Inorganic Chemistry
including bioinorganic chemistry
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1. X-ray data for $P_2(tmpB)_2(GePh_2)$, 10

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{30} H_{46} B_2 Ge N_2 P_2$
Color; Habit	colorless, transparent prism
Crystal size (mm)	0.253 x 0.253 x 0.920
Crystal System	Orthorhombic
Space Group	$P2_12_12_1$
Unit Cell Dimensions	a = 8.586(2) Å
	b = 16.809(3) Å
	c = 22.240(4) Å
Volume	3209.7(11) $Å^3$
Z	4
Formula weight	590.8
Density(calc.)	1.223 Mg/m^3
Absorption Coefficient	1.075 mm^{-1}
F(000)	1248

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 50.0°
Scan Type	ω
Scan Speed	Variable; 8.00 to 32.00°/min. in ω
Scan Range (ω)	1.60°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections Observed standard intensity ratios showed no substantial changes during course of data collection; observed range was 1.03-.96. Intensities were scaled on standard intensity ratios.
Index Ranges	$-10 \leq h \leq 10$, $-19 \leq k \leq 19$ $-26 \leq l \leq 26$
Reflections Collected	6464
Independent Reflections	5651 (R_{int} = 1.61%)
Observed Reflections	3434 ($F > 2.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.8069 / 1.8957

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U set to 1.25U(equiv) of parent atom.
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0007F^2$
Number of Parameters Refined	334
Final R Indices (obs. data)	R = 6.25 %, wR = 6.00 % Rw = 5.50 %
R Indices (all data)	R = 9.83 %, wR = 6.44 %
Goodness-of-Fit	1.01
Largest and Mean Δ/σ	0.002, 0.000
Data-to-Parameter Ratio	10.3:1
Largest Difference Peak	1.06 eÅ^{-3}
Largest Difference Hole	-0.60 eÅ^{-3}

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2x10^3$)

	x	y	z	U(eq)
Ge	2018(1)	8468(1)	3826(1)	41(1)
P(1)	2115(3)	9683(1)	3326(1)	42(1)
P(2)	4630(3)	8773(1)	3971(1)	40(1)
B(1)	3497(11)	9800(6)	4025(4)	35(4)
B(2)	4123(14)	9177(6)	3156(5)	41(4)
N(1)	3704(9)	10447(4)	4424(3)	37(3)
N(2)	5068(10)	9147(4)	2629(3)	41(3)
C(1)	862(11)	8436(6)	4590(4)	38(3)
C(2)	-715(12)	8410(6)	4610(5)	55(4)
C(3)	-1513(13)	8398(6)	5151(5)	63(5)
C(4)	-650(15)	8417(7)	5685(5)	66(5)
C(5)	922(14)	8452(7)	5666(4)	61(4)
C(6)	1716(12)	8458(6)	5120(4)	53(4)
C(7)	1358(12)	7573(6)	3316(5)	49(4)
C(8)	541(12)	6944(6)	3554(5)	60(4)
C(9)	33(14)	6332(7)	3187(6)	79(5)
C(10)	352(16)	6347(8)	2579(7)	91(7)
C(11)	1188(16)	6950(8)	2348(6)	95(6)
C(12)	1680(15)	7581(6)	2701(5)	73(5)
C(13)	5170(13)	10537(6)	4772(5)	54(4)
C(14)	5416(14)	11415(6)	4958(5)	82(5)
C(15)	4089(15)	11782(7)	5297(5)	90(6)
C(16)	2549(13)	11413(6)	5143(4)	72(5)
C(17)	2447(11)	11064(6)	4501(4)	49(4)
C(18)	6592(12)	10333(7)	4400(5)	87(5)
C(19)	5143(15)	10001(6)	5329(5)	84(5)
C(20)	821(12)	10702(6)	4469(5)	67(5)
C(21)	2587(13)	11710(5)	4027(4)	79(5)
C(22)	6465(13)	8631(6)	2580(4)	56(5)
C(23)	6766(19)	8420(8)	1921(5)	126(7)
C(24)	6836(22)	9063(9)	1485(6)	153(9)
C(25)	6057(19)	9758(9)	1676(6)	154(9)
C(26)	4721(15)	9724(6)	2119(5)	63(5)
C(27)	6218(14)	7810(6)	2879(5)	82(5)
C(28)	7890(14)	9022(7)	2860(6)	102(6)
C(29)	3193(17)	9487(7)	1814(4)	104(6)

C(30)	4512(16)	10563(6)	2352(5)	87(6)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

Ge-P(1)	2.326 (3)
Ge-C(1)	1.969 (9)
P(1)-B(1)	1.966 (10)
P(2)-B(1)	1.985 (11)
B(1)-N(1)	1.415 (13)
N(1)-C(13)	1.486 (13)
N(2)-C(22)	1.484 (13)
C(1)-C(2)	1.356 (14)
C(2)-H(2)	0.960
C(3)-H(3)	0.960
C(4)-H(4)	0.960
C(5)-H(5)	0.960
C(6)-H(6)	0.960
C(7)-C(12)	1.395 (15)
C(8)-C(9)	1.384 (16)
C(9)-C(10)	1.379 (21)
C(10)-C(11)	1.344 (20)
C(11)-C(12)	1.386 (18)
C(13)-C(14)	1.548 (15)
C(13)-C(19)	1.532 (15)
C(14)-H(14B)	0.960
C(15)-H(15A)	0.960
C(15)-C(16)	1.501 (17)
C(16)-H(16B)	0.960
C(17)-C(20)	1.524 (14)
C(18)-H(18A)	0.960
C(18)-H(18C)	0.960
C(19)-H(19B)	0.960
C(20)-H(20A)	0.960
C(20)-H(20C)	0.960
C(21)-H(21B)	0.960
C(22)-C(23)	1.530 (15)
C(22)-C(28)	1.521 (16)
C(23)-H(23B)	0.960
C(24)-H(24A)	0.960
C(24)-C(25)	1.414 (22)
C(25)-H(25B)	0.960
Ge-P(2)	2.322 (3)
Ge-C(7)	1.968 (10)
P(1)-B(2)	1.958 (12)
P(2)-B(2)	1.983 (12)
B(2)-N(2)	1.426 (14)
N(1)-C(17)	1.507 (12)
N(2)-C(26)	1.522 (13)
C(1)-C(6)	1.389 (13)
C(2)-C(3)	1.385 (16)
C(3)-C(4)	1.399 (17)
C(4)-C(5)	1.352 (18)
C(5)-C(6)	1.392 (14)
C(7)-C(8)	1.376 (14)
C(8)-H(8)	0.960
C(9)-H(9)	0.960
C(10)-H(10)	0.960
C(11)-H(11)	0.960
C(12)-H(12)	0.960
C(13)-C(18)	1.514 (15)
C(14)-H(14A)	0.960
C(14)-C(15)	1.499 (17)
C(15)-H(15B)	0.960
C(16)-H(16A)	0.960
C(16)-C(17)	1.546 (14)
C(17)-C(21)	1.518 (13)
C(18)-H(18B)	0.960
C(19)-H(19A)	0.960
C(19)-H(19C)	0.960
C(20)-H(20B)	0.960
C(21)-H(21A)	0.960
C(21)-H(21C)	0.960
C(22)-C(27)	1.547 (14)
C(23)-H(23A)	0.960
C(23)-C(24)	1.454 (18)
C(24)-H(24B)	0.960
C(25)-H(25A)	0.960
C(25)-C(26)	1.513 (20)

C(26)-C(29)	1.530 (18)	C(26)-C(30)	1.513 (14)
C(27)-H(27A)	0.960	C(27)-H(27B)	0.960
C(27)-H(27C)	0.960	C(28)-H(28A)	0.960
C(28)-H(28B)	0.960	C(28)-H(28C)	0.960
C(29)-H(29A)	0.960	C(29)-H(29B)	0.960
C(29)-H(29C)	0.960	C(30)-H(30A)	0.960
C(30)-H(30B)	0.960	C(30)-H(30C)	0.960

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Table 3. Bond angles (^{o})

