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SUPPORTING INFORMATION of SYNTHESES, STRUCTURES, AND COMPUTATIONS

Carbene-Stabilized Diphosphorus: Bidentate Complexation of BH_2^+

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All reactions were performed under purified argon using Schlenk techniques and an inert atmosphere drybox (M-Braun LabMaster 130). Chemicals were purchased from commercial sources and used as received. Solvents were dried and distilled under argon from Na/benzophenone prior to use. Compound **1** (L:P–P:L, L: = = :C{N(2,6-$Pr^i_2C_6H_3$)CH}$_2$) was prepared according to the literature method.[1] ^{1}H NMR spectra were recorded on a Varian Mercury Plus 400 MHz spectrometer. ^{11}B NMR and ^{31}P{^{1}H} NMR spectra were recorded on a Varian Unity Inova 500 MHz spectrometer. X-ray intensity data for compound **2** were collected on a Bruker SMART APEX II X-ray diffractometer system with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å), using the ω-scan technique.

Compound 2. 1.0 M BH_3·THF in THF (3.60 mL, 3.60 mmol) was added into a Schlenk tube containing **1** (0.600 g, 0.715 mmol) in 15 mL of THF at ambient temperature. After the mixture was stirred over night, the solvent was removed. The resulting solid was rinsed using 70 mL toluene and then filtered. The residue was vacuumed, giving the raw product of **2** as off-white powder (0.51 g, 85.0% yield). X-ray quality single crystals of **2** were obtained by recrystallization of **2** in THF. Mp: melt and decomposed at 174 °C. ^{1}H NMR (THF-d$_8$): δ 1.00 [d, 12H, CH(C*H*$_3$)$_2$], 1.01 [d, 12H, CH(C*H*$_3$)$_2$], 1.06 [d, 12H, CH(C*H*$_3$)$_2$], 1.27 [d, 12H, CH(C*H*$_3$)$_2$], 2.19 [m, 4H, C*H*(CH$_3$)$_2$], 2.27 [m, 4H, C*H*(CH$_3$)$_2$], 7.25 (d, 4H, Ar-*H*), 7.32 (d, 4H, Ar-*H*), 7.48 (t, 4H, Ar-*H*), 7.62 (s, 4H, C*H*). ^{11}B NMR (THF-d$_8$): δ -31.59 (s, $w_{1/2}$ = 443 Hz, BH_2^+), -25.05 (q, $^1J_{BH}$ = 101 Hz, $B_2H_7^-$). ^{31}P{^{1}H} NMR (THF-d$_8$): δ -185.9 (s). Anal. (Lab ID: 3992.1; Complete Analysis Laboratories Inc., Parsippany, NJ) Calcd (found) for $C_{54}H_{81}N_4P_2B_3$ (880.65): C, 73.65 (73.71); H, 9.27 (9.27); N, 6.36 (6.33). Crystal data for **2**·(THF)$_2$: $C_{62}H_{97}N_4B_3O_2P_2$, fw = 1024.81, triclinic, *P*-1 (No. 2), a = 14.459(3) Å, b = 15.275(3) Å, c = 16.847(4) Å, α = 63.054(3)º, β = 79.702(3)º, γ = 66.638(3)º, V = 3045.1(11) Å^3, Z = 2, R1 = 0.0561 for 9200 data ($I > 2\sigma(I)$), wR$_2$ = 0.1535 (all data).

Reference:

1. Y. Wang, Y. Xie, P. Wei, R. B. King, H. F. Schaefer, III, P. v. R. Schleyer and G. H. Robinson, *J. Am. Chem. Soc.*, 2008, **130**, 14970-14971.

X-ray Structural Data of Compound 2

Experimental

Data Collection

Colorless crystals were mounted on the top of glass fiber. The X-ray intensity data were measured at 100 K temperature on a Bruker SMART APEX II X-ray diffractometer system with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) using ω-scan technique. The data were collected in 1464 frames with 10 second exposure times. Crystallographic data: $C_{62}H_{97}N_4B_3O_2P_2$: a = 14.459(3) Å, b = 15.275(3) Å, c = 16.847(4) Å, α= 63.054(3) °, β = 79.702(3) °, γ = 66.638(3) °, V = 3045.1(11) Å^3, Z = 2, F.W. = 1024.81, μ = 0.115 mm-1, d = 1.118 g/cm3, F(000) = 1116.

Data Reduction [1]

Of the 11671 unique reflections collected, 9200 were observed ($I > 2\,\sigma(I)$). The linear absorption coefficient for Mo Kα radiation is 0.115 mm^{-1}. The data were corrected for Lorentz and polarization effects and integrated with the manufacturer's SAINT software. Absorption corrections were applied with the SADABS.

Structure Solution and Refinement [2]

Subsequent solution and refinement was performed using the SHELXTL 6.1[3] solution package operating on a Pentium computer. The structure was solved by direct methods using the SHELXTL 6.1 Software Package. Non-hydrogen atomic scattering factors were taken from the literature tabulations.[4] Non-hydrogen atoms were located from successive difference Fourier map calculations. In the final cycles of each refinement, all the non-hydrogen atoms were refined with anisotropic displacement parameters. The two hydrogen atoms (H(1A), H(1B)) bonded on B(1) and seven hydrogen atoms (H(1C), H(2A),H(2B),H(2C), H(3A), H(3B), H(3C)) bonded with B(2) and B(3) were located from difference Fourier map and refined with proper restraints of B-H bonds around 1.150 Å. The coordinates and thermal parameters of three located hydrogen atoms of H(3A), H(3B), H(3C) had to be fixed because they were unstable and exploded during refinement. The rest of hydrogen atom positions were calculated and allowed to ride on the carbon to which they are bonded assuming a C–H bond length of m Å (m = 0.98 for CH groups, m = 0.96 for CH_3 groups, m = 0.93 for Ph-H groups). Hydrogen atom temperature factors were fixed at n (n = 1.2 for CH groups, n = 1.5 for CH_3 groups, m = 1.2 for Ph-H groups) times the isotropic temperature factor of the C-atom to which they are bonded. The crystal system of compound is triclinic, space group P-1 (No. 2) and the final residual values based on 683 variable parameters and

