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Table 1s. Crystal data for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

Identification code	bc61x
Empirical formula	$C_{36}H_{54}B_{30}$
Formula mass	811.09
Crystal size	0.04 x 0.28 x 0.28 mm
Crystal color, habit	white plate
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	
a = 7.3774(5) Å	α = 109.7368(6)°
b = 15.6765(10) Å	β = 96.4756(12)°
c = 22.645(2) Å	γ = 95.2715(11)°
Volume	2425.6(3) Å^3
Z	2
Density (calculated)	1.111 Mg·m^{-3}
Absorption coefficient	0.053 mm^{-1}
F(000)	840
Absorption correction	Semi-empirical from psi-scans
Max. and min. trans. coeff.	1.0000 and 0.5321

Table 2s. Data collection for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

Diffractometer	Siemens SMART CCD
Temperature	146(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
Cell measurement	
Reflections used	4077
θ range	$1.39 < \theta < 28.29$
θ range, data coll'n	$1.39 < \theta < 25.00$
Scan type	0.3° ω scans
Index ranges	$-9 \leq h \leq 9$, $-20 \leq k \leq 20$, $-29 \leq l \leq 14$
Reflections collected	12975
Independent reflections	8404 (R(int) = 0.0770)
Standard reflections	50 frames re-measured on completion
Stability of standards	no decay observed

Table 3s. Solution and refinement of bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

System for solution	Siemens SHELXTL[1,2]
Structure solution	direct
System for refinement	Siemens SHELXTL[1,2]
Hydrogen atoms	riding w/riding isotropic U
Data/ restraints/ parameters	8095 / 23 / 637
Final R indices[3] [I>2σ(I)]	R1 = 0.0952, wR2 = 0.2153
Reflections observed	5387
R indices (all data)	R1 = 0.1483, wR2 = 0.2784
Goodness-of-fit[4] on F^2	1.085
Largest diff. peak and hole	0.386 and -0.325 e·Å^{-3}

1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5 beta, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $$R1 = \frac{\sum \left| |Fo| - |Fc| \right|}{\sum |Fo|} \; ; \quad wR2 = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{\sum \left[w\left(Fo^2\right)^2 \right]}}$$

4) $$Goodness - of - Fit = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{(M - N)}}$$

where M is the number of reflections and N is the number of parameters refined.

Notes on the structure determination for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

A suitable crystal was selected and mounted with silicone grease in the 123 K N_2 cold stream of a Siemens SMART 3-circle goniometer. Indexing was determined after collection of three sets of twenty 0.3°(ω) scans. Least-squares refinement of final cell dimensions was performed using all reflections harvested during data collection. A hemisphere of data was collected. Equivalent reflections were merged and all data were corrected for Lorentz and polarization effects. Structure solution by direct methods in the centrosymmetric space group $P\bar{1}$ revealed most of the non-hydrogen structure. The asymmetric unit contains 1.5 carborane molecules as well as 1.5 benzene molecules. Inversion completes the fractional molecules.

Rotational disorder about the long axis of the molecule was observed in the phenyl ring C(3) to C(8). A second orientation was added to the model; refinement indicates occupancies of 0.46(4) and 0.54(4) for groups {C(4),C(5),C(7),C(8)} and {C(4'),C(5'),C(7'),C(8')}, respectively. The benzene molecules neatly cap the ends of the carboranes, with a contact distance of 2.45 Å from H(1C) to the ring centroid and 2.56 Å from H(18C) by translation.

The structure determination was performed using equipment acquired under National Science Foundation grant CHE-9505926. This equipment includes a Siemens SMART CCD diffractometer system, LT-2A low-temperature apparatus and Silicon Graphics Indigo2 XL workstation.

Table 4s. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
B(1)	-458(6)	7332(3)	-1554(2)	29(1)
B(2)	-265(5)	6199(3)	-2051(2)	27(1)
B(3)	-2145(6)	5455(3)	-1986(2)	30(1)
B(4)	-3496(5)	6126(3)	-1447(2)	27(1)
B(5)	-2442(6)	7290(3)	-1176(2)	30(1)
B(6)	-2541(6)	7645(3)	-1845(2)	30(1)
B(7)	-1191(6)	6975(3)	-2380(2)	31(1)
B(8)	-2243(6)	5810(3)	-2649(2)	30(1)
B(9)	-4221(6)	5766(3)	-2275(2)	32(1)
B(10)	-4396(6)	6898(3)	-1781(2)	30(1)
B(11)	9554(6)	5911(3)	3871(2)	30(1)
B(12)	11242(5)	6605(3)	3659(2)	29(1)
B(13)	10740(5)	7750(3)	3934(2)	30(1)
B(14)	8768(6)	7775(3)	4328(2)	29(1)
B(15)	8024(6)	6634(3)	4281(2)	29(1)
B(16)	9795(6)	6287(3)	4706(2)	35(1)
B(17)	11782(6)	6270(3)	4323(2)	33(1)
B(18)	12515(6)	7407(3)	4367(2)	35(1)
B(19)	10974(6)	8123(3)	4778(2)	30(1)
B(20)	9308(6)	7438(3)	4985(2)	33(1)
C(1)	-3508(5)	6694(2)	-2463(2)	29(1)
C(2)	-1123(5)	6409(2)	-1342(2)	26(1)
C(3)	30(4)	6300(2)	-780(2)	27(1)
C(6)	2196(4)	6223(3)	289(2)	31(1)
C(4)	1942(6)	6479(24)	-705(8)	59(8)
C(5)	3009(7)	6446(21)	-172(7)	45(5)
C(7)	284(6)	6049(18)	216(7)	32(5)
C(8)	-784(7)	6093(16)	-314(6)	25(4)
C(4')	1867(10)	6167(17)	-793(5)	37(4)
C(5')	2916(12)	6097(17)	-269(4)	40(4)
C(7')	349(10)	6339(15)	297(4)	31(4)
C(8')	-712(10)	6388(16)	-231(4)	32(4)
C(9)	3336(5)	6231(3)	855(2)	35(1)
C(10)	4297(5)	6279(3)	1332(2)	32(1)
C(11)	5446(5)	6394(2)	1916(2)	28(1)
C(12)	7188(5)	6091(2)	1914(2)	31(1)