P(1)-Ge-P(2)	80.7(1)	P(1)-Ge-C(1)	117.1(3)
P(2)-Ge-C(1)	111.9(3)	P(1)-Ge-C(7)	113.9(3)
P(2)-Ge-C(7)	121.8(3)	C(1)-Ge-C(7)	109.4(4)
Ge-P(1)-B(1)	74.4(3)	Ge-P(1)-B(2)	75.1(3)
B(1)-P(1)-B(2)	70.4(5)	Ge-P(2)-B(1)	74.1(3)
Ge-P(2)-B(2)	74.7(4)	B(1)-P(2)-B(2)	69.5(4)
P(1)-B(1)-P(2)	99.3(5)	P(1)-B(1)-N(1)	130.4(7)
P(2)-B(1)-N(1)	130.2(7)	P(1)-B(2)-P(2)	99.5(5)
P(1)-B(2)-N(2)	132.4(8)	P(2)-B(2)-N(2)	127.8(8)
B(1)-N(1)-C(13)	120.8(8)	B(1)-N(1)-C(17)	120.7(7)
C(13)-N(1)-C(17)	118.5(7)	B(2)-N(2)-C(22)	122.8(8)
B(2)-N(2)-C(26)	118.6(8)	C(22)-N(2)-C(26)	118.4(8)
Ge-C(1)-C(2)	122.2(7)	Ge-C(1)-C(6)	117.8(7)
C(2)-C(1)-C(6)	120.0(9)	C(1)-C(2)-H(2)	119.2(6)
C(1)-C(2)-C(3)	121.6(10)	H(2)-C(2)-C(3)	119.2(6)
C(2)-C(3)-H(3)	120.8(6)	C(2)-C(3)-C(4)	118.3(10)
H(3)-C(3)-C(4)	120.9(7)	C(3)-C(4)-H(4)	119.9(7)
C(3)-C(4)-C(5)	120.3(11)	H(4)-C(4)-C(5)	119.9(6)
C(4)-C(5)-H(5)	119.5(6)	C(4)-C(5)-C(6)	121.0(10)
H(5)-C(5)-C(6)	119.5(6)	C(1)-C(6)-C(5)	118.8(10)
C(1)-C(6)-H(6)	120.6(6)	C(5)-C(6)-H(6)	120.6(6)
Ge-C(7)-C(8)	120.8(8)	Ge-C(7)-C(12)	120.0(7)
C(8)-C(7)-C(12)	119.1(9)	C(7)-C(8)-H(8)	119.9(6)
C(7)-C(8)-C(9)	120.2(10)	H(8)-C(8)-C(9)	119.9(7)
C(8)-C(9)-H(9)	119.9(7)	C(8)-C(9)-C(10)	120.2(11)
H(9)-C(9)-C(10)	119.9(7)	C(9)-C(10)-H(10)	120.2(7)
C(9)-C(10)-C(11)	119.6(13)	H(10)-C(10)-C(11)	120.2(9)
C(10)-C(11)-H(11)	119.2(9)	C(10)-C(11)-C(12)	121.6(13)
H(11)-C(11)-C(12)	119.2(7)	C(7)-C(12)-C(11)	119.2(10)
C(7)-C(12)-H(12)	120.4(6)	C(11)-C(12)-H(12)	120.4(7)
N(1)-C(13)-C(14)	110.7(8)	N(1)-C(13)-C(18)	112.0(8)
C(14)-C(13)-C(18)	104.6(9)	N(1)-C(13)-C(19)	110.4(8)
C(14)-C(13)-C(19)	110.3(9)	C(18)-C(13)-C(19)	108.7(9)
C(13)-C(14)-H(14A)	108.0(6)	C(13)-C(14)-H(14B)	108.1(6)
H(14A)-C(14)-H(14B)	109.5(1)	C(13)-C(14)-C(15)	115.0(9)
H(14A)-C(14)-C(15)	108.2(6)	H(14B)-C(14)-C(15)	108.0(7)

C(14)-C(15)-H(15A)	108.8(6)	C(14)-C(15)-H(15B)	108.6(6)
H(15A)-C(15)-H(15B)	109.5(1)	C(14)-C(15)-C(16)	112.6(9)
H(15A)-C(15)-C(16)	108.8(6)	H(15B)-C(15)-C(16)	108.6(6)
C(15)-C(16)-H(16A)	108.1(6)	C(15)-C(16)-H(16B)	108.2(6)
H(16A)-C(16)-H(16B)	109.5(1)	C(15)-C(16)-C(17)	114.7(9)
H(16A)-C(16)-C(17)	108.2(5)	H(16B)-C(16)-C(17)	108.1(5)
N(1)-C(17)-C(16)	109.0(8)	N(1)-C(17)-C(20)	112.1(8)
C(16)-C(17)-C(20)	104.3(8)	N(1)-C(17)-C(21)	110.9(8)
C(16)-C(17)-C(21)	111.4(8)	C(20)-C(17)-C(21)	109.0(8)
C(13)-C(18)-H(18A)	109.5(6)	C(13)-C(18)-H(18B)	109.5(6)
H(18A)-C(18)-H(18B)	109.5(1)	C(13)-C(18)-H(18C)	109.4(6)
H(18A)-C(18)-H(18C)	109.5(1)	H(18B)-C(18)-H(18C)	109.5(1)
C(13)-C(19)-H(19A)	109.5(6)	C(13)-C(19)-H(19B)	109.5(6)
H(19A)-C(19)-H(19B)	109.5(1)	C(13)-C(19)-H(19C)	109.5(5)
H(19A)-C(19)-H(19C)	109.5(1)	H(19B)-C(19)-H(19C)	109.5(1)
C(17)-C(20)-H(20A)	109.5(6)	C(17)-C(20)-H(20B)	109.5(5)
H(20A)-C(20)-H(20B)	109.5(1)	C(17)-C(20)-H(20C)	109.4(5)
H(20A)-C(20)-H(20C)	109.5(1)	H(20B)-C(20)-H(20C)	109.5(1)
C(17)-C(21)-H(21A)	109.5(6)	C(17)-C(21)-H(21B)	109.5(5)
H(21A)-C(21)-H(21B)	109.5(1)	C(17)-C(21)-H(21C)	109.5(5)
H(21A)-C(21)-H(21C)	109.5(1)	H(21B)-C(21)-H(21C)	109.5(1)
N(2)-C(22)-C(23)	110.0(9)	N(2)-C(22)-C(27)	112.3(9)
C(23)-C(22)-C(27)	103.2(9)	N(2)-C(22)-C(28)	111.6(9)
C(23)-C(22)-C(28)	110.9(10)	C(27)-C(22)-C(28)	108.7(9)
C(22)-C(23)-H(23A)	107.2(7)	C(22)-C(23)-H(23B)	107.2(7)
H(23A)-C(23)-H(23B)	109.5(1)	C(22)-C(23)-C(24)	118.3(11)
H(23A)-C(23)-C(24)	107.3(9)	H(23B)-C(23)-C(24)	107.1(9)
C(23)-C(24)-H(24A)	108.5(8)	C(23)-C(24)-H(24B)	108.6(10)
H(24A)-C(24)-H(24B)	109.5(1)	C(23)-C(24)-C(25)	113.2(12)
H(24A)-C(24)-C(25)	108.4(9)	H(24B)-C(24)-C(25)	108.7(10)
C(24)-C(25)-H(25A)	106.2(10)	C(24)-C(25)-H(25B)	106.5(8)
H(25A)-C(25)-H(25B)	109.5(1)	C(24)-C(25)-C(26)	121.6(13)
H(25A)-C(25)-C(26)	106.3(7)	H(25B)-C(25)-C(26)	106.5(7)
N(2)-C(26)-C(25)	111.2(10)	N(2)-C(26)-C(29)	109.4(9)
C(25)-C(26)-C(29)	111.8(10)	N(2)-C(26)-C(30)	111.3(8)
C(25)-C(26)-C(30)	106.0(10)	C(29)-C(26)-C(30)	107.0(10)
C(22)-C(27)-H(27A)	109.5(5)	C(22)-C(27)-H(27B)	109.5(6)
H(27A)-C(27)-H(27B)	109.5(1)	C(22)-C(27)-H(27C)	109.4(6)
H(27A)-C(27)-H(27C)	109.5(1)	H(27B)-C(27)-H(27C)	109.5(1)