9200 observed reflections ($I > 2\,\sigma(I)$) are $R1 = 0.0561$, $wR2 = 0.1404$, and those for all unique reflections are $R1 = 0.0767$, $wR2 = 0.1535$. The goodness-of-fit indicator for all data is 1.036. Peaks on the final difference map ranged from 0.399 to -0.505 e/Å^3, which are of no chemical significance.

Summary

The compound crystallizes in triclinic, space group P-1 (No. 2). The asymmetric unit contains one molecule (a cation-anion pair) in the form of $C_{54}H_{81}N_4B_3P_2$ plus two solvent THF molecules. The total form is $C_{62}H_{97}N_4B_3O_2P_2$. Structure solution, refinement and the calculation of derived results were performed using the SHELXTL 6.1[3] package of computer programs. Neutral atom scattering factors were those of Cromer and Waber,[4] and the real and imaginary anomalous dispersion corrections were those of Cromer.[5]

References

1. Data Reduction:

Intensity

$$I = [S - B/R]\cdot V$$

Standard Deviation in Intensity

$$s(I) = [S + B/R^2]^{1/2}\cdot V$$

Structure Factor

$$F = (I/Lp)^{1/2}$$

Standard Deviation in Structure Factor

$$\sigma(F) = \sigma(I)/(2\cdot F\cdot Lp)$$

Where:
S = total scan count
B = sum of background counts
R = ratio of background counting time to scan counting time
V = scan rate
Lp = Lorentz-polarization correction

2. Least-Squares Refinement:

Weighting Scheme

$$w = 1/[\sigma^2(F_o^2) + (0.0883*P)^2 + 0.3162*P] \quad \text{where } P = [\mathrm{Max}(F_o^2, 0) + 2*F_c^2]/3;$$

Residuals

R-factors:

$R = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$;

Weighted R-factor on F^2:

$wR2 = [\Sigma[w\,(F_o^2 - F_c^2)^2] \,/\, \Sigma[w(F_o^2)^2]]^{1/2}$;

Goodness of Fit Indicator:

goodness-of-fit = $[\Sigma[w\,(F_o^2 - F_c^2)^2] \,/ (N_{observns} - N_{params})\,]^{1/2}$.

3. Sheldrick, G.M. *A Short History of SHELX*, Acta Cryst. 2008, A64, 112.

4. Cromer, D.T. and Waber, J.T. International Tables for X-ray Crystallography, Vol. IV, Table 2.2B, The Kynoch Press, Birmingham England, 1974.

5. Cromer, D.T. International Tables for X-ray Crystallography, Vol. IV, Table 2.3.1, The Kynoch Press, Birmingham England, 1974.

Table 1. Crystal data and structure refinement for **2**.

Identification code	**2**
Empirical formula	C62 H97 B3 N4 O2 P2
Formula weight	1024.81
Temperature	100 K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 14.459(3) A alpha = 63.054(3) deg. b = 15.275(3) A beta = 79.702(3) deg. c = 16.847(4) A gamma = 66.638(3) deg.
Volume	3045.1(11) A^3
Z, Calculated density	2, 1.118 Mg/m^3
Absorption coefficient	0.115 mm^-1
F(000)	1116
Crystal size	0.20 x 0.17 x 0.06 mm
Theta range for data collection	2.50 to 25.81 deg.
Limiting indices	-17<=h<=17, -18<=k<=18, -20<=l<=20
Reflections collected / unique	34171 / 11671 [R(int) = 0.0540]
Completeness to theta = 25.81	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9931 and 0.9773
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11671 / 7 / 683
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0561, wR2 = 0.1404

R indices (all data)	R1 = 0.0767, wR2 = 0.1535
Largest diff. peak and hole	0.399 and -0.505 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1)	1798(1)	8368(1)	3252(1)	28(1)
P(2)	3317(1)	8359(1)	3277(1)	27(1)
B(1)	2547(4)	7783(4)	4358(2)	37(1)
N(1)	1495(2)	6597(2)	3488(2)	26(1)
N(2)	2880(2)	6584(2)	2764(2)	27(1)
N(3)	2257(2)	10588(2)	2945(2)	26(1)
N(4)	3662(2)	9762(2)	3676(2)	25(1)
C(1)	2124(2)	7141(2)	3145(2)	24(1)
C(2)	1841(2)	5712(3)	3331(2)	33(1)
C(3)	2718(2)	5698(3)	2883(2)	32(1)
C(4)	3679(2)	6896(3)	2201(2)	30(1)
C(5)	4629(2)	6477(3)	2573(2)	29(1)
C(6)	5383(3)	6747(3)	1999(3)	38(1)
C(7)	5191(3)	7416(3)	1127(3)	44(1)
C(8)	4247(3)	7816(3)	774(3)	45(1)
C(9)	3460(3)	7551(3)	1301(2)	37(1)
C(10)	2429(3)	7969(3)	896(3)	43(1)
C(11)	1855(3)	9121(3)	723(3)	56(1)
C(12)	2504(4)	7830(4)	46(3)	68(1)
C(13)	4870(2)	5720(3)	3540(2)	32(1)
C(14)	5559(3)	5934(3)	3962(3)	38(1)
C(15)	5329(3)	4584(3)	3643(3)	44(1)
C(16)	542(2)	6958(2)	3909(2)	25(1)
C(17)	499(2)	6524(2)	4836(2)	27(1)
C(18)	-429(2)	6901(3)	5211(2)	30(1)
C(19)	-1254(2)	7677(3)	4677(3)	34(1)
C(20)	-1183(2)	8070(3)	3778(2)	32(1)
C(21)	-281(2)	7728(2)	3346(2)	29(1)
C(22)	-221(3)	8141(3)	2338(2)	38(1)
C(23)	-464(3)	7464(3)	2028(3)	49(1)
C(24)	-873(3)	9290(3)	1864(3)	49(1)
C(25)	1377(2)	5647(3)	5429(2)	29(1)
C(26)	1526(3)	5836(3)	6196(3)	38(1)
C(27)	1233(3)	4592(3)	5784(3)	44(1)
C(28)	3017(2)	9639(2)	3278(2)	24(1)
C(29)	2440(2)	11302(3)	3133(2)	31(1)
C(30)	3303(2)	10788(2)	3596(2)	30(1)