C(13)	8304(5)	6230(2)	2475(2)	30(1)
C(14)	7759(5)	6672(2)	3058(2)	26(1)
C(15)	6017(5)	6957(2)	3062(2)	30(1)
C(16)	4892(5)	6822(2)	2497(2)	29(1)
C(17)	8994(5)	6839(2)	3674(2)	24(1)
C(18)	11523(5)	7198(3)	4954(2)	32(1)
B(21)	-431(6)	10370(3)	2188(2)	34(1)
B(22)	1040(6)	9608(3)	1772(2)	34(1)
B(23)	208(6)	8484(3)	1728(2)	30(1)
B(24)	-1770(6)	8549(3)	2122(2)	30(1)
B(25)	-2182(6)	9708(3)	2395(2)	32(1)
B(26)	-2666(6)	10048(3)	1733(2)	38(1)
B(27)	-677(6)	9986(3)	1345(2)	37(1)
B(28)	-287(6)	8819(3)	1069(2)	38(1)
B(29)	-2020(6)	8165(3)	1284(2)	36(1)
B(30)	-3477(6)	8925(3)	1694(2)	36(1)
C(19)	-2464(5)	9107(3)	1103(2)	38(1)
C(20)	41(5)	9434(2)	2379(2)	26(1)
C(21)	1264(5)	9598(2)	3001(2)	28(1)
C(22)	2989(5)	9294(3)	3007(2)	35(1)
C(23)	4089(5)	9430(3)	3574(2)	34(1)
C(24)	3516(5)	9859(2)	4151(2)	32(1)
C(25)	1803(6)	10173(3)	4142(2)	39(1)
C(26)	712(6)	10046(3)	3578(2)	37(1)
C(27)	4587(5)	9960(3)	4746(2)	35(1)
C(28)	-5392(6)	8097(3)	-3358(2)	48(1)
C(29)	-4207(6)	7655(3)	-3744(2)	50(1)
C(30)	-4604(6)	6719(3)	-4067(2)	51(1)
C(31)	-6198(6)	6231(3)	-4003(2)	45(1)
C(32)	-7377(6)	6685(3)	-3615(2)	43(1)
C(33)	-6983(6)	7618(3)	-3297(2)	44(1)
C(34)	-3493(6)	10596(3)	25(2)	48(1)
C(35)	-4695(6)	10879(3)	445(2)	48(1)
C(36)	-6220(6)	10273(3)	422(2)	49(1)

(') denotes second atom of a disordered group

Table 5s. Bond lengths [Å] for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

B(1)-C(2)	1.719(5)	B(1)-B(7)	1.764(6)
B(1)-B(6)	1.779(6)	B(1)-B(2)	1.781(6)
B(1)-B(5)	1.784(6)	B(2)-C(2)	1.730(5)
B(2)-B(7)	1.775(6)	B(2)-B(3)	1.780(6)
B(2)-B(8)	1.780(6)	B(3)-C(2)	1.733(5)
B(3)-B(8)	1.765(6)	B(3)-B(9)	1.771(6)
B(3)-B(4)	1.786(6)	B(4)-C(2)	1.735(5)
B(4)-B(9)	1.767(6)	B(4)-B(10)	1.770(6)
B(4)-B(5)	1.785(6)	B(5)-C(2)	1.725(5)
B(5)-B(10)	1.776(6)	B(5)-B(6)	1.780(7)
B(6)-C(1)	1.690(5)	B(6)-B(10)	1.769(6)
B(6)-B(7)	1.779(6)	B(7)-C(1)	1.699(5)
B(7)-B(8)	1.786(6)	B(8)-C(1)	1.703(5)
B(8)-B(9)	1.775(6)	B(9)-C(1)	1.704(6)
B(9)-B(10)	1.775(6)	B(10)-C(1)	1.688(6)
B(11)-C(17)	1.731(5)	B(11)-B(16)	1.763(6)
B(11)-B(17)	1.769(6)	B(11)-B(15)	1.784(6)
B(11)-B(12)	1.789(6)	B(12)-C(17)	1.733(5)
B(12)-B(18)	1.766(6)	B(12)-B(17)	1.768(7)
B(12)-B(13)	1.779(6)	B(13)-C(17)	1.722(5)
B(13)-B(18)	1.778(6)	B(13)-B(19)	1.783(6)
B(13)-B(14)	1.787(6)	B(14)-C(17)	1.734(5)
B(14)-B(19)	1.752(6)	B(14)-B(20)	1.758(7)
B(14)-B(15)	1.787(6)	B(15)-C(17)	1.728(5)
B(15)-B(20)	1.764(6)	B(15)-B(16)	1.769(6)
B(16)-C(18)	1.715(6)	B(16)-B(20)	1.784(6)
B(16)-B(17)	1.784(6)	B(17)-C(18)	1.704(6)
B(17)-B(18)	1.780(7)	B(18)-C(18)	1.696(6)
B(18)-B(19)	1.784(6)	B(19)-C(18)	1.699(6)
B(19)-B(20)	1.765(6)	B(20)-C(18)	1.714(6)
C(2)-C(3)	1.518(5)	C(3)-C(8')	1.383(4)
C(3)-C(8)	1.385(5)	C(3)-C(4')	1.392(4)
C(3)-C(4)	1.392(5)	C(6)-C(5)	1.387(5)
C(6)-C(5')	1.387(4)	C(6)-C(7)	1.391(4)
C(6)-C(7')	1.392(4)	C(6)-C(9)	1.446(5)
C(4)-C(5)	1.384(5)	C(7)-C(8)	1.385(5)
C(4')-C(5')	1.384(5)	C(7')-C(8')	1.382(5)
C(9)-C(10)	1.199(5)	C(10)-C(11)	1.434(5)
C(11)-C(16)	1.386(5)	C(11)-C(12)	1.411(5)
C(12)-C(13)	1.374(5)	C(13)-C(14)	1.391(5)
C(14)-C(15)	1.399(5)	C(14)-C(17)	1.505(5)
C(15)-C(16)	1.386(5)	B(21)-C(20)	1.716(6)