C(22)-C(28)-H(28A)	109.5(6)	C(22)-C(28)-H(28B)	109.5(6)
H(28A)-C(28)-H(28B)	109.5(1)	C(22)-C(28)-H(28C)	109.5(6)
H(28A)-C(28)-H(28C)	109.5(1)	H(28B)-C(28)-H(28C)	109.5(1)
C(26)-C(29)-H(29A)	109.5(6)	C(26)-C(29)-H(29B)	109.5(6)
H(29A)-C(29)-H(29B)	109.5(1)	C(26)-C(29)-H(29C)	109.5(6)
H(29A)-C(29)-H(29C)	109.5(1)	H(29B)-C(29)-H(29C)	109.5(1)
C(26)-C(30)-H(30A)	109.5(7)	C(26)-C(30)-H(30B)	109.5(6)
H(30A)-C(30)-H(30B)	109.5(1)	C(26)-C(30)-H(30C)	109.5(7)
H(30A)-C(30)-H(30C)	109.5(1)	H(30B)-C(30)-H(30C)	109.5(1)

Table 4. Anisotropic displacement coefficients ($\AA^2 x10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ge	48(1)	38(1)	36(1)	-4(1)	0(1)	-2(1)
P(1)	47(2)	40(2)	40(1)	5(2)	-6(2)	1(1)
P(2)	44(2)	41(1)	36(2)	4(1)	-5(1)	2(1)
B(1)	25(6)	41(7)	38(7)	1(5)	-3(5)	12(6)
B(2)	48(8)	33(7)	40(7)	-11(6)	-11(6)	4(6)
N(1)	38(5)	34(5)	39(5)	-4(4)	-2(4)	-1(4)
N(2)	47(5)	41(5)	35(5)	8(4)	3(5)	5(4)
C(1)	46(6)	29(5)	40(6)	0(6)	8(5)	0(6)
C(2)	55(8)	53(7)	58(7)	-10(7)	3(6)	4(7)
C(3)	59(8)	48(7)	84(9)	-2(7)	23(7)	-6(8)
C(4)	85(10)	46(7)	67(9)	-13(9)	22(7)	0(7)
C(5)	83(9)	64(7)	37(7)	-20(9)	4(6)	-4(7)
C(6)	56(7)	50(6)	53(6)	-16(7)	8(6)	3(6)
C(7)	54(7)	35(6)	59(7)	-3(5)	-8(6)	-8(6)
C(8)	67(8)	50(7)	62(7)	-18(6)	-14(6)	3(6)
C(9)	85(10)	53(9)	100(10)	-16(7)	-36(9)	2(8)
C(10)	87(11)	68(10)	119(13)	-6(8)	-33(10)	-35(9)
C(11)	121(13)	90(10)	74(9)	-25(10)	-6(9)	-47(8)
C(12)	100(11)	69(8)	50(7)	-26(8)	4(8)	-15(6)
C(13)	47(7)	52(7)	62(8)	-16(6)	-2(6)	-9(6)
C(14)	81(9)	56(8)	108(10)	-12(8)	-31(8)	-27(8)
C(15)	94(11)	78(10)	98(10)	-4(9)	-27(9)	-40(8)
C(16)	102(12)	51(7)	62(7)	9(7)	6(6)	-14(6)
C(17)	56(8)	43(6)	48(6)	8(5)	10(6)	-4(5)
C(18)	49(8)	88(9)	125(11)	-22(7)	-30(8)	-11(9)
C(19)	118(11)	72(8)	61(8)	-2(8)	-39(8)	-5(7)
C(20)	58(8)	58(8)	85(9)	9(7)	18(8)	-22(7)
C(21)	122(12)	51(7)	64(7)	21(7)	5(7)	13(5)
C(22)	62(8)	55(8)	52(7)	2(6)	15(6)	4(6)
C(23)	196(16)	114(11)	68(8)	60(14)	51(10)	9(9)
C(24)	240(20)	126(13)	94(11)	71(15)	98(14)	48(10)
C(25)	223(19)	126(14)	113(12)	84(14)	107(13)	73(11)
C(26)	96(10)	53(7)	40(7)	17(7)	11(7)	11(6)
C(27)	108(11)	47(7)	90(9)	32(7)	22(8)	6(7)
C(28)	65(8)	109(10)	132(12)	8(10)	-4(10)	18(9)
C(29)	178(14)	81(9)	53(8)	16(11)	-53(10)	5(6)

C(30)	143(13)	42(7)	76(9)	-3(8)	-6(9)	20(6)

The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2x10^3$)

	x	y	z	U
H(2)	-1293	8401	4241	69
H(3)	-2630	8378	5160	79
H(4)	-1177	8403	6065	82
H(5)	1500	8475	6035	77
H(6)	2833	8476	5110	66
H(8)	323	6929	3978	75
H(9)	-543	5897	3355	99
H(10)	-21	5929	2322	114
H(11)	1451	6943	1928	119
H(12)	2236	8019	2524	91
H(14A)	5584	11721	4599	102
H(14B)	6327	11442	5208	102
H(15A)	4272	11718	5720	112
H(15B)	4046	12339	5202	112
H(16A)	2354	10991	5424	90
H(16B)	1758	11813	5183	90
H(18A)	6523	9791	4267	109
H(18B)	7513	10400	4639	109
H(18C)	6640	10679	4057	109
H(19A)	4246	10125	5569	105
H(19B)	6070	10087	5562	105
H(19C)	5096	9454	5206	105
H(20A)	663	10470	4079	83
H(20B)	57	11110	4535	83
H(20C)	718	10299	4772	83
H(21A)	3608	11941	4044	99
H(21B)	1820	12114	4101	99
H(21C)	2420	11484	3636	99
H(23A)	5949	8067	1797	157
H(23B)	7747	8146	1905	157
H(24A)	6362	8883	1118	192
H(24B)	7910	9190	1411	192
H(25A)	6836	10093	1856	192
H(25B)	5658	10009	1321	192
H(27A)	6018	7881	3301	102
H(27B)	7137	7491	2828	102

H(27C)	5347	7548	2695	102
H(28A)	8771	8675	2821	128
H(28B)	7695	9125	3278	128
H(28C)	8102	9515	2657	128
H(29A)	3280	8955	1660	130
H(29B)	2980	9847	1489	130
H(29C)	2360	9510	2102	130
H(30A)	3672	10575	2636	109
H(30B)	4279	10912	2022	109
H(30C)	5455	10735	2544	109

2. X-ray data for $P_2(tmpB)_2(GePh_2){\cdot}Cr(CO)_5$, 13

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{35}H_{46}B_2CrGeN_2O_5P_2$
Color; Habit	clear yellow prism
Crystal size (mm)	0.207 x 0.575 x 0.690
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 12.040(2) Å
	$\underline{b}$ = 19.862(4) Å
	$\underline{c}$ = 16.680(3) Å
	β = 104.06(3)°
Volume	3869.4(12) $Å^3$
Z	4
Formula weight	782.9
Density(calc.)	1.344 Mg/m^3
Absorption Coefficient	1.181 mm^{-1}
F(000)	1624

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 47.0°
Scan Type	ω
Scan Speed	Variable; 6.00 to 32.00°/min. in ω
Scan Range (ω)	1.60°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections Observed standard intensity ratios showed no substantial changes during course of data collection; observed range was 1.03-.93. Intensities were scaled on standard intensity ratios.
Index Ranges	$-13 \leq h \leq 13$, $-22 \leq k \leq 22$ $-18 \leq l \leq 18$
Reflections Collected	11367
Independent Reflections	5689 (R_{int} = 1.43%)
Observed Reflections	5231 ($F > 1.4\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.6664 / 1.0000

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U set to 1.25U(equiv) of parent atom.
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.00001F^2$
Number of Parameters Refined	433
Final R Indices (obs. data)	R = 5.40 %, wR = 2.48 % Rw = 3.11 %
R Indices (all data)	R = 6.01 %, wR = 2.51 %
Goodness-of-Fit	1.19
Largest and Mean Δ/σ	0.001, 0.000
Data-to-Parameter Ratio	12.1:1
Largest Difference Peak	0.73 $eÅ^{-3}$
Largest Difference Hole	-0.45 $eÅ^{-3}$