C(31)	4568(2)	8952(2)	4156(2)	26(1)
C(32)	4539(2)	8507(2)	5075(2)	28(1)
C(33)	5429(2)	7743(3)	5531(2)	31(1)
C(34)	6299(2)	7448(3)	5067(3)	36(1)
C(35)	6304(2)	7905(3)	4154(3)	33(1)
C(36)	5447(2)	8672(3)	3655(2)	30(1)
C(37)	5445(3)	9172(3)	2643(2)	34(1)
C(38)	5473(3)	10272(3)	2241(3)	42(1)
C(39)	6309(3)	8495(3)	2257(3)	46(1)
C(40)	3593(2)	8840(3)	5593(2)	29(1)
C(41)	3379(3)	7897(3)	6337(2)	36(1)
C(42)	3692(3)	9540(3)	5971(3)	40(1)
C(43)	1533(2)	10935(2)	2277(2)	29(1)
C(44)	536(2)	11020(2)	2534(2)	32(1)
C(45)	-138(3)	11457(3)	1844(3)	39(1)
C(46)	169(3)	11762(3)	967(3)	44(1)
C(47)	1147(3)	11662(3)	746(3)	42(1)
C(48)	1864(3)	11253(3)	1399(2)	34(1)
C(49)	2928(3)	11236(3)	1156(2)	40(1)
C(50)	3432(3)	10716(4)	526(3)	56(1)
C(51)	2936(3)	12351(3)	770(3)	48(1)
C(52)	212(2)	10731(3)	3500(2)	33(1)
C(53)	-270(3)	11735(3)	3663(3)	45(1)
C(54)	-520(3)	10155(3)	3775(3)	45(1)
O(1)	4446(2)	4006(2)	2166(2)	62(1)
C(55)	4978(5)	4621(4)	1498(3)	77(2)
C(56)	5686(5)	3903(4)	1094(4)	83(2)
C(57)	4289(4)	3377(5)	1823(4)	76(2)
C(58)	5058(5)	3294(5)	1116(4)	96(2)
O(2)	7764(2)	5781(2)	1446(2)	67(1)
C(59)	7495(5)	5091(4)	1280(4)	93(2)
C(60)	8381(9)	4229(6)	1248(8)	206(6)
C(61)	9187(5)	4613(12)	1105(8)	215(8)
C(62)	8823(4)	5563(6)	1295(5)	122(3)
B(2)	1418(4)	4164(4)	2477(4)	53(1)
B(3)	1660(6)	5432(6)	1105(5)	93(2)

Table 3. Bond lengths [A] and angles [deg] for **2**.

P(1)-C(1)	1.830(3)
P(1)-B(1)	1.972(4)
P(1)-P(2)	2.1993(11)
P(2)-C(28)	1.828(3)
P(2)-B(1)	1.982(4)
B(1)-H(1A)	1.169(18)
B(1)-H(1B)	1.125(19)
N(1)-C(1)	1.351(4)
N(1)-C(2)	1.375(4)
N(1)-C(16)	1.452(4)
N(2)-C(1)	1.356(4)
N(2)-C(3)	1.384(4)
N(2)-C(4)	1.447(4)
N(3)-C(28)	1.358(4)
N(3)-C(29)	1.389(4)
N(3)-C(43)	1.443(4)
N(4)-C(28)	1.354(4)
N(4)-C(30)	1.390(4)
N(4)-C(31)	1.445(4)
C(2)-C(3)	1.353(4)
C(2)-H(2)	0.9300
C(3)-H(3)	0.9300
C(4)-C(5)	1.392(5)
C(4)-C(9)	1.394(5)
C(5)-C(6)	1.382(5)
C(5)-C(13)	1.514(5)
C(6)-C(7)	1.356(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.375(6)
C(7)-H(7)	0.9300
C(8)-C(9)	1.388(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.519(5)
C(10)-C(11)	1.528(6)
C(10)-C(12)	1.519(6)
C(10)-H(10)	0.9800
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.525(5)
C(13)-C(15)	1.529(5)
C(13)-H(13)	0.9800