B(21)-B(26)	1.774(6)	B(21)-B(27)	1.779(7)
B(21)-B(25)	1.784(6)	B(21)-B(22)	1.789(6)
B(22)-C(20)	1.717(6)	B(22)-B(28)	1.766(6)
B(22)-B(27)	1.772(6)	B(22)-B(23)	1.777(6)
B(23)-C(20)	1.731(5)	B(23)-B(28)	1.754(7)
B(23)-B(29)	1.760(6)	B(23)-B(24)	1.786(6)
B(24)-C(20)	1.728(5)	B(24)-B(30)	1.765(7)
B(24)-B(29)	1.767(6)	B(24)-B(25)	1.777(6)
B(25)-C(20)	1.734(5)	B(25)-B(30)	1.752(6)
B(25)-B(26)	1.765(7)	B(26)-C(19)	1.704(6)
B(26)-B(30)	1.777(7)	B(26)-B(27)	1.787(7)
B(27)-C(19)	1.712(6)	B(27)-B(28)	1.786(7)
B(28)-C(19)	1.711(6)	B(28)-B(29)	1.777(6)
B(29)-C(19)	1.709(6)	B(29)-B(30)	1.775(6)
B(30)-C(19)	1.696(6)	C(20)-C(21)	1.514(5)
C(21)-C(26)	1.385(5)	C(21)-C(22)	1.400(5)
C(22)-C(23)	1.379(5)	C(23)-C(24)	1.386(5)
C(24)-C(25)	1.398(5)	C(24)-C(27)	1.434(5)
C(25)-C(26)	1.373(6)	C(27)-C(27)#1	1.202(8)
C(28)-C(29)	1.372(6)	C(28)-C(33)	1.380(6)
C(29)-C(30)	1.386(6)	C(30)-C(31)	1.392(6)
C(31)-C(32)	1.377(6)	C(32)-C(33)	1.380(6)
C(34)-C(35)	1.366(6)	C(34)-C(36)#2	1.375(6)
C(35)-C(36)	1.388(7)	C(36)-C(34)#2	1.375(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 -x-1,-y+2,-z

(') denotes second atom of a disordered group

Table 6s. Bond angles [°] for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

C(2)-B(1)-B(7)	105.6(3)	C(2)-B(1)-B(6)	105.4(3)
B(7)-B(1)-B(6)	60.3(2)	C(2)-B(1)-B(2)	59.2(2)
B(7)-B(1)-B(2)	60.1(2)	B(6)-B(1)-B(2)	108.4(3)
C(2)-B(1)-B(5)	59.0(2)	B(7)-B(1)-B(5)	108.3(3)
B(6)-B(1)-B(5)	59.9(2)	B(2)-B(1)-B(5)	108.4(3)
C(2)-B(2)-B(7)	104.6(3)	C(2)-B(2)-B(3)	59.1(2)
B(7)-B(2)-B(3)	107.6(3)	C(2)-B(2)-B(8)	104.9(3)
B(7)-B(2)-B(8)	60.3(2)	B(3)-B(2)-B(8)	59.4(2)
C(2)-B(2)-B(1)	58.6(2)	B(7)-B(2)-B(1)	59.5(2)
B(3)-B(2)-B(1)	107.7(3)	B(8)-B(2)-B(1)	107.6(3)
C(2)-B(3)-B(8)	105.5(3)	C(2)-B(3)-B(9)	105.2(3)
B(8)-B(3)-B(9)	60.3(2)	C(2)-B(3)-B(2)	59.0(2)
B(8)-B(3)-B(2)	60.3(2)	B(9)-B(3)-B(2)	108.5(3)
C(2)-B(3)-B(4)	59.1(2)	B(8)-B(3)-B(4)	108.0(3)
B(9)-B(3)-B(4)	59.6(2)	B(2)-B(3)-B(4)	108.3(3)
C(2)-B(4)-B(9)	105.3(3)	C(2)-B(4)-B(10)	104.9(3)
B(9)-B(4)-B(10)	60.3(2)	C(2)-B(4)-B(5)	58.7(2)
B(9)-B(4)-B(5)	108.3(3)	B(10)-B(4)-B(5)	60.0(2)
C(2)-B(4)-B(3)	58.9(2)	B(9)-B(4)-B(3)	59.8(2)
B(10)-B(4)-B(3)	107.7(3)	B(5)-B(4)-B(3)	107.8(3)
C(2)-B(5)-B(10)	105.0(3)	C(2)-B(5)-B(6)	105.1(3)
B(10)-B(5)-B(6)	59.7(2)	C(2)-B(5)-B(1)	58.6(2)
B(10)-B(5)-B(1)	107.4(3)	B(6)-B(5)-B(1)	59.9(2)
C(2)-B(5)-B(4)	59.2(2)	B(10)-B(5)-B(4)	59.6(2)
B(6)-B(5)-B(4)	107.6(3)	B(1)-B(5)-B(4)	107.7(3)
C(1)-B(6)-B(10)	58.3(2)	C(1)-B(6)-B(7)	58.6(2)
B(10)-B(6)-B(7)	107.9(3)	C(1)-B(6)-B(1)	103.7(3)
B(10)-B(6)-B(1)	107.9(3)	B(7)-B(6)-B(1)	59.4(2)
C(1)-B(6)-B(5)	104.1(3)	B(10)-B(6)-B(5)	60.1(2)
B(7)-B(6)-B(5)	107.8(3)	B(1)-B(6)-B(5)	60.2(2)
C(1)-B(7)-B(1)	104.0(3)	C(1)-B(7)-B(2)	104.3(3)
B(1)-B(7)-B(2)	60.4(2)	C(1)-B(7)-B(6)	58.1(2)
B(1)-B(7)-B(6)	60.3(2)	B(2)-B(7)-B(6)	108.7(3)
C(1)-B(7)-B(8)	58.4(2)	B(1)-B(7)-B(8)	108.1(3)
B(2)-B(7)-B(8)	60.0(2)	B(6)-B(7)-B(8)	107.9(3)
C(1)-B(8)-B(3)	104.1(3)	C(1)-B(8)-B(9)	58.6(2)
B(3)-B(8)-B(9)	60.0(2)	C(1)-B(8)-B(2)	103.9(3)
B(3)-B(8)-B(2)	60.3(2)	B(9)-B(8)-B(2)	108.3(3)
C(1)-B(8)-B(7)	58.2(2)	B(3)-B(8)-B(7)	107.8(3)
B(9)-B(8)-B(7)	107.9(3)	B(2)-B(8)-B(7)	59.7(2)
C(1)-B(9)-B(4)	103.8(3)	C(1)-B(9)-B(3)	103.8(3)
B(4)-B(9)-B(3)	60.6(2)	C(1)-B(9)-B(8)	58.6(2)