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\mathring{A}^2 \times 10^3$)

	x	y	z	U(eq)
Cr	25356(5)	3116(3)	11464(4)	427(3)
C(1)	22400(36)	7998(20)	1273(25)	519(19)
O(1)	20994(27)	10257(15)	-5103(17)	801(15)
C(2)	41249(38)	4082(23)	12084(27)	671(22)
O(2)	50620(27)	3857(18)	11900(23)	1122(19)
C(3)	28908(37)	-2066(21)	21193(25)	599(21)
O(3)	30924(31)	-5421(16)	26917(18)	991(18)
C(4)	9642(37)	1003(21)	10162(24)	547(20)
O(4)	480(26)	-757(17)	9243(19)	932(17)
C(5)	26094(37)	-4353(21)	5061(24)	550(20)
O(5)	26567(28)	-8926(14)	905(18)	836(16)
Ge	16058(4)	10953(2)	32468(2)	366(2)
C(6)	1079(32)	6808(18)	31044(24)	401(16)
C(7)	-6975(35)	7003(20)	23455(25)	555(19)
C(8)	-17759(37)	4403(22)	22591(28)	679(22)
C(9)	-20810(38)	1578(21)	29185(31)	661(23)
C(10)	-12947(39)	1285(20)	36765(28)	604(22)
C(11)	-2159(34)	3932(19)	37657(24)	467(18)
C(12)	26772(31)	7288(19)	42205(21)	366(16)
C(13)	27032(31)	498(19)	44220(23)	443(17)
C(14)	34472(34)	-1758(22)	51484(26)	563(20)
C(15)	41547(36)	2559(24)	56652(26)	625(22)
C(16)	41322(34)	9292(22)	54746(24)	584(20)
C(17)	34041(31)	11672(20)	47557(22)	481(17)
P(1)	22302(8)	12795(5)	20470(5)	316(4)
P(2)	16578(9)	22573(5)	32156(6)	373(4)
B(1)	11436(35)	20556(21)	20404(25)	341(18)
B(2)	30081(37)	20103(20)	27972(23)	316(17)
N(1)	4135(23)	24307(14)	14268(17)	334(12)
N(2)	40811(24)	23128(14)	29492(16)	337(12)
C(18)	5442(32)	24505(19)	5567(21)	400(16)
C(19)	1001(35)	31252(20)	1411(23)	638(20)
C(20)	-11213(37)	32963(25)	1372(26)	931(25)
C(21)	-15029(32)	29704(21)	8509(26)	718(22)
C(22)	-5240(34)	28693(21)	16383(25)	505(19)
C(23)	18273(29)	24327(18)	5551(19)	472(17)

C(24)	-763(31)	18637(19)	536(22)	647(19)
C(25)	-426(33)	35492(19)	19911(24)	708(22)
C(26)	-10846(30)	25115(22)	22467(25)	794(23)
C(27)	42945(32)	30176(19)	33071(23)	406(17)
C(28)	53190(35)	33438(20)	30638(25)	730(22)
C(29)	64265(39)	29502(24)	33055(35)	1126(31)
C(30)	62340(31)	21990(22)	33398(26)	715(22)
C(31)	50997(33)	19468(19)	27665(24)	426(17)
C(32)	32978(31)	34826(17)	29359(22)	594(19)
C(33)	44748(31)	30049(18)	42453(21)	630(20)
C(34)	50527(28)	12003(18)	29993(20)	492(17)
C(35)	51056(32)	20158(18)	18576(21)	617(20)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

Cr-C(1)	1.914 (4)	Cr-C(2)	1.901 (5)
Cr-C(3)	1.881 (4)	Cr-C(4)	1.898 (5)
Cr-C(5)	1.843 (4)	Cr-P(1)	2.521 (1)
C(1)-O(1)	1.129 (5)	C(2)-O(2)	1.137 (6)
C(3)-O(3)	1.141 (5)	C(4)-O(4)	1.131 (5)
C(5)-O(5)	1.152 (5)	Ge-C(6)	1.944 (4)
Ge-C(12)	1.953 (3)	Ge-P(1)	2.331 (1)
Ge-P(2)	2.310 (1)	C(6)-C(7)	1.396 (5)
C(6)-C(11)	1.380 (6)	C(7)-H(7A)	0.960
C(7)-C(8)	1.372 (6)	C(8)-H(8A)	0.960
C(8)-C(9)	1.362 (7)	C(9)-H(9A)	0.960
C(9)-C(10)	1.384 (6)	C(10)-H(10A)	0.960
C(10)-C(11)	1.375 (6)	C(11)-H(11A)	0.960
C(12)-C(13)	1.388 (5)	C(12)-C(17)	1.393 (5)
C(13)-H(13A)	0.960	C(13)-C(14)	1.394 (5)
C(14)-H(14A)	0.960	C(14)-C(15)	1.359 (6)
C(15)-H(15A)	0.960	C(15)-C(16)	1.373 (7)
C(16)-H(16A)	0.960	C(16)-C(17)	1.385 (5)
C(17)-H(17A)	0.960	P(1)-B(1)	2.020 (4)
P(1)-B(2)	1.995 (4)	P(2)-B(1)	1.949 (4)
P(2)-B(2)	1.980 (5)	B(1)-N(1)	1.392 (5)
B(2)-N(2)	1.391 (5)	N(1)-C(18)	1.498 (5)
N(1)-C(22)	1.533 (5)	N(2)-C(27)	1.519 (5)
N(2)-C(31)	1.519 (5)	C(18)-C(19)	1.543 (5)
C(18)-C(23)	1.546 (5)	C(18)-C(24)	1.522 (5)
C(19)-H(19A)	0.960	C(19)-H(19B)	0.960
C(19)-C(20)	1.508 (6)	C(20)-H(20A)	0.960
C(20)-H(20B)	0.960	C(20)-C(21)	1.521 (7)
C(21)-H(21A)	0.960	C(21)-H(21B)	0.960
C(21)-C(22)	1.550 (5)	C(22)-C(25)	1.530 (5)
C(22)-C(26)	1.524 (6)	C(23)-H(23A)	0.960
C(23)-H(23B)	0.960	C(23)-H(23C)	0.960
C(24)-H(24A)	0.960	C(24)-H(24B)	0.960
C(24)-H(24C)	0.960	C(25)-H(25A)	0.960
C(25)-H(25B)	0.960	C(25)-H(25C)	0.960
C(26)-H(26A)	0.960	C(26)-H(26B)	0.960
C(26)-H(26C)	0.960	C(27)-C(28)	1.533 (6)

C(27)-C(32)	1.522 (5)	C(27)-C(33)	1.527 (5)
C(28)-H(28A)	0.960	C(28)-H(28B)	0.960
C(28)-C(29)	1.514 (6)	C(29)-H(29A)	0.960
C(29)-H(29B)	0.960	C(29)-C(30)	1.513 (6)
C(30)-H(30A)	0.960	C(30)-H(30B)	0.960
C(30)-C(31)	1.548 (5)	C(31)-C(34)	1.537 (5)
C(31)-C(35)	1.524 (5)	C(32)-H(32A)	0.960
C(32)-H(32B)	0.960	C(32)-H(32C)	0.960
C(33)-H(33A)	0.960	C(33)-H(33B)	0.960
C(33)-H(33C)	0.960	C(34)-H(34A)	0.960
C(34)-H(34B)	0.960	C(34)-H(34C)	0.960
C(35)-H(35A)	0.960	C(35)-H(35B)	0.960
C(35)-H(35C)	0.960		

Table 3. Bond angles (°)