C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-C(17)	1.393(5)
C(16)-C(21)	1.408(4)
C(17)-C(18)	1.396(4)
C(17)-C(25)	1.515(5)
C(18)-C(19)	1.391(5)
C(18)-H(18)	0.9300
C(19)-C(20)	1.354(5)
C(19)-H(19)	0.9300
C(20)-C(21)	1.403(4)
C(20)-H(20)	0.9300
C(21)-C(22)	1.521(5)
C(22)-C(24)	1.515(5)
C(22)-C(23)	1.519(5)
C(22)-H(22)	0.9800
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.512(5)
C(25)-C(27)	1.532(5)
C(25)-H(25)	0.9800
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(29)-C(30)	1.341(5)
C(29)-H(29)	0.9300
C(30)-H(30)	0.9300
C(31)-C(32)	1.380(5)
C(31)-C(36)	1.422(4)
C(32)-C(33)	1.399(5)
C(32)-C(40)	1.522(4)
C(33)-C(34)	1.383(5)
C(33)-H(33)	0.9300
C(34)-C(35)	1.372(5)
C(34)-H(34)	0.9300
C(35)-C(36)	1.393(5)
C(35)-H(35)	0.9300
C(36)-C(37)	1.520(5)
C(37)-C(39)	1.532(5)

C(37)-C(38)	1.516(5)
C(37)-H(37)	0.9800
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
C(40)-C(42)	1.530(5)
C(40)-C(41)	1.523(5)
C(40)-H(40)	0.9800
C(41)-H(41A)	0.9600
C(41)-H(41B)	0.9600
C(41)-H(41C)	0.9600
C(42)-H(42A)	0.9600
C(42)-H(42B)	0.9600
C(42)-H(42C)	0.9600
C(43)-C(48)	1.389(5)
C(43)-C(44)	1.402(5)
C(44)-C(45)	1.390(5)
C(44)-C(52)	1.517(5)
C(45)-C(46)	1.379(6)
C(45)-H(45)	0.9300
C(46)-C(47)	1.362(5)
C(46)-H(46)	0.9300
C(47)-C(48)	1.394(5)
C(47)-H(47)	0.9300
C(48)-C(49)	1.514(5)
C(49)-C(51)	1.528(5)
C(49)-C(50)	1.521(5)
C(49)-H(49)	0.9800
C(50)-H(50A)	0.9600
C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600
C(51)-H(51A)	0.9600
C(51)-H(51B)	0.9600
C(51)-H(51C)	0.9600
C(52)-C(53)	1.543(5)
C(52)-C(54)	1.518(5)
C(52)-H(52)	0.9800
C(53)-H(53A)	0.9600
C(53)-H(53B)	0.9600
C(53)-H(53C)	0.9600
C(54)-H(54A)	0.9600
C(54)-H(54B)	0.9600
C(54)-H(54C)	0.9600
O(1)-C(55)	1.430(6)
O(1)-C(57)	1.426(6)
C(55)-C(56)	1.500(7)
C(55)-H(55A)	0.9700

C(55)-H(55B)	0.9700
C(56)-C(58)	1.522(8)
C(56)-H(56A)	0.9700
C(56)-H(56B)	0.9700
C(57)-C(58)	1.492(7)
C(57)-H(57A)	0.9700
C(57)-H(57B)	0.9700
C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
O(2)-C(59)	1.405(6)
O(2)-C(62)	1.433(6)
C(59)-C(60)	1.441(9)
C(59)-H(59A)	0.9700
C(59)-H(59B)	0.9700
C(60)-C(61)	1.440(13)
C(60)-H(60A)	0.9700
C(60)-H(60B)	0.9700
C(61)-C(62)	1.497(11)
C(61)-H(61A)	0.9700
C(61)-H(61B)	0.9700
C(62)-H(62A)	0.9700
C(62)-H(62B)	0.9700
B(2)-H(1C)	1.103(18)
B(2)-H(2A)	1.28(4)
B(2)-H(2B)	1.09(4)
B(2)-H(2C)	1.18(4)
B(3)-H(1C)	1.296(18)
B(3)-H(3A)	1.324(7)
B(3)-H(3B)	1.308(8)
B(3)-H(3C)	1.244(8)

C(1)-P(1)-B(1)	98.15(18)
C(1)-P(1)-P(2)	99.79(9)
B(1)-P(1)-P(2)	56.43(13)
C(28)-P(2)-B(1)	97.52(18)
C(28)-P(2)-P(1)	100.87(10)
B(1)-P(2)-P(1)	56.00(13)
P(1)-B(1)-P(2)	67.57(12)
P(1)-B(1)-H(1A)	109.1(17)
P(2)-B(1)-H(1A)	115.7(17)
P(1)-B(1)-H(1B)	112(2)
P(2)-B(1)-H(1B)	121(2)
H(1A)-B(1)-H(1B)	119(3)
C(1)-N(1)-C(2)	111.4(3)
C(1)-N(1)-C(16)	123.5(3)
C(2)-N(1)-C(16)	125.0(3)
C(1)-N(2)-C(3)	109.9(3)
C(1)-N(2)-C(4)	127.4(3)
C(3)-N(2)-C(4)	122.1(3)
C(28)-N(3)-C(29)	109.5(3)