B(4)-B(9)-B(8)	108.4(3)	B(3)-B(9)-B(8)	59.7(2)
C(1)-B(9)-B(10)	58.0(2)	B(4)-B(9)-B(10)	60.0(2)
B(3)-B(9)-B(10)	108.1(3)	B(8)-B(9)-B(10)	107.8(3)
C(1)-B(10)-B(6)	58.5(2)	C(1)-B(10)-B(4)	104.4(3)
B(6)-B(10)-B(4)	108.7(3)	C(1)-B(10)-B(9)	58.9(2)
B(6)-B(10)-B(9)	108.5(3)	B(4)-B(10)-B(9)	59.8(2)
C(1)-B(10)-B(5)	104.4(3)	B(6)-B(10)-B(5)	60.3(2)
B(4)-B(10)-B(5)	60.4(2)	B(9)-B(10)-B(5)	108.3(3)
C(17)-B(11)-B(16)	105.3(3)	C(17)-B(11)-B(17)	105.2(3)
B(16)-B(11)-B(17)	60.7(2)	C(17)-B(11)-B(15)	58.9(2)
B(16)-B(11)-B(15)	59.8(2)	B(17)-B(11)-B(15)	108.3(3)
C(17)-B(11)-B(12)	59.0(2)	B(16)-B(11)-B(12)	108.2(3)
B(17)-B(11)-B(12)	59.6(2)	B(15)-B(11)-B(12)	108.0(3)
C(17)-B(12)-B(18)	105.1(3)	C(17)-B(12)-B(17)	105.1(3)
B(18)-B(12)-B(17)	60.5(3)	C(17)-B(12)-B(13)	58.7(2)
B(18)-B(12)-B(13)	60.2(2)	B(17)-B(12)-B(13)	108.6(3)
C(17)-B(12)-B(11)	58.8(2)	B(18)-B(12)-B(11)	107.9(3)
B(17)-B(12)-B(11)	59.6(2)	B(13)-B(12)-B(11)	107.9(3)
C(17)-B(13)-B(18)	105.0(3)	C(17)-B(13)-B(12)	59.3(2)
B(18)-B(13)-B(12)	59.5(2)	C(17)-B(13)-B(19)	104.4(3)
B(18)-B(13)-B(19)	60.1(2)	B(12)-B(13)-B(19)	107.5(3)
C(17)-B(13)-B(14)	59.2(2)	B(18)-B(13)-B(14)	107.3(3)
B(12)-B(13)-B(14)	108.3(3)	B(19)-B(13)-B(14)	58.8(2)
C(17)-B(14)-B(19)	105.2(3)	C(17)-B(14)-B(20)	105.0(3)
B(19)-B(14)-B(20)	60.4(2)	C(17)-B(14)-B(15)	58.7(2)
B(19)-B(14)-B(15)	108.0(3)	B(20)-B(14)-B(15)	59.7(2)
C(17)-B(14)-B(13)	58.5(2)	B(19)-B(14)-B(13)	60.5(2)
B(20)-B(14)-B(13)	108.6(3)	B(15)-B(14)-B(13)	107.7(3)
C(17)-B(15)-B(20)	105.1(3)	C(17)-B(15)-B(16)	105.2(3)
B(20)-B(15)-B(16)	60.7(2)	C(17)-B(15)-B(11)	59.0(2)
B(20)-B(15)-B(11)	108.0(3)	B(16)-B(15)-B(11)	59.5(2)
C(17)-B(15)-B(14)	59.1(2)	B(20)-B(15)-B(14)	59.4(2)
B(16)-B(15)-B(14)	108.0(3)	B(11)-B(15)-B(14)	108.1(3)
C(18)-B(16)-B(11)	104.0(3)	C(18)-B(16)-B(15)	104.1(3)
B(11)-B(16)-B(15)	60.7(2)	C(18)-B(16)-B(20)	58.6(2)
B(11)-B(16)-B(20)	108.0(3)	B(15)-B(16)-B(20)	59.5(2)
C(18)-B(16)-B(17)	58.2(2)	B(11)-B(16)-B(17)	59.8(3)
B(15)-B(16)-B(17)	108.2(3)	B(20)-B(16)-B(17)	107.8(3)
C(18)-B(17)-B(12)	104.0(3)	C(18)-B(17)-B(11)	104.2(3)
B(12)-B(17)-B(11)	60.8(2)	C(18)-B(17)-B(18)	58.2(2)
B(12)-B(17)-B(18)	59.7(3)	B(11)-B(17)-B(18)	108.2(3)
C(18)-B(17)-B(16)	58.8(2)	B(12)-B(17)-B(16)	108.2(3)
B(11)-B(17)-B(16)	59.5(3)	B(18)-B(17)-B(16)	107.9(3)
C(18)-B(18)-B(12)	104.4(3)	C(18)-B(18)-B(13)	104.6(3)
B(12)-B(18)-B(13)	60.3(2)	C(18)-B(18)-B(17)	58.6(2)