C(1)-Cr-C(2)	88.0(2)	C(1)-Cr-C(3)	176.1(2)
C(2)-Cr-C(3)	89.6(2)	C(1)-Cr-C(4)	92.6(2)
C(2)-Cr-C(4)	172.2(2)	C(3)-Cr-C(4)	89.4(2)
C(1)-Cr-C(5)	85.3(2)	C(2)-Cr-C(5)	85.6(2)
C(3)-Cr-C(5)	91.5(2)	C(4)-Cr-C(5)	86.7(2)
C(1)-Cr-P(1)	96.9(1)	C(2)-Cr-P(1)	100.4(1)
C(3)-Cr-P(1)	86.5(1)	C(4)-Cr-P(1)	87.2(1)
C(5)-Cr-P(1)	173.6(1)	Cr-C(1)-O(1)	172.5(4)
Cr-C(2)-O(2)	170.8(4)	Cr-C(3)-O(3)	177.4(4)
Cr-C(4)-O(4)	174.6(4)	Cr-C(5)-O(5)	178.4(4)
C(6)-Ge-C(12)	110.5(2)	C(6)-Ge-P(1)	116.4(1)
C(12)-Ge-P(1)	119.1(1)	C(6)-Ge-P(2)	116.7(1)
C(12)-Ge-P(2)	112.0(1)	P(1)-Ge-P(2)	78.9(1)
Ge-C(6)-C(7)	121.2(3)	Ge-C(6)-C(11)	120.8(3)
C(7)-C(6)-C(11)	117.9(4)	C(6)-C(7)-H(7A)	118.5(3)
C(6)-C(7)-C(8)	121.1(4)	H(7A)-C(7)-C(8)	120.4(3)
C(7)-C(8)-H(8A)	121.4(3)	C(7)-C(8)-C(9)	120.3(4)
H(8A)-C(8)-C(9)	118.3(2)	C(8)-C(9)-H(9A)	121.6(2)
C(8)-C(9)-C(10)	119.7(4)	H(9A)-C(9)-C(10)	118.6(3)
C(9)-C(10)-H(10A)	120.8(3)	C(9)-C(10)-C(11)	120.1(4)
H(10A)-C(10)-C(11)	119.2(2)	C(6)-C(11)-C(10)	121.0(3)
C(6)-C(11)-H(11A)	118.0(2)	C(10)-C(11)-H(11A)	121.1(2)
Ge-C(12)-C(13)	122.3(3)	Ge-C(12)-C(17)	119.0(3)
C(13)-C(12)-C(17)	118.6(3)	C(12)-C(13)-H(13A)	120.3(2)
C(12)-C(13)-C(14)	119.6(3)	H(13A)-C(13)-C(14)	120.1(2)
C(13)-C(14)-H(14A)	119.4(2)	C(13)-C(14)-C(15)	121.3(4)
H(14A)-C(14)-C(15)	119.2(3)	C(14)-C(15)-H(15A)	120.0(3)
C(14)-C(15)-C(16)	119.6(4)	H(15A)-C(15)-C(16)	120.4(2)
C(15)-C(16)-H(16A)	120.3(2)	C(15)-C(16)-C(17)	120.4(4)
H(16A)-C(16)-C(17)	119.4(2)	C(12)-C(17)-C(16)	120.6(4)
C(12)-C(17)-H(17A)	119.1(2)	C(16)-C(17)-H(17A)	120.3(2)
Cr-P(1)-Ge	121.1(1)	Cr-P(1)-B(1)	140.0(1)
Ge-P(1)-B(1)	77.3(1)	Cr-P(1)-B(2)	144.5(1)
Ge-P(1)-B(2)	77.1(1)	B(1)-P(1)-B(2)	69.7(2)
Ge-P(2)-B(1)	79.2(1)	Ge-P(2)-B(2)	77.8(1)
B(1)-P(2)-B(2)	71.5(2)	P(1)-B(1)-P(2)	96.0(2)

P(1)-B(1)-N(1)	134.8(3)	P(2)-B(1)-N(1)	128.2(3)
P(1)-B(2)-P(2)	95.8(2)	P(1)-B(2)-N(2)	134.6(3)
P(2)-B(2)-N(2)	129.4(3)	B(1)-N(1)-C(18)	122.0(3)
B(1)-N(1)-C(22)	120.2(3)	C(18)-N(1)-C(22)	117.7(3)
B(2)-N(2)-C(27)	122.0(3)	B(2)-N(2)-C(31)	121.1(3)
C(27)-N(2)-C(31)	116.9(3)	N(1)-C(18)-C(19)	110.6(3)
N(1)-C(18)-C(23)	110.0(3)	C(19)-C(18)-C(23)	104.9(3)
N(1)-C(18)-C(24)	111.2(3)	C(19)-C(18)-C(24)	110.3(3)
C(23)-C(18)-C(24)	109.8(3)	C(18)-C(19)-H(19A)	108.7(2)
C(18)-C(19)-H(19B)	107.2(2)	H(19A)-C(19)-H(19B)	107.5(1)
C(18)-C(19)-C(20)	115.4(4)	H(19A)-C(19)-C(20)	109.3(2)
H(19B)-C(19)-C(20)	108.5(2)	C(19)-C(20)-H(20A)	108.7(2)
C(19)-C(20)-H(20B)	108.8(2)	H(20A)-C(20)-H(20B)	107.9(1)
C(19)-C(20)-C(21)	112.4(3)	H(20A)-C(20)-C(21)	110.4(2)
H(20B)-C(20)-C(21)	108.6(2)	C(20)-C(21)-H(21A)	108.2(2)
C(20)-C(21)-H(21B)	109.1(2)	H(21A)-C(21)-H(21B)	107.9(1)
C(20)-C(21)-C(22)	114.0(3)	H(21A)-C(21)-C(22)	106.7(2)
H(21B)-C(21)-C(22)	110.7(2)	N(1)-C(22)-C(21)	109.2(3)
N(1)-C(22)-C(25)	111.0(3)	C(21)-C(22)-C(25)	110.5(3)
N(1)-C(22)-C(26)	111.0(3)	C(21)-C(22)-C(26)	104.8(3)
C(25)-C(22)-C(26)	110.1(3)	C(18)-C(23)-H(23A)	108.8(2)
C(18)-C(23)-H(23B)	112.0(2)	H(23A)-C(23)-H(23B)	109.5(1)
C(18)-C(23)-H(23C)	107.6(2)	H(23A)-C(23)-H(23C)	109.5(1)
H(23B)-C(23)-H(23C)	109.5(1)	C(18)-C(24)-H(24A)	108.9(2)
C(18)-C(24)-H(24B)	110.3(2)	H(24A)-C(24)-H(24B)	109.5(1)
C(18)-C(24)-H(24C)	109.2(2)	H(24A)-C(24)-H(24C)	109.5(1)
H(24B)-C(24)-H(24C)	109.5(1)	C(22)-C(25)-H(25A)	108.9(2)
C(22)-C(25)-H(25B)	109.2(2)	H(25A)-C(25)-H(25B)	109.5(1)
C(22)-C(25)-H(25C)	110.3(2)	H(25A)-C(25)-H(25C)	109.5(1)
H(25B)-C(25)-H(25C)	109.5(1)	C(22)-C(26)-H(26A)	109.4(2)
C(22)-C(26)-H(26B)	111.7(2)	H(26A)-C(26)-H(26B)	109.5(1)
C(22)-C(26)-H(26C)	107.3(2)	H(26A)-C(26)-H(26C)	109.5(1)
H(26B)-C(26)-H(26C)	109.5(1)	N(2)-C(27)-C(28)	110.8(3)
N(2)-C(27)-C(32)	111.0(3)	C(28)-C(27)-C(32)	104.0(3)
N(2)-C(27)-C(33)	110.8(3)	C(28)-C(27)-C(33)	110.8(3)
C(32)-C(27)-C(33)	109.2(3)	C(27)-C(28)-H(28A)	109.4(2)
C(27)-C(28)-H(28B)	107.5(2)	H(28A)-C(28)-H(28B)	108.0(1)
C(27)-C(28)-C(29)	115.1(4)	H(28A)-C(28)-C(29)	109.0(2)
H(28B)-C(28)-C(29)	107.6(3)	C(28)-C(29)-H(29A)	107.6(3)

