1.878740	-0.625562
C	-0.645637	-1.833234	3.250497	H	3.709139	2.491800	0.987540
H	-0.972482	-1.583362	4.238239	H	3.603453	0.769313	0.713795
H	-1.389522	-2.433677	2.769870	C	-3.169616	1.179826	-0.470889
H	0.272551	-2.379792	3.306222	H	-4.227332	1.034965	-0.542665
C	0.715872	0.915746	3.217136	H	-2.954084	1.835429	0.346810
H	0.747800	1.857987	2.711110	H	-2.806309	1.611952	-1.379831
H	0.321692	1.053176	4.202344	C	-2.831505	-1.032919	1.525432
H	1.704625	0.511892	3.281706	H	-3.883757	-1.226038	1.544712
C	-2.052400	0.568030	2.314182	H	-2.300068	-1.927526	1.774735
H	-2.340318	0.732435	3.331519	H	-2.596105	-0.268441	2.236107
H	-1.998142	1.506336	1.802774	C	-3.112682	-1.568310	-1.481292
H	-2.776223	-0.057824	1.835342	H	-4.140130	-1.736668	-1.234497
C	2.834767	-0.622533	-2.294658	H	-3.048863	-1.093439	-2.438018
H	3.102399	-0.873166	-3.299873	H	-2.595355	-2.504417	-1.512525
H	2.923885	0.434543	-2.154841	C	1.041780	2.059392	2.520752
H	3.488056	-1.128547	-1.614905	H	1.685129	2.827537	2.896192
				H	0.021284	2.352831	2.652590
				H	1.223151	1.149853	3.054365

Cartesian coordinates for $[Pt(PCy_3)_2]_{OPT}$

$[Pt(PCy_3)_2]_{OPT}$			
Pt	-1.13873400	-0.20070800	-0.42663000
P	-0.76892100	-0.07845700	-2.67331900
P	-1.45913400	-0.18311600	1.84213000
C	-1.53265000	-4.18221600	-5.07093900
C	-1.79188900	-4.09327200	-3.55737000
C	-1.03555800	-2.91410300	-2.91977600
C	-3.43884900	3.76925700	-3.34369100
C	-1.39344300	-1.58676700	-3.62468000
C	-1.91891900	3.90773500	-3.51528400
C	-1.09726600	-1.67613100	-5.13535600
C	-1.86050600	-2.85400200	-5.77311000
C	-3.11752400	0.62325700	2.25850600
C	-3.45012300	1.03597100	3.70822600
C	-4.27101200	-0.19692700	1.63508300
C	-4.78798900	1.80129600	3.76529100
C	-5.60406100	0.56785200	1.70758100
C	-1.73243000	-3.00669200	1.68717800
C	-5.93691000	0.98808000	3.14840900
C	-1.31400400	-1.88295500	2.66388400
C	-1.98416500	-2.10073200	4.03796500
C	-1.39012700	-4.39528500	2.25406800
C	-1.63378300	-3.48908000	4.60960400
C	-2.02147300	-4.61562700	3.63867100
C	-0.09657100	0.84303200	2.66077600
C	0.15193800	0.71542100	4.17861000
C	-0.21180500	2.32206100	2.23136100
C	1.38923000	1.53324900	4.60125100
C	1.02262600	3.13033200	2.66789100
C	1.27088400	3.00655500	4.18001800
C	1.05196600	0.24479800	-3.06959600
C	1.44361600	0.66714100	-4.50158900
C	1.95685400	-0.90253300	-2.57077400
C	2.93041000	1.07178200	-4.55927000
C	-1.65816900	1.36181700	-3.51047000
C	-3.18969000	1.23741800	-3.34536400
C	-1.16883900	2.70343800	-2.91824500
C	-3.93399600	2.44491700	-3.94366000
C	3.44144200	-0.50154000	-2.63418200
C	3.84477400	-0.05412600	-4.04908300
H	-0.46581600	-4.42690900	-5.24195200
H	-2.11805200	-5.00639100	-5.51638200
H	-1.50561700	-5.03837900	-3.06214600
H	-2.87781700	-3.96250500	-3.38109800
H	0.05255000	-3.09808400	-2.99713000
H	-1.26611900	-2.82520800	-1.84254700
H	-3.68728500	3.79541800	-2.26473300
H	-3.96066400	4.62434600	-3.80941500
H	-2.49024500	-1.46528400	-3.50562700
H	-1.55862600	4.84049800	-3.04549200
H	-1.68155500	3.98865000	-4.59465200
H	-1.35632300	-0.73391700	-5.65035900
H	-0.01298600	-1.83421000	-5.28736000
H	-2.94880300	-2.66092800	-5.70056400
H	-1.62451800	-2.91814500	-6.85064700
H	-3.03548000	1.55419500	1.65958200
H	-2.64957400	1.66852300	4.12744400
H	-3.51951800	0.14252200	4.35338600
H	-4.37768400	-1.15689700	2.17724100
H	-4.01290800	-0.44498000	0.58887800
H	-4.68177700	2.75545000	3.21253800
H	-5.02129800	2.06963300	4.81136100
H	-5.53538800	1.47199300	1.07118600

H	-6.41713100	-0.05084500	1.28735900
H	-2.82231700	-2.94307100	1.50304900
H	-1.24569200	-2.83705100	0.70947700
H	-6.87626900	1.56878600	3.17547400
H	-6.11016400	0.08138400	3.76099600
H	-0.21478100	-1.97143500	2.80330200
H	-1.69570300	-1.31599900	4.75672400
H	-3.08221100	-2.03352300	3.91922900
H	-0.28922500	-4.48962400	2.33711700
H	-1.71931200	-5.18126700	1.55101300
H	-0.54434500	-3.53408200	4.80572300
H	-2.13328100	-3.62987500	5.58507400
H	-1.72384400	-5.59690100	4.04968200
H	-3.12402800	-4.63950500	3.53478000
H	0.79608100	0.43137200	2.14532600
H	0.29992800	-0.34130100	4.46134600
H	-0.72712500	1.07538500	4.74431600
H	-1.11476000	2.77303800	2.68802800
H	-0.34597000	2.36756200	1.13453900
H	2.28949900	1.09281000	4.12952200
H	1.53646900	1.45260200	5.69325600
H	1.91015100	2.75650800	2.12075600
H	0.90016300	4.19021500	2.38142400
H	2.18017200	3.56272400	4.47007700
H	0.42852800	3.47457900	4.72665800
H	1.24908400	1.10877300	-2.40157500
H	0.81702300	1.50467200	-4.85495000
H	1.27376300	-0.17034600	-5.20206600
H	1.80106700	-1.79754100	-3.20351100
H	1.66407800	-1.17844600	-1.54130700
H	3.08285600	1.97493300	-3.93617900
H	3.20411600	1.35378800	-5.59190300
H	-1.41680300	1.34050900	-4.59275700
H	-3.55943400	0.31079500	-3.81834400
H	-3.41413100	1.15162000	-2.26370200
H	-1.32028400	2.66661700	-1.82104900
H	-0.08379000	2.82908400	-3.08042500
H	-3.77936100	2.46326800	-5.04073800
H	-5.02080000	2.32838100	-3.78311600
H	3.62072400	0.32884900	-1.92332400
H	4.07518400	-1.34276100	-2.30069500
H	4.90038100	0.27107700	-4.06619600
H	3.77166600	-0.91927500	-4.73719700

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