C(28)-N(3)-C(43)	126.6(3)
C(29)-N(3)-C(43)	121.4(3)
C(28)-N(4)-C(30)	109.9(3)
C(28)-N(4)-C(31)	126.3(3)
C(30)-N(4)-C(31)	123.8(3)
N(1)-C(1)-N(2)	105.1(3)
N(1)-C(1)-P(1)	119.0(2)
N(2)-C(1)-P(1)	135.9(2)
C(3)-C(2)-N(1)	106.1(3)
C(3)-C(2)-H(2)	126.9
N(1)-C(2)-H(2)	126.9
N(2)-C(3)-C(2)	107.4(3)
N(2)-C(3)-H(3)	126.3
C(2)-C(3)-H(3)	126.3
C(5)-C(4)-C(9)	123.9(3)
C(5)-C(4)-N(2)	118.5(3)
C(9)-C(4)-N(2)	117.5(3)
C(4)-C(5)-C(6)	116.5(3)
C(4)-C(5)-C(13)	123.4(3)
C(6)-C(5)-C(13)	120.0(3)
C(7)-C(6)-C(5)	121.4(3)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(6)-C(7)-C(8)	121.0(3)
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-H(7)	119.5
C(7)-C(8)-C(9)	121.0(4)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(4)-C(9)-C(8)	116.1(3)
C(4)-C(9)-C(10)	123.5(3)
C(8)-C(9)-C(10)	120.4(3)
C(9)-C(10)-C(11)	111.7(3)
C(9)-C(10)-C(12)	111.7(3)
C(11)-C(10)-C(12)	110.4(4)
C(9)-C(10)-H(10)	107.6
C(11)-C(10)-H(10)	107.6
C(12)-C(10)-H(10)	107.6
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

C(14)-C(13)-C(5)	113.5(3)
C(14)-C(13)-C(15)	110.1(3)
C(5)-C(13)-C(15)	110.4(3)
C(14)-C(13)-H(13)	107.5
C(5)-C(13)-H(13)	107.5
C(15)-C(13)-H(13)	107.5
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	124.4(3)
C(17)-C(16)-N(1)	118.3(3)
C(21)-C(16)-N(1)	117.3(3)
C(16)-C(17)-C(18)	116.4(3)
C(16)-C(17)-C(25)	123.5(3)
C(18)-C(17)-C(25)	120.1(3)
C(19)-C(18)-C(17)	120.9(3)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(20)-C(19)-C(18)	120.8(3)
C(20)-C(19)-H(19)	119.6
C(18)-C(19)-H(19)	119.6
C(19)-C(20)-C(21)	122.0(3)
C(19)-C(20)-H(20)	119.0
C(21)-C(20)-H(20)	119.0
C(16)-C(21)-C(20)	115.5(3)
C(16)-C(21)-C(22)	122.9(3)
C(20)-C(21)-C(22)	121.5(3)
C(24)-C(22)-C(21)	112.9(3)
C(24)-C(22)-C(23)	111.2(3)
C(21)-C(22)-C(23)	111.0(3)
C(24)-C(22)-H(22)	107.1
C(21)-C(22)-H(22)	107.1
C(23)-C(22)-H(22)	107.1
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5

H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(17)-C(25)-C(26)	112.8(3)
C(17)-C(25)-C(27)	110.0(3)
C(26)-C(25)-C(27)	109.9(3)
C(17)-C(25)-H(25)	108.0
C(26)-C(25)-H(25)	108.0
C(27)-C(25)-H(25)	108.0
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(3)-C(28)-N(4)	106.1(3)
N(3)-C(28)-P(2)	135.0(2)
N(4)-C(28)-P(2)	118.9(2)
C(30)-C(29)-N(3)	107.5(3)
C(30)-C(29)-H(29)	126.3
N(3)-C(29)-H(29)	126.3
C(29)-C(30)-N(4)	107.1(3)
C(29)-C(30)-H(30)	126.5
N(4)-C(30)-H(30)	126.5
C(32)-C(31)-C(36)	123.6(3)
C(32)-C(31)-N(4)	118.3(3)
C(36)-C(31)-N(4)	118.1(3)
C(31)-C(32)-C(33)	117.7(3)
C(31)-C(32)-C(40)	122.4(3)
C(33)-C(32)-C(40)	119.9(3)
C(34)-C(33)-C(32)	120.5(3)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	120.5(3)
C(33)-C(34)-H(34)	119.7
C(35)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	122.2(3)
C(34)-C(35)-H(35)	118.9
C(36)-C(35)-H(35)	118.9
C(31)-C(36)-C(35)	115.6(3)
C(31)-C(36)-C(37)	122.0(3)
C(35)-C(36)-C(37)	122.4(3)
C(36)-C(37)-C(39)	112.5(3)

C(36)-C(37)-C(38)	113.1(3)
C(39)-C(37)-C(38)	109.2(3)
C(36)-C(37)-H(37)	107.2
C(39)-C(37)-H(37)	107.2
C(38)-C(37)-H(37)	107.2
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(32)-C(40)-C(42)	109.8(3)
C(32)-C(40)-C(41)	112.0(3)
C(42)-C(40)-C(41)	110.4(3)
C(32)-C(40)-H(40)	108.2
C(42)-C(40)-H(40)	108.2
C(41)-C(40)-H(40)	108.2
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(48)-C(43)-C(44)	124.2(3)
C(48)-C(43)-N(3)	116.6(3)
C(44)-C(43)-N(3)	119.0(3)
C(45)-C(44)-C(43)	115.6(3)
C(45)-C(44)-C(52)	123.0(3)
C(43)-C(44)-C(52)	121.3(3)
C(46)-C(45)-C(44)	121.7(3)
C(46)-C(45)-H(45)	119.1
C(44)-C(45)-H(45)	119.1
C(45)-C(46)-C(47)	120.8(3)
C(45)-C(46)-H(46)	119.6
C(47)-C(46)-H(46)	119.6
C(48)-C(47)-C(46)	120.9(4)
C(48)-C(47)-H(47)	119.5
C(46)-C(47)-H(47)	119.5