C(28)-C(29)-H(29B)	110.8(3)
C(28)-C(29)-C(30)	112.7(4)
H(29B)-C(29)-C(30)	108.2(3)
C(29)-C(30)-H(30B)	108.8(3)
C(29)-C(30)-C(31)	114.6(3)
H(30B)-C(30)-C(31)	110.3(2)
N(2)-C(31)-C(34)	109.3(3)
N(2)-C(31)-C(35)	110.8(3)
C(34)-C(31)-C(35)	110.3(3)
C(27)-C(32)-H(32B)	110.8(2)
C(27)-C(32)-H(32C)	108.3(2)
H(32B)-C(32)-H(32C)	109.5(1)
C(27)-C(33)-H(33B)	110.2(2)
C(27)-C(33)-H(33C)	109.4(2)
H(33B)-C(33)-H(33C)	109.5(1)
C(31)-C(34)-H(34B)	110.6(2)
C(31)-C(34)-H(34C)	108.1(2)
H(34B)-C(34)-H(34C)	109.5(1)
C(31)-C(35)-H(35B)	109.1(2)
C(31)-C(35)-H(35C)	111.5(2)
H(35B)-C(35)-H(35C)	109.5(1)
H(29A)-C(29)-H(29B)	107.4(1)
H(29A)-C(29)-C(30)	109.9(2)
C(29)-C(30)-H(30A)	108.3(3)
H(30A)-C(30)-H(30B)	108.0(1)
H(30A)-C(30)-C(31)	106.7(2)
N(2)-C(31)-C(30)	110.8(3)
C(30)-C(31)-C(34)	103.7(3)
C(30)-C(31)-C(35)	111.6(3)
C(27)-C(32)-H(32A)	109.3(2)
H(32A)-C(32)-H(32B)	109.5(1)
H(32A)-C(32)-H(32C)	109.5(1)
C(27)-C(33)-H(33A)	108.8(2)
H(33A)-C(33)-H(33B)	109.5(1)
H(33A)-C(33)-H(33C)	109.5(1)
C(31)-C(34)-H(34A)	109.7(2)
H(34A)-C(34)-H(34B)	109.5(1)
H(34A)-C(34)-H(34C)	109.5(1)
C(31)-C(35)-H(35A)	107.8(2)
H(35A)-C(35)-H(35B)	109.5(1)
H(35A)-C(35)-H(35C)	109.5(1)

Table 4. Anisotropic displacement coefficients ($Å^2 x10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cr	456(5)	390(4)	428(4)	-6(4)	90(3)	-44(3)
C(1)	651(34)	465(30)	516(30)	-44(25)	287(27)	-60(24)
O(1)	1190(29)	760(24)	522(20)	-83(22)	342(21)	125(19)
C(2)	558(35)	684(35)	785(35)	-47(32)	188(30)	-324(27)
O(2)	451(22)	1281(33)	1699(37)	-94(25)	384(25)	-622(28)
C(3)	789(37)	436(32)	556(32)	200(27)	134(29)	-77(24)
O(3)	1572(36)	781(26)	599(23)	455(25)	226(24)	187(19)
C(4)	625(35)	524(31)	493(29)	-180(28)	138(28)	-145(23)
O(4)	663(25)	1257(32)	921(26)	-485(24)	281(22)	-374(22)
C(5)	711(34)	453(31)	495(30)	43(27)	166(25)	35(24)
O(5)	1195(30)	521(23)	793(24)	61(21)	242(21)	-218(18)
Ge	363(3)	395(3)	345(2)	-16(3)	95(2)	67(2)
C(6)	400(28)	347(25)	499(27)	3(22)	196(23)	-3(22)
C(7)	431(31)	710(33)	520(30)	-129(27)	110(25)	26(25)
C(8)	445(33)	830(39)	711(36)	-124(30)	39(27)	-134(30)
C(9)	499(35)	511(33)	1049(43)	-150(27)	338(34)	-173(32)
C(10)	620(36)	513(32)	790(37)	-68(28)	385(30)	21(28)
C(11)	421(29)	498(29)	520(28)	-25(25)	187(23)	14(23)
C(12)	373(27)	431(27)	347(24)	27(23)	189(21)	67(21)
C(13)	372(28)	462(29)	516(28)	58(23)	147(22)	125(23)
C(14)	504(32)	558(34)	655(33)	141(27)	192(26)	276(27)
C(15)	507(34)	834(42)	506(30)	114(31)	71(25)	203(30)
C(16)	551(33)	698(38)	453(29)	-7(28)	27(24)	23(26)
C(17)	565(30)	384(27)	466(26)	79(26)	74(23)	57(23)
P(1)	300(6)	334(6)	309(6)	6(5)	63(5)	19(5)
P(2)	417(7)	385(7)	344(6)	47(6)	142(5)	28(5)
B(1)	295(29)	333(28)	447(29)	-76(24)	190(24)	37(23)
B(2)	424(31)	282(26)	241(25)	85(25)	80(22)	128(21)
N(1)	234(19)	381(20)	381(20)	73(16)	66(16)	83(16)
N(2)	319(21)	318(20)	377(19)	-12(17)	87(16)	-75(16)
C(18)	382(28)	448(28)	345(24)	76(23)	38(21)	42(21)
C(19)	722(36)	713(35)	463(28)	207(29)	112(25)	263(25)
C(20)	733(38)	1178(46)	811(37)	491(38)	48(30)	341(35)
C(21)	398(30)	743(36)	986(39)	288(27)	114(29)	172(30)
C(22)	331(28)	576(32)	615(31)	138(25)	128(24)	130(25)
C(23)	576(30)	540(29)	321(24)	4(25)	153(21)	154(21)

C(24)	482(29)	786(35)	609(29)	-30(27)	6(23)	-87(27)
C(25)	600(34)	662(35)	851(36)	279(28)	156(28)	29(28)
C(26)	407(31)	1057(41)	1029(38)	291(29)	389(28)	293(33)
C(27)	363(27)	337(25)	526(28)	-49(22)	122(22)	-37(21)
C(28)	727(36)	543(32)	1046(38)	-286(32)	461(31)	-279(30)
C(29)	549(39)	760(41)	2174(66)	-280(35)	534(41)	-614(44)
C(30)	290(29)	818(40)	1012(39)	-48(27)	111(27)	-324(31)
C(31)	341(27)	386(26)	540(28)	-53(22)	88(23)	-92(22)
C(32)	698(33)	296(27)	795(32)	-34(25)	193(27)	22(23)
C(33)	760(35)	556(30)	558(30)	-64(27)	127(26)	-160(24)
C(34)	352(26)	514(29)	574(27)	88(25)	42(21)	17(24)
C(35)	734(34)	573(30)	667(31)	12(26)	412(27)	-43(25)

The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2x10^3$)

	x	y	z	U
H(7A)	-479	897	1881	69
H(8A)	-2331	449	1737	85
H(9A)	-2837	-18	2875	83
H(10A)	-1490	-79	4144	76
H(11A)	333	387	4290	58
H(13A)	2217	-264	4061	55
H(14A)	3464	-646	5286	70
H(15A)	4660	91	6163	78
H(16A)	4615	1240	5842	73
H(17A)	3404	1636	4615	60
H(19A)	185	3121	-416	80
H(19B)	589	3473	433	80
H(20A)	-1608	3157	-381	116
H(20B)	-1188	3776	179	116
H(21A)	-1799	2531	678	90
H(21B)	-2113	3232	973	90
H(23A)	2153	2019	803	59
H(23B)	1941	2467	7	59
H(23C)	2193	2806	881	59
H(24A)	-876	1889	44	81
H(24B)	17	1882	-501	81
H(24C)	233	1448	307	81
H(25A)	558	3473	2479	88
H(25B)	262	3782	1587	88
H(25C)	-634	3816	2129	88
H(26A)	-528	2447	2761	99
H(26B)	-1722	2762	2342	99
H(26C)	-1345	2081	2012	99
H(28A)	5442	3786	3300	91
H(28B)	5125	3390	2473	91
H(29A)	6841	3110	3837	141
H(29B)	6893	3033	2924	141
H(30A)	6209	2083	3894	89
H(30B)	6873	1969	3215	89
H(32A)	2616	3316	3069	74
H(32B)	3449	3932	3147	74