B(12)-B(18)-B(17)	59.8(3)	B(13)-B(18)-B(17)	108.1(3)
C(18)-B(18)-B(19)	58.4(2)	B(12)-B(18)-B(19)	108.0(3)
B(13)-B(18)-B(19)	60.1(2)	B(17)-B(18)-B(19)	107.8(3)
C(18)-B(19)-B(14)	105.1(3)	C(18)-B(19)-B(20)	59.3(2)
B(14)-B(19)-B(20)	60.0(3)	C(18)-B(19)-B(13)	104.3(3)
B(14)-B(19)-B(13)	60.7(2)	B(20)-B(19)-B(13)	108.5(3)
C(18)-B(19)-B(18)	58.2(2)	B(14)-B(19)-B(18)	108.6(3)
B(20)-B(19)-B(18)	108.4(3)	B(13)-B(19)-B(18)	59.8(2)
C(18)-B(20)-B(14)	104.2(3)	C(18)-B(20)-B(15)	104.3(3)
B(14)-B(20)-B(15)	61.0(2)	C(18)-B(20)-B(19)	58.5(2)
B(14)-B(20)-B(19)	59.6(2)	B(15)-B(20)-B(19)	108.4(3)
C(18)-B(20)-B(16)	58.7(2)	B(14)-B(20)-B(16)	108.6(3)
B(15)-B(20)-B(16)	59.8(2)	B(19)-B(20)-B(16)	108.1(3)
B(10)-C(1)-B(6)	63.2(2)	B(10)-C(1)-B(7)	115.8(3)
B(6)-C(1)-B(7)	63.3(2)	B(10)-C(1)-B(8)	115.6(3)
B(6)-C(1)-B(8)	116.3(3)	B(7)-C(1)-B(8)	63.4(2)
B(10)-C(1)-B(9)	63.1(2)	B(6)-C(1)-B(9)	116.0(3)
B(7)-C(1)-B(9)	115.6(3)	B(8)-C(1)-B(9)	62.8(2)
C(3)-C(2)-B(1)	117.9(3)	C(3)-C(2)-B(5)	116.6(3)
B(1)-C(2)-B(5)	62.4(2)	C(3)-C(2)-B(2)	119.7(3)
B(1)-C(2)-B(2)	62.2(2)	B(5)-C(2)-B(2)	113.7(3)
C(3)-C(2)-B(3)	120.4(3)	B(1)-C(2)-B(3)	112.8(3)
B(5)-C(2)-B(3)	113.2(3)	B(2)-C(2)-B(3)	61.9(2)
C(3)-C(2)-B(4)	118.5(3)	B(1)-C(2)-B(4)	113.1(3)
B(5)-C(2)-B(4)	62.1(2)	B(2)-C(2)-B(4)	113.1(3)
B(3)-C(2)-B(4)	62.0(2)	C(8')-C(3)-C(4')	119.2(3)
C(8)-C(3)-C(4)	119.2(3)	C(8')-C(3)-C(2)	119.9(3)
C(8)-C(3)-C(2)	121.2(3)	C(4')-C(3)-C(2)	120.8(3)
C(4)-C(3)-C(2)	119.4(3)	C(5)-C(6)-C(7)	119.1(3)
C(5')-C(6)-C(7')	118.9(3)	C(5)-C(6)-C(9)	119.6(3)
C(5')-C(6)-C(9)	120.8(3)	C(7)-C(6)-C(9)	121.2(4)
C(7')-C(6)-C(9)	120.4(3)	C(5)-C(4)-C(3)	120.2(4)
C(4)-C(5)-C(6)	120.6(4)	C(8)-C(7)-C(6)	120.2(5)
C(3)-C(8)-C(7)	120.7(4)	C(5')-C(4')-C(3)	120.2(3)
C(4')-C(5')-C(6)	120.6(3)	C(8')-C(7')-C(6)	120.3(3)
C(7')-C(8')-C(3)	120.6(3)	C(10)-C(9)-C(6)	177.1(4)
C(9)-C(10)-C(11)	176.6(4)	C(16)-C(11)-C(12)	118.2(3)
C(16)-C(11)-C(10)	121.0(3)	C(12)-C(11)-C(10)	120.7(3)
C(13)-C(12)-C(11)	120.4(4)	C(12)-C(13)-C(14)	121.4(3)
C(13)-C(14)-C(15)	118.5(3)	C(13)-C(14)-C(17)	121.4(3)
C(15)-C(14)-C(17)	120.1(3)	C(16)-C(15)-C(14)	120.3(4)
C(15)-C(16)-C(11)	121.3(3)	C(14)-C(17)-B(13)	118.3(3)
C(14)-C(17)-B(15)	118.2(3)	B(13)-C(17)-B(15)	113.6(3)
C(14)-C(17)-B(11)	119.0(3)	B(13)-C(17)-B(11)	113.4(3)
B(15)-C(17)-B(11)	62.1(2)	C(14)-C(17)-B(12)	119.3(3)