C(47)-C(48)-C(43)	116.8(3)
C(47)-C(48)-C(49)	121.3(3)
C(43)-C(48)-C(49)	121.7(3)
C(51)-C(49)-C(48)	110.0(3)
C(51)-C(49)-C(50)	111.2(3)
C(48)-C(49)-C(50)	113.0(3)
C(51)-C(49)-H(49)	107.5
C(48)-C(49)-H(49)	107.5
C(50)-C(49)-H(49)	107.5
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-C(54)	109.5(3)
C(53)-C(52)-C(44)	109.5(3)
C(54)-C(52)-C(44)	112.9(3)
C(53)-C(52)-H(52)	108.2
C(54)-C(52)-H(52)	108.2
C(44)-C(52)-H(52)	108.2
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(55)-O(1)-C(57)	107.0(4)
O(1)-C(55)-C(56)	104.6(4)
O(1)-C(55)-H(55A)	110.8
C(56)-C(55)-H(55A)	110.8
O(1)-C(55)-H(55B)	110.8
C(56)-C(55)-H(55B)	110.8
H(55A)-C(55)-H(55B)	108.9
C(58)-C(56)-C(55)	101.9(5)
C(58)-C(56)-H(56A)	111.4
C(55)-C(56)-H(56A)	111.4
C(58)-C(56)-H(56B)	111.4

C(55)-C(56)-H(56B)	111.4
H(56A)-C(56)-H(56B)	109.3
O(1)-C(57)-C(58)	107.2(4)
O(1)-C(57)-H(57A)	110.3
C(58)-C(57)-H(57A)	110.3
O(1)-C(57)-H(57B)	110.3
C(58)-C(57)-H(57B)	110.3
H(57A)-C(57)-H(57B)	108.5
C(56)-C(58)-C(57)	105.3(4)
C(56)-C(58)-H(58A)	110.7
C(57)-C(58)-H(58A)	110.7
C(56)-C(58)-H(58B)	110.7
C(57)-C(58)-H(58B)	110.7
H(58A)-C(58)-H(58B)	108.8
C(59)-O(2)-C(62)	109.0(5)
C(60)-C(59)-O(2)	110.4(7)
C(60)-C(59)-H(59A)	109.6
O(2)-C(59)-H(59A)	109.6
C(60)-C(59)-H(59B)	109.6
O(2)-C(59)-H(59B)	109.6
H(59A)-C(59)-H(59B)	108.1
C(59)-C(60)-C(61)	103.6(7)
C(59)-C(60)-H(60A)	111.0
C(61)-C(60)-H(60A)	111.0
C(59)-C(60)-H(60B)	111.0
C(61)-C(60)-H(60B)	111.0
H(60A)-C(60)-H(60B)	109.0
C(60)-C(61)-C(62)	109.6(6)
C(60)-C(61)-H(61A)	109.8
C(62)-C(61)-H(61A)	109.8
C(60)-C(61)-H(61B)	109.8
C(62)-C(61)-H(61B)	109.8
H(61A)-C(61)-H(61B)	108.2
O(2)-C(62)-C(61)	104.2(6)
O(2)-C(62)-H(62A)	110.9
C(61)-C(62)-H(62A)	110.9
O(2)-C(62)-H(62B)	110.9
C(61)-C(62)-H(62B)	110.9
H(62A)-C(62)-H(62B)	108.9
H(1C)-B(2)-H(2A)	103(4)
H(1C)-B(2)-H(2B)	94(4)
H(2A)-B(2)-H(2B)	112(3)
H(1C)-B(2)-H(2C)	116(3)
H(2A)-B(2)-H(2C)	113(3)
H(2B)-B(2)-H(2C)	117(3)
H(1C)-B(3)-H(3A)	116(3)
H(1C)-B(3)-H(3B)	94(2)
H(3A)-B(3)-H(3B)	94.9(5)
H(1C)-B(3)-H(3C)	95(3)
H(3A)-B(3)-H(3C)	142.1(7)

H(3B)-B(3)-H(3C)	103.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
P(1)	14(1)	26(1)	45(1)	-20(1)	0(1)	-2(1)
P(2)	15(1)	24(1)	45(1)	-19(1)	2(1)	-4(1)
B(1)	49(2)	39(2)	31(2)	-15(2)	1(2)	-25(2)
N(1)	16(1)	28(1)	38(2)	-19(1)	2(1)	-6(1)
N(2)	18(1)	28(1)	38(2)	-20(1)	3(1)	-7(1)
N(3)	19(1)	22(1)	31(1)	-11(1)	0(1)	-2(1)
N(4)	21(1)	20(1)	32(1)	-12(1)	0(1)	-5(1)
C(1)	15(1)	25(2)	30(2)	-14(1)	0(1)	-4(1)
C(2)	22(2)	30(2)	54(2)	-26(2)	4(2)	-8(1)
C(3)	23(2)	33(2)	51(2)	-29(2)	3(2)	-9(1)
C(4)	23(2)	34(2)	39(2)	-24(2)	8(1)	-9(1)
C(5)	20(2)	28(2)	42(2)	-22(2)	8(1)	-7(1)
C(6)	20(2)	43(2)	56(2)	-31(2)	11(2)	-10(2)
C(7)	31(2)	53(2)	55(2)	-31(2)	18(2)	-20(2)
C(8)	49(2)	52(2)	34(2)	-19(2)	9(2)	-21(2)
C(9)	30(2)	40(2)	43(2)	-24(2)	4(2)	-9(2)
C(10)	40(2)	55(2)	39(2)	-24(2)	4(2)	-17(2)
C(11)	42(2)	52(2)	57(3)	-12(2)	-6(2)	-11(2)
C(12)	55(3)	99(4)	62(3)	-51(3)	-1(2)	-20(3)
C(13)	16(2)	28(2)	50(2)	-21(2)	3(1)	-3(1)
C(14)	27(2)	30(2)	54(2)	-20(2)	-6(2)	-3(2)
C(15)	34(2)	30(2)	68(3)	-26(2)	0(2)	-7(2)
C(16)	14(1)	24(2)	39(2)	-17(1)	3(1)	-5(1)
C(17)	17(2)	22(2)	45(2)	-17(2)	2(1)	-6(1)
C(18)	19(2)	31(2)	41(2)	-19(2)	2(1)	-7(1)
C(19)	13(2)	31(2)	62(2)	-28(2)	7(2)	-6(1)
C(20)	15(2)	29(2)	51(2)	-18(2)	0(1)	-4(1)
C(21)	16(1)	26(2)	44(2)	-15(2)	0(1)	-6(1)
C(22)	19(2)	45(2)	45(2)	-13(2)	-3(2)	-12(2)
C(23)	46(2)	47(2)	50(2)	-26(2)	-6(2)	-4(2)
C(24)	47(2)	45(2)	49(2)	-12(2)	-10(2)	-14(2)
C(25)	16(2)	26(2)	42(2)	-15(2)	3(1)	-5(1)
C(26)	26(2)	40(2)	46(2)	-21(2)	-1(2)	-6(2)
C(27)	29(2)	26(2)	68(3)	-18(2)	-3(2)	-3(2)
C(28)	18(1)	23(2)	26(2)	-9(1)	3(1)	-5(1)
C(29)	29(2)	21(2)	39(2)	-14(2)	1(2)	-5(1)