H(32C)	3194	3487	2347	74
H(33A)	5112	2716	4476	79
H(33B)	4631	3451	4467	79
H(33C)	3799	2833	4383	79
H(34A)	4380	995	2659	62
H(34B)	5720	967	2928	62
H(34C)	5022	1176	3568	62
H(35A)	4381	1857	1535	77
H(35B)	5198	2482	1735	77
H(35C)	5712	1757	1726	77

3. X-ray data for $P_2(tmpB)_2(GeMe_2)\cdot Cr(CO)_5$, 14

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{25}H_{42}B_2CrGeN_2O_5P_2$
Color; Habit	transparent, yellow chip
Crystal size (mm)	0.230 x 0.460 x 0.667
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 14.969(1) Å
	$\underline{b}$ = 12.011(1) Å
	$\underline{c}$ = 18.185(2) Å
	β = 97.95(1)°
Volume	3237.9(5) Å^3
	Cell determination used 54 reflections in 2θ range from 4.39° to 25.00°
Z	4
Formula weight	658.8
Density(calc.)	1.351 Mg/m^3
Absorption Coefficient	1.397 mm^{-1}
F(000)	1368

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 52.0°
Scan Type	ω
Scan Speed	Variable; 9.00 to 48.00°/min. in ω
Scan Range (ω)	2.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections Observed standard intensity ratios showed a 6.5% decline during the data collection; Intensities were scaled on standard intensity ratios.
Index Ranges	$-18 \leq h \leq 18$, $-14 \leq k \leq 14$ $-22 \leq l \leq 22$
Reflections Collected	13488
Independent Reflections	6360 (R_{int} = 1.73%)
Observed Reflections	3534 ($F > 2.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.7398 / 1.0000

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 52.0°
Scan Type	ω
Scan Speed	Variable; 9.00 to 48.00°/min. in ω
Scan Range (ω)	2.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections Observed standard intensity ratios showed a 6.5% decline during the data collection; Intensities were scaled on standard intensity ratios.
Index Ranges	$-18 \leq h \leq 18$, $-14 \leq k \leq 14$ $-22 \leq l \leq 22$
Reflections Collected	13488
Independent Reflections	6360 (R_{int} = 1.73%)
Observed Reflections	3534 ($F > 2.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.7398 / 1.0000

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Patterson Map Interpretation
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U set to 1.25U(equiv) of parent atom.
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0001F^2$
Number of Parameters Refined	343
Final R Indices (obs. data)	R = 4.24 %, wR = 3.29 % Rw = 3.32 %
R Indices (all data)	R = 8.94 %, wR = 3.96 %
Goodness-of-Fit	1.05
Largest and Mean Δ/σ	0.024, 0.004
Data-to-Parameter Ratio	10.3:1
Largest Difference Peak	0.43 eÅ^{-3}
Largest Difference Hole	-0.30 eÅ^{-3}

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2x10^3$)

	x	y	z	U(eq)
Ge	1758(1)	1610(1)	246(1)	56(1)
Cr	2184(1)	424(1)	2381(1)	55(1)
P(1)	2480(1)	1865(1)	1450(1)	45(1)
P(2)	2677(1)	3117(1)	109(1)	55(1)
O(1)	3913(3)	642(3)	3456(2)	89(2)
O(2)	408(3)	-41(4)	1411(2)	117(2)
O(3)	3109(3)	-1200(3)	1462(2)	93(2)
O(4)	1229(2)	1841(3)	3411(2)	101(2)
O(5)	1725(3)	-1473(3)	3324(2)	112(2)
N(1)	4390(2)	2145(3)	928(2)	41(1)
N(2)	1941(3)	4397(3)	1346(2)	64(2)
B(1)	3458(3)	2247(4)	855(2)	42(2)
B(2)	2243(3)	3422(5)	1071(3)	52(2)
C(1)	3277(3)	605(4)	3035(3)	63(2)
C(2)	1076(4)	165(4)	1771(3)	76(2)
C(3)	2758(3)	-568(4)	1803(3)	68(2)
C(4)	1592(3)	1361(4)	2999(3)	71(2)
C(5)	1908(4)	-737(5)	2957(3)	78(2)
C(6)	468(3)	1930(4)	73(2)	85(2)
C(7)	2016(3)	197(4)	-185(2)	80(2)
C(8)	4879(3)	2295(3)	258(2)	47(2)
C(9)	5759(3)	1644(4)	369(3)	68(2)
C(10)	6404(3)	1938(5)	1051(3)	89(2)
C(11)	5914(3)	2409(4)	1666(2)	71(2)
C(12)	4960(3)	1941(3)	1667(2)	48(2)
C(13)	5058(3)	3541(3)	131(2)	62(2)
C(14)	4334(3)	1807(3)	-443(2)	65(2)
C(15)	4570(3)	2601(4)	2270(2)	66(2)
C(16)	4986(3)	706(3)	1857(2)	64(2)
C(17)	1599(4)	4392(4)	2097(3)	82(3)
C(18)	1306(7)	5521(6)	2348(5)	211(6)
C(19)	1136(7)	6388(6)	1901(5)	160(5)
C(20)	1605(6)	6460(5)	1318(5)	186(6)
C(21)	1932(4)	5468(4)	907(3)	76(2)
C(22)	2339(4)	4001(5)	2693(3)	108(3)
C(23)	776(3)	3628(5)	2018(3)	99(3)

C(24)	2880(4)	5738(5)	774(4)	135(4)
C(25)	1313(4)	5326(5)	190(4)	144(4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

Ge-P(1)	2.324 (1)	Ge-P(2)	2.308 (1)
Ge-C(6)	1.951 (4)	Ge-C(7)	1.931 (5)
Cr-P(1)	2.503 (1)	Cr-C(1)	1.898 (5)
Cr-C(2)	1.889 (5)	Cr-C(3)	1.874 (5)
Cr-C(4)	1.895 (5)	Cr-C(5)	1.827 (6)
P(1)-B(1)	1.990 (5)	P(1)-B(2)	2.008 (6)
P(2)-B(1)	1.965 (5)	P(2)-B(2)	1.982 (5)
O(1)-C(1)	1.137 (6)	O(2)-C(2)	1.145 (6)
O(3)-C(3)	1.152 (6)	O(4)-C(4)	1.141 (6)
O(5)-C(5)	1.162 (7)	N(1)-B(1)	1.389 (6)
N(1)-C(8)	1.515 (5)	N(1)-C(12)	1.509 (5)
N(2)-B(2)	1.374 (7)	N(2)-C(17)	1.523 (7)
N(2)-C(21)	1.513 (7)	C(8)-C(9)	1.522 (6)
C(8)-C(13)	1.543 (6)	C(8)-C(14)	1.532 (5)
C(9)-C(10)	1.505 (6)	C(10)-C(11)	1.529 (7)
C(11)-C(12)	1.534 (6)	C(12)-C(15)	1.532 (6)
C(12)-C(16)	1.523 (6)	C(17)-C(18)	1.514 (10)
C(17)-C(22)	1.513 (8)	C(17)-C(23)	1.526 (8)
C(18)-C(19)	1.324 (11)	C(19)-C(20)	1.352 (14)
C(20)-C(21)	1.523 (10)	C(21)-C(24)	1.509 (8)
C(21)-C(25)	1.502 (8)		

Table 3. Bond angles (°)