B(13)-C(17)-B(12)	62.0(2)	B(15)-C(17)-B(12)	113.2(3)
B(11)-C(17)-B(12)	62.2(2)	C(14)-C(17)-B(14)	118.2(3)
B(13)-C(17)-B(14)	62.3(2)	B(15)-C(17)-B(14)	62.1(2)
B(11)-C(17)-B(14)	113.0(3)	B(12)-C(17)-B(14)	112.9(3)
B(18)-C(18)-B(19)	63.4(3)	B(18)-C(18)-B(17)	63.1(3)
B(19)-C(18)-B(17)	115.5(3)	B(18)-C(18)-B(20)	115.1(3)
B(19)-C(18)-B(20)	62.3(2)	B(17)-C(18)-B(20)	115.0(3)
B(18)-C(18)-B(16)	115.3(3)	B(19)-C(18)-B(16)	114.6(3)
B(17)-C(18)-B(16)	62.9(3)	B(20)-C(18)-B(16)	62.7(2)
C(20)-B(21)-B(26)	105.3(3)	C(20)-B(21)-B(27)	104.9(3)
B(26)-B(21)-B(27)	60.4(3)	C(20)-B(21)-B(25)	59.3(2)
B(26)-B(21)-B(25)	59.5(3)	B(27)-B(21)-B(25)	107.8(3)
C(20)-B(21)-B(22)	58.6(2)	B(26)-B(21)-B(22)	107.9(3)
B(27)-B(21)-B(22)	59.6(3)	B(25)-B(21)-B(22)	107.8(3)
C(20)-B(22)-B(28)	105.1(3)	C(20)-B(22)-B(27)	105.1(3)
B(28)-B(22)-B(27)	60.6(3)	C(20)-B(22)-B(23)	59.4(2)
B(28)-B(22)-B(23)	59.3(3)	B(27)-B(22)-B(23)	108.1(3)
C(20)-B(22)-B(21)	58.6(2)	B(28)-B(22)-B(21)	108.2(3)
B(27)-B(22)-B(21)	59.9(3)	B(23)-B(22)-B(21)	108.1(3)
C(20)-B(23)-B(28)	105.0(3)	C(20)-B(23)-B(29)	105.1(3)
B(28)-B(23)-B(29)	60.7(3)	C(20)-B(23)-B(22)	58.6(2)
B(28)-B(23)-B(22)	60.0(3)	B(29)-B(23)-B(22)	108.5(3)
C(20)-B(23)-B(24)	58.8(2)	B(28)-B(23)-B(24)	108.3(3)
B(29)-B(23)-B(24)	59.8(2)	B(22)-B(23)-B(24)	107.9(3)
C(20)-B(24)-B(30)	104.7(3)	C(20)-B(24)-B(29)	104.9(3)
B(30)-B(24)-B(29)	60.3(3)	C(20)-B(24)-B(25)	59.3(2)
B(30)-B(24)-B(25)	59.3(2)	B(29)-B(24)-B(25)	107.9(3)
C(20)-B(24)-B(23)	59.0(2)	B(30)-B(24)-B(23)	107.5(3)
B(29)-B(24)-B(23)	59.4(2)	B(25)-B(24)-B(23)	108.2(3)
C(20)-B(25)-B(30)	105.1(3)	C(20)-B(25)-B(26)	104.9(3)
B(30)-B(25)-B(26)	60.7(3)	C(20)-B(25)-B(24)	58.9(2)
B(30)-B(25)-B(24)	60.0(3)	B(26)-B(25)-B(24)	108.7(3)
C(20)-B(25)-B(21)	58.4(2)	B(30)-B(25)-B(21)	108.3(3)
B(26)-B(25)-B(21)	60.0(3)	B(24)-B(25)-B(21)	108.0(3)
C(19)-B(26)-B(25)	103.9(3)	C(19)-B(26)-B(21)	104.3(3)
B(25)-B(26)-B(21)	60.5(3)	C(19)-B(26)-B(30)	58.3(3)
B(25)-B(26)-B(30)	59.3(3)	B(21)-B(26)-B(30)	107.7(3)
C(19)-B(26)-B(27)	58.7(3)	B(25)-B(26)-B(27)	108.2(3)
B(21)-B(26)-B(27)	59.9(3)	B(30)-B(26)-B(27)	107.7(3)
C(19)-B(27)-B(22)	104.0(3)	C(19)-B(27)-B(21)	103.8(3)
B(22)-B(27)-B(21)	60.5(3)	C(19)-B(27)-B(28)	58.5(2)
B(22)-B(27)-B(28)	59.5(3)	B(21)-B(27)-B(28)	107.8(3)
C(19)-B(27)-B(26)	58.2(3)	B(22)-B(27)-B(26)	108.0(3)
B(21)-B(27)-B(26)	59.7(3)	B(28)-B(27)-B(26)	107.7(3)
C(19)-B(28)-B(23)	104.4(3)	C(19)-B(28)-B(22)	104.3(3)