C(30)	27(2)	21(2)	43(2)	-17(2)	1(1)	-7(1)
C(31)	15(1)	21(2)	41(2)	-15(2)	-3(1)	-2(1)
C(32)	20(2)	24(2)	44(2)	-20(2)	0(1)	-5(1)
C(33)	20(2)	26(2)	43(2)	-14(2)	-4(1)	-2(1)
C(34)	18(2)	28(2)	58(2)	-18(2)	-2(2)	-4(1)
C(35)	17(2)	28(2)	56(2)	-23(2)	2(2)	-5(1)
C(36)	22(2)	30(2)	45(2)	-22(2)	4(1)	-12(1)
C(37)	24(2)	43(2)	41(2)	-23(2)	5(2)	-15(2)
C(38)	41(2)	47(2)	43(2)	-21(2)	4(2)	-20(2)
C(39)	40(2)	54(2)	58(2)	-37(2)	15(2)	-20(2)
C(40)	23(2)	25(2)	35(2)	-16(1)	2(1)	-1(1)
C(41)	26(2)	30(2)	42(2)	-14(2)	2(2)	0(1)
C(42)	34(2)	39(2)	52(2)	-29(2)	-1(2)	-4(2)
C(43)	22(2)	22(2)	38(2)	-12(1)	-5(1)	-1(1)
C(44)	20(2)	18(2)	50(2)	-16(2)	-2(2)	1(1)
C(45)	28(2)	30(2)	58(2)	-18(2)	-9(2)	-4(2)
C(46)	42(2)	39(2)	45(2)	-14(2)	-18(2)	-5(2)
C(47)	39(2)	42(2)	37(2)	-14(2)	-5(2)	-9(2)
C(48)	30(2)	27(2)	38(2)	-12(2)	-2(2)	-5(1)
C(49)	37(2)	37(2)	34(2)	-11(2)	6(2)	-9(2)
C(50)	49(2)	63(3)	61(3)	-34(2)	21(2)	-25(2)
C(51)	45(2)	50(2)	48(2)	-19(2)	11(2)	-22(2)
C(52)	18(2)	28(2)	43(2)	-14(2)	0(1)	0(1)
C(53)	39(2)	42(2)	55(2)	-30(2)	9(2)	-8(2)
C(54)	29(2)	36(2)	64(3)	-23(2)	14(2)	-9(2)
O(1)	63(2)	63(2)	67(2)	-40(2)	10(2)	-20(2)
C(55)	106(4)	71(3)	67(3)	-41(3)	23(3)	-41(3)
C(56)	104(4)	75(4)	74(3)	-39(3)	33(3)	-41(3)
C(57)	63(3)	96(4)	90(4)	-66(3)	3(3)	-19(3)
C(58)	119(5)	109(5)	105(5)	-76(4)	56(4)	-69(4)
O(2)	39(2)	57(2)	87(2)	-26(2)	2(2)	-6(1)
C(59)	118(5)	61(3)	107(5)	-48(3)	56(4)	-48(3)
C(60)	254(14)	80(6)	203(11)	-81(7)	-41(10)	61(7)
C(61)	39(4)	412(19)	266(13)	-287(15)	-20(5)	28(7)
C(62)	59(4)	116(6)	101(5)	33(4)	-19(3)	-29(4)
B(2)	57(3)	39(3)	68(3)	-27(3)	4(3)	-17(2)
B(3)	101(6)	110(6)	71(4)	-30(4)	6(4)	-53(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(1A)	2160(20)	8320(20)	4730(20)	35(9)
H(1B)	2730(30)	6910(16)	4740(30)	63(13)
H(2)	1533	5222	3499	39
H(3)	3135	5187	2691	39
H(6)	6035	6463	2215	45
H(7)	5707	7608	763	53
H(8)	4135	8270	173	54
H(10)	2040	7557	1327	52
H(11A)	1186	9339	521	84
H(11B)	2199	9550	275	84
H(11C)	1818	9199	1263	84
H(12A)	1840	8042	-162	101
H(12B)	2869	7104	164	101
H(12C)	2851	8256	-401	101
H(13)	4233	5800	3870	38
H(14A)	5687	5427	4571	57
H(14B)	5239	6629	3938	57
H(14C)	6184	5880	3642	57
H(15A)	4876	4448	3399	65
H(15B)	5439	4111	4262	65
H(15C)	5959	4479	3331	65
H(18)	-497	6630	5827	36
H(19)	-1863	7929	4940	41
H(20)	-1749	8582	3437	39
H(22)	478	8081	2170	46
H(23A)	-33	6742	2330	73
H(23B)	-357	7696	1397	73
H(23C)	-1155	7524	2161	73
H(24A)	-794	9514	1232	74
H(24B)	-671	9706	2040	74
H(24C)	-1566	9381	2021	74
H(25)	1990	5606	5066	35
H(26A)	2102	5272	6539	57
H(26B)	938	5868	6568	57
H(26C)	1633	6490	5968	57
H(27A)	1797	4041	6151	65
H(27B)	1185	4455	5293	65
H(27C)	626	4620	6130	65
H(29)	2037	12006	2969	37