P(1)-Ge-P(2)	78.0(1)	P(1)-Ge-C(6)	116.6(1)
P(2)-Ge-C(6)	114.8(2)	P(1)-Ge-C(7)	113.9(1)
P(2)-Ge-C(7)	119.3(2)	C(6)-Ge-C(7)	111.0(2)
P(1)-Cr-C(1)	97.3(2)	P(1)-Cr-C(2)	86.6(2)
C(1)-Cr-C(2)	176.1(2)	P(1)-Cr-C(3)	85.6(2)
C(1)-Cr-C(3)	90.1(2)	C(2)-Cr-C(3)	90.0(2)
P(1)-Cr-C(4)	97.6(2)	C(1)-Cr-C(4)	89.6(2)
C(2)-Cr-C(4)	90.1(2)	C(3)-Cr-C(4)	176.8(2)
P(1)-Cr-C(5)	172.6(2)	C(1)-Cr-C(5)	88.3(2)
C(2)-Cr-C(5)	87.8(2)	C(3)-Cr-C(5)	89.6(2)
C(4)-Cr-C(5)	87.2(2)	Ge-P(1)-Cr	116.3(1)
Ge-P(1)-B(1)	78.5(1)	Cr-P(1)-B(1)	137.7(1)
Ge-P(1)-B(2)	76.3(1)	Cr-P(1)-B(2)	146.8(2)
B(1)-P(1)-B(2)	73.0(2)	Ge-P(2)-B(1)	79.3(1)
Ge-P(2)-B(2)	77.1(2)	B(1)-P(2)-B(2)	74.0(2)
B(1)-N(1)-C(8)	120.3(3)	B(1)-N(1)-C(12)	122.4(3)
C(8)-N(1)-C(12)	117.3(3)	B(2)-N(2)-C(17)	119.5(4)
B(2)-N(2)-C(21)	120.7(4)	C(17)-N(2)-C(21)	119.8(4)
P(1)-B(1)-P(2)	94.9(2)	P(1)-B(1)-N(1)	137.1(3)
P(2)-B(1)-N(1)	127.3(3)	P(1)-B(2)-P(2)	93.8(2)
P(1)-B(2)-N(2)	136.0(4)	P(2)-B(2)-N(2)	130.1(4)
Cr-C(1)-O(1)	174.7(4)	Cr-C(2)-O(2)	176.9(5)
Cr-C(3)-O(3)	178.2(4)	Cr-C(4)-O(4)	173.7(5)
Cr-C(5)-O(5)	179.5(6)	N(1)-C(8)-C(9)	109.8(3)
N(1)-C(8)-C(13)	110.4(3)	C(9)-C(8)-C(13)	110.6(3)
N(1)-C(8)-C(14)	111.3(3)	C(9)-C(8)-C(14)	105.4(3)
C(13)-C(8)-C(14)	109.2(3)	C(8)-C(9)-C(10)	115.7(4)
C(9)-C(10)-C(11)	111.9(4)	C(10)-C(11)-C(12)	113.9(4)
N(1)-C(12)-C(11)	110.6(3)	N(1)-C(12)-C(15)	109.2(3)
C(11)-C(12)-C(15)	104.9(3)	N(1)-C(12)-C(16)	110.7(3)
C(11)-C(12)-C(16)	111.3(3)	C(15)-C(12)-C(16)	110.0(3)
N(2)-C(17)-C(18)	114.4(5)	N(2)-C(17)-C(22)	109.8(5)
C(18)-C(17)-C(22)	106.0(5)	N(2)-C(17)-C(23)	106.6(4)
C(18)-C(17)-C(23)	107.7(6)	C(22)-C(17)-C(23)	112.4(5)
C(17)-C(18)-C(19)	123.9(8)	C(18)-C(19)-C(20)	117.0(8)
C(19)-C(20)-C(21)	124.8(6)	N(2)-C(21)-C(20)	112.7(5)

N(2)-C(21)-C(24)	109.1(4)	C(20)-C(21)-C(24)	106.5(5)
N(2)-C(21)-C(25)	108.7(4)	C(20)-C(21)-C(25)	108.3(5)
C(24)-C(21)-C(25)	111.5(5)		

Table 4. Anisotropic displacement coefficients ($Å^2 x10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ge	53(1)	71(1)	43(1)	-3(1)	-2(1)	0(1)
Cr	61(1)	64(1)	40(1)	-7(1)	8(1)	5(1)
P(1)	45(1)	52(1)	38(1)	2(1)	4(1)	-2(1)
P(2)	53(1)	63(1)	50(1)	9(1)	7(1)	14(1)
O(1)	97(3)	100(3)	61(2)	1(3)	-19(2)	0(2)
O(2)	84(3)	181(4)	80(3)	-52(3)	-10(2)	1(3)
O(3)	116(3)	68(3)	98(3)	-10(2)	28(2)	-18(2)
O(4)	98(3)	148(4)	61(2)	29(3)	25(2)	-2(2)
O(5)	119(3)	117(3)	101(3)	-22(3)	26(3)	48(3)
N(1)	43(2)	33(2)	46(2)	0(2)	6(2)	-3(2)
N(2)	64(3)	50(3)	83(3)	12(2)	26(2)	2(2)
B(1)	52(3)	34(3)	39(3)	0(3)	5(3)	-10(2)
B(2)	35(3)	56(4)	65(3)	4(3)	3(3)	10(3)
C(1)	79(4)	59(4)	50(3)	4(3)	7(3)	-2(3)
C(2)	90(4)	92(4)	51(3)	-20(4)	23(3)	3(3)
C(3)	82(4)	57(4)	65(3)	-16(3)	13(3)	3(3)
C(4)	69(4)	100(5)	45(3)	4(3)	9(3)	13(3)
C(5)	83(4)	93(5)	60(3)	-9(4)	15(3)	12(3)
C(6)	50(3)	116(5)	82(4)	-7(3)	-13(3)	18(3)
C(7)	99(4)	86(4)	53(3)	-14(3)	8(3)	-16(3)
C(8)	49(3)	38(3)	56(3)	0(2)	17(2)	-4(2)
C(9)	60(3)	62(3)	90(4)	11(3)	30(3)	10(3)
C(10)	47(3)	121(5)	99(4)	12(4)	11(3)	17(4)
C(11)	51(3)	80(4)	77(4)	-7(3)	-8(3)	5(3)
C(12)	48(3)	46(3)	49(3)	4(2)	-2(2)	2(2)
C(13)	65(3)	51(3)	73(3)	-2(3)	20(3)	9(3)
C(14)	76(3)	63(3)	62(3)	3(3)	27(3)	-7(3)
C(15)	69(3)	72(4)	50(3)	1(3)	-16(3)	-13(3)
C(16)	69(3)	54(3)	66(3)	11(3)	3(3)	6(3)
C(17)	84(4)	60(4)	107(5)	17(3)	34(4)	-13(3)
C(18)	328(13)	98(7)	241(11)	97(8)	161(10)	6(7)
C(19)	209(9)	96(7)	188(9)	60(7)	71(7)	-34(6)
C(20)	242(10)	61(5)	283(12)	41(6)	140(9)	11(6)
C(21)	66(4)	56(4)	109(4)	11(3)	18(3)	1(4)
C(22)	128(6)	116(5)	78(4)	-14(5)	14(4)	-41(4)
C(23)	63(4)	141(6)	99(4)	31(4)	30(3)	22(4)

C(24)	116(6)	84(5)	214(7)	-25(4)	53(5)	14(5)
C(25)	138(6)	100(5)	180(7)	35(5)	-31(6)	57(5)

The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(6A)	355	2635	291	106
H(6B)	146	1356	293	106
H(6C)	267	1957	-452	106
H(7A)	2654	58	-93	100
H(7B)	1823	216	-711	100
H(7C)	1702	-385	35	100
H(9A)	6061	1771	-56	86
H(9B)	5614	868	398	86
H(10A)	6726	1280	1232	112
H(10B)	6823	2485	921	112
H(11A)	6263	2240	2136	89
H(11B)	5870	3202	1605	89
H(13A)	5399	3849	570	78
H(13B)	4494	3928	24	78
H(13C)	5393	3620	-280	78
H(14A)	3766	2186	-544	82
H(14B)	4232	1029	-370	82
H(14C)	4665	1902	-856	82
H(15A)	3968	2350	2301	82
H(15B)	4559	3379	2147	82
H(15C)	4940	2489	2739	82
H(16A)	5351	593	2328	80
H(16B)	5239	300	1480	80
H(16C)	4385	446	1882	80
H(18A)	1774	5758	2731	263
H(18B)	762	5391	2558	263
H(19A)	507	6368	1706	200
H(19B)	1262	7048	2195	200
H(20A)	1230	6884	948	232
H(20B)	2137	6880	1495	232
H(22A)	2550	3283	2560	134
H(22B)	2106	3948	3158	134
H(22C)	2829	4523	2738	134
H(23A)	537	3600	2481	124
H(23B)	950	2893	1887	124
H(23C)	325	3911	1638	124