B(23)-B(28)-B(22)	60.6(3)	C(19)-B(28)-B(29)	58.7(3)
B(23)-B(28)-B(29)	59.8(3)	B(22)-B(28)-B(29)	108.3(3)
C(19)-B(28)-B(27)	58.6(3)	B(23)-B(28)-B(27)	108.5(3)
B(22)-B(28)-B(27)	59.9(3)	B(29)-B(28)-B(27)	108.2(3)
C(19)-B(29)-B(23)	104.2(3)	C(19)-B(29)-B(24)	104.2(3)
B(23)-B(29)-B(24)	60.9(2)	C(19)-B(29)-B(30)	58.2(3)
B(23)-B(29)-B(30)	108.3(3)	B(24)-B(29)-B(30)	59.8(3)
C(19)-B(29)-B(28)	58.7(2)	B(23)-B(29)-B(28)	59.4(3)
B(24)-B(29)-B(28)	108.2(3)	B(30)-B(29)-B(28)	107.8(3)
C(19)-B(30)-B(25)	104.8(3)	C(19)-B(30)-B(24)	104.8(3)
B(25)-B(30)-B(24)	60.7(2)	C(19)-B(30)-B(29)	58.9(3)
B(25)-B(30)-B(29)	108.6(3)	B(24)-B(30)-B(29)	59.9(3)
C(19)-B(30)-B(26)	58.7(3)	B(25)-B(30)-B(26)	60.0(3)
B(24)-B(30)-B(26)	108.7(3)	B(29)-B(30)-B(26)	108.6(3)
B(30)-C(19)-B(26)	63.0(3)	B(30)-C(19)-B(29)	62.8(3)
B(26)-C(19)-B(29)	115.3(3)	B(30)-C(19)-B(28)	114.8(3)
B(26)-C(19)-B(28)	115.2(3)	B(29)-C(19)-B(28)	62.6(3)
B(30)-C(19)-B(27)	115.2(3)	B(26)-C(19)-B(27)	63.1(3)
B(29)-C(19)-B(27)	115.0(3)	B(28)-C(19)-B(27)	62.9(3)
C(21)-C(20)-B(21)	118.0(3)	C(21)-C(20)-B(22)	118.2(3)
B(21)-C(20)-B(22)	62.8(3)	C(21)-C(20)-B(24)	118.7(3)
B(21)-C(20)-B(24)	113.5(3)	B(22)-C(20)-B(24)	113.5(3)
C(21)-C(20)-B(23)	118.7(3)	B(21)-C(20)-B(23)	113.7(3)
B(22)-C(20)-B(23)	62.1(2)	B(24)-C(20)-B(23)	62.2(2)
C(21)-C(20)-B(25)	118.8(3)	B(21)-C(20)-B(25)	62.3(2)
B(22)-C(20)-B(25)	113.6(3)	B(24)-C(20)-B(25)	61.8(2)
B(23)-C(20)-B(25)	112.9(3)	C(26)-C(21)-C(22)	118.2(4)
C(26)-C(21)-C(20)	121.3(3)	C(22)-C(21)-C(20)	120.5(3)
C(23)-C(22)-C(21)	120.5(4)	C(22)-C(23)-C(24)	121.3(4)
C(23)-C(24)-C(25)	118.0(4)	C(23)-C(24)-C(27)	122.3(4)
C(25)-C(24)-C(27)	119.8(4)	C(26)-C(25)-C(24)	120.9(4)
C(25)-C(26)-C(21)	121.2(4)	C(27)#1-C(27)-C(24)	177.1(6)
C(29)-C(28)-C(33)	120.4(4)	C(28)-C(29)-C(30)	119.6(4)
C(29)-C(30)-C(31)	120.2(4)	C(32)-C(31)-C(30)	119.5(4)
C(31)-C(32)-C(33)	120.1(4)	C(28)-C(33)-C(32)	120.2(4)
C(35)-C(34)-C(36)#2	121.1(4)	C(34)-C(35)-C(36)	119.2(4)
C(34)#2-C(36)-C(35)	119.7(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 -x-1,-y+2,-z

(') denotes second atom of a disordered group

Table 7s. Anisotropic displacement parameters [Å^2 x 10^3] for bis[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 5

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B(1)	22(2)	18(2)	41(3)	4(2)	4(2)	-3(2)
B(2)	16(2)	24(2)	38(2)	6(2)	7(2)	1(2)
B(3)	20(2)	18(2)	46(3)	5(2)	4(2)	-2(2)
B(4)	16(2)	27(2)	34(2)	7(2)	4(2)	-1(2)
B(5)	20(2)	23(2)	40(2)	4(2)	2(2)	5(2)
B(6)	24(2)	16(2)	43(3)	2(2)	4(2)	2(2)
B(7)	21(2)	26(2)	44(3)	9(2)	7(2)	-2(2)
B(8)	27(2)	23(2)	32(2)	1(2)	2(2)	7(2)
B(9)	25(2)	22(2)	42(3)	4(2)	6(2)	-1(2)
B(10)	18(2)	27(2)	40(2)	6(2)	2(2)	1(2)
B(11)	25(2)	19(2)	40(2)	6(2)	1(2)	5(2)
B(12)	14(2)	29(2)	35(2)	1(2)	1(2)	3(2)
B(13)	17(2)	26(2)	40(2)	6(2)	3(2)	-4(2)
B(14)	23(2)	19(2)	37(2)	1(2)	5(2)	5(2)
B(15)	23(2)	26(2)	34(2)	9(2)	7(2)	-1(2)
B(16)	32(2)	25(2)	50(3)	17(2)	2(2)	-1(2)
B(17)	25(2)	30(2)	38(2)	4(2)	1(2)	7(2)
B(18)	23(2)	32(2)	43(3)	5(2)	6(2)	2(2)
B(19)	20(2)	26(2)	38(2)	4(2)	1(2)	2(2)
B(20)	24(2)	32(2)	38(2)	7(2)	10(2)	4(2)
C(1)	24(2)	25(2)	34(2)	8(2)	-1(2)	4(2)
C(2)	15(2)	21(2)	35(2)	3(2)	4(2)	2(1)
C(3)	17(2)	23(2)	34(2)	3(2)	0(2)	1(1)
C(6)	25(2)	27(2)	35(2)	4(2)	-1(2)	1(2)
C(4)	24(8)	76(18)	83(13)	34(10)	8(7)	8(6)
C(5)	16(6)	61(14)	57(8)	22(8)	-2(5)	4(5)
C(7)	27(6)	25(11)	40(7)	12(6)	-8(5)	1(4)
C(8)	15(5)	5(9)	48(7)	3(5)	2(4)	-1(3)
C(4')	19(5)	64(12)	32(5)	21(6)	6(4)	3(4)
C(5')	17(5)	63(12)	48(6)	27(6)	8(4)	9(4)
C(7')	31(6)	28(10)	27(5)	0(5)	5(4)	7(3)
C(8')	30(5)	15(9)	40(5)	-6(4)	10(4)	6(3)
C(9)	26(2)	30(2)	44(2)	10(2)	3(2)	0(2)
C(10)	23(2)	25(2)	43(2)	10(2)	1(2)	-2(2)
C(11)	20(2)	21(2)	38(2)	8(2)	-3(2)	-5(1)
C(12)	29(2)	25(2)	35(2)	7(2)	0(2)	0(2)
C(13)	24(2)	25(2)	39(2)	6(2)	4(2)	5(2)
C(14)	19(2)	15(2)	40(2)	5(2)	-1(2)	-2(1)
C(15)	19(2)	26(2)	42(2)	10(2)	5(2)	0(2)