H(30)	3604	11066	3820	36
H(33)	5436	7431	6150	37
H(34)	6885	6936	5377	43
H(35)	6898	7695	3857	40
H(37)	4813	9230	2452	41
H(38A)	5451	10555	1604	63
H(38B)	6082	10245	2419	63
H(38C)	4903	10713	2446	63
H(39A)	6262	8828	1619	69
H(39B)	6263	7813	2476	69
H(39C)	6941	8418	2434	69
H(40)	3021	9254	5180	35
H(41A)	2786	8139	6655	55
H(41B)	3941	7467	6739	55
H(41C)	3274	7491	6087	55
H(42A)	3094	9747	6298	61
H(42B)	3779	10155	5492	61
H(42C)	4265	9157	6361	61
H(45)	-813	11546	1976	47
H(46)	-297	12039	522	53
H(47)	1340	11871	151	50
H(49)	3324	10823	1707	48
H(50A)	3414	10019	783	83
H(50B)	4119	10677	432	83
H(50C)	3080	11124	-33	83
H(51A)	3619	12327	667	73
H(51B)	2622	12658	1182	73
H(51C)	2572	12770	217	73
H(52)	814	10270	3876	40
H(53A)	180	12117	3461	68
H(53B)	-395	11544	4288	68
H(53C)	-894	12169	3342	68
H(54A)	-211	9517	3693	67
H(54B)	-1117	10595	3416	67
H(54C)	-696	9987	4390	67
H(55A)	5346	4835	1760	92
H(55B)	4516	5244	1053	92
H(56A)	5864	4298	490	100
H(56B)	6295	3438	1446	100
H(57A)	3616	3702	1576	91
H(57B)	4363	2683	2294	91
H(58A)	5476	2564	1259	116
H(58B)	4737	3600	544	116
H(59A)	7050	4819	1746	111
H(59B)	7138	5468	718	111
H(60A)	8339	4069	763	248
H(60B)	8473	3603	1803	248
H(61A)	9418	4795	493	258
H(61B)	9750	4069	1493	258
H(62A)	9154	5417	1817	146

H(62B)	8947	6152	792	146
H(1C)	1670(40)	4580(30)	1800(20)	120(20)
H(2A)	2220(30)	3710(30)	2940(20)	45(10)
H(2B)	1260(30)	3630(30)	2310(30)	60(12)
H(2C)	750(30)	4700(30)	2760(30)	64(13)
H(3A)	2332	5829	1087	150
H(3B)	2195	4937	619	150
H(3C)	775	5694	896	150

Computation of 2

All computations employed the Gaussian 94 and Gaussian03 programs:
For Gaussian 94: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Gill, P. M. W.; Johnson, B. G.; Robb, M. A.; Cheeseman, J. R.; Keith, T.; Petersson, G. A.; Montgomery, J. A.; Raghavachari, K.; Al-Laham, M. A.; Zakrzewski, V. G.; Ortiz, J. V.; Foresman, J. B.; Peng, C. Y.; Ayala, P. Y.; Chen, W.; Wong, M. W.; Andes, J. L.; Replogle, E. S.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Binkley, J. S.; Defrees, D. J.; Baker, J.; Stewart, J. J. P.; Head-Gordon, M.; Gonzalez, C.; Pople, J. A. Gaussian 94, Revision B.3; Gaussian Inc.: Pittsburgh, PA, 1995.
For Gaussian 03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr. J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision C.02; Gaussian, Inc.: Wallingford, CT, 2004.

The DFT computation of the simplified **2-H** cation model at the B3LYP/DZP level:

The optimized geometry of the simplified **2-H** cation model:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.898570	0.673000	0.351284
2	15	0	0.898570	-0.673000	0.351284
3	5	0	0.000000	0.000000	2.012120
4	7	0	-0.458027	3.468413	0.194565
5	7	0	1.168558	2.405327	-0.720730
6	7	0	-1.168558	-2.405327	-0.720730
7	7	0	0.458027	-3.468413	0.194565
8	6	0	0.000000	2.218745	-0.064033
9	6	0	0.415789	4.432162	-0.288861
10	6	0	1.451421	3.755595	-0.869878
11	6	0	0.000000	-2.218745	-0.064033

12	6	0	-1.451421	-3.755595	-0.869878
13	6	0	-0.415789	-4.432162	-0.288861
14	1	0	-0.719581	-0.753710	2.591986
15	1	0	0.719581	0.753710	2.591986
16	1	0	2.344194	4.117447	-1.360937
17	1	0	0.236471	5.492914	-0.179931
18	1	0	-0.236471	-5.492914	-0.179931
19	1	0	-2.344194	-4.117447	-1.360937
20	1	0	1.318410	-3.654709	0.700386
21	1	0	-1.745433	-1.627112	-1.031275
22	1	0	1.745433	1.627112	-1.031275
23	1	0	-1.318410	3.654709	0.700386