C(16)	15(2)	28(2)	42(2)	12(2)	0(2)	1(2)
C(17)	17(2)	19(2)	33(2)	5(2)	3(2)	0(1)
C(18)	26(2)	32(2)	35(2)	9(2)	1(2)	5(2)
B(21)	25(2)	28(2)	48(3)	12(2)	2(2)	4(2)
B(22)	21(2)	34(2)	46(3)	15(2)	2(2)	-2(2)
B(23)	22(2)	24(2)	40(2)	7(2)	2(2)	2(2)
B(24)	21(2)	23(2)	42(3)	10(2)	3(2)	-6(2)
B(25)	17(2)	31(2)	41(3)	7(2)	2(2)	1(2)
B(26)	24(2)	36(3)	50(3)	12(2)	2(2)	5(2)
B(27)	28(2)	39(3)	48(3)	22(2)	0(2)	1(2)
B(28)	23(2)	44(3)	43(3)	11(2)	3(2)	1(2)
B(29)	26(2)	33(2)	40(3)	6(2)	0(2)	-7(2)
B(30)	19(2)	40(3)	44(3)	10(2)	5(2)	-3(2)
C(19)	21(2)	47(3)	44(2)	17(2)	0(2)	1(2)
C(20)	20(2)	21(2)	35(2)	7(2)	4(2)	-2(1)
C(21)	23(2)	19(2)	38(2)	8(2)	1(2)	-3(2)
C(22)	21(2)	37(2)	41(2)	10(2)	3(2)	0(2)
C(23)	17(2)	39(2)	46(2)	17(2)	-2(2)	-4(2)
C(24)	25(2)	23(2)	43(2)	10(2)	-5(2)	-10(2)
C(25)	43(2)	24(2)	39(2)	0(2)	1(2)	8(2)
C(26)	34(2)	25(2)	43(2)	2(2)	-1(2)	12(2)
C(27)	31(2)	23(2)	44(2)	9(2)	-4(2)	-6(2)
C(28)	42(3)	31(2)	69(3)	13(2)	13(2)	0(2)
C(29)	40(3)	48(3)	60(3)	18(2)	13(2)	-5(2)
C(30)	40(3)	63(3)	48(3)	10(2)	14(2)	14(2)
C(31)	48(3)	33(2)	47(3)	8(2)	-2(2)	4(2)
C(32)	30(2)	40(2)	60(3)	21(2)	4(2)	-2(2)
C(33)	33(2)	42(3)	60(3)	18(2)	12(2)	10(2)
C(34)	33(2)	56(3)	51(3)	14(2)	3(2)	4(2)
C(35)	41(3)	43(3)	45(3)	-4(2)	-1(2)	11(2)
C(36)	36(2)	67(3)	42(3)	10(2)	12(2)	22(2)

(') denotes second atom of a disordered group

Table 8s. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for bis[4-(1,12-dicarba-closo-dodecaboran-1-yl)phenyl]acetylene, 5

	x	y	z	U_{eq}
H(1)	794(6)	7846(3)	-1312(2)	35
H(2)	1105(5)	5967(3)	-2136(2)	33
H(3)	-2003(6)	4733(3)	-2028(2)	36
H(4)	-4246(5)	5845(3)	-1135(2)	32
H(5)	-2497(6)	7773(3)	-686(2)	35
H(6)	-2692(6)	8365(3)	-1809(2)	36
H(7)	-451(6)	7257(3)	-2694(2)	37
H(8)	-2202(6)	5327(3)	-3140(2)	36
H(9)	-5473(6)	5253(3)	-2519(2)	38
H(10)	-5769(6)	7130(3)	-1701(2)	36
H(11)	9069(6)	5179(3)	3566(2)	36
H(12)	11868(5)	6330(3)	3216(2)	35
H(13)	11033(5)	8224(3)	3670(2)	36
H(14)	7771(6)	8272(3)	4325(2)	34
H(15)	6534(6)	6377(3)	4246(2)	34
H(16)	9500(6)	5810(3)	4967(2)	42
H(17)	12789(6)	5780(3)	4331(2)	40
H(18)	14006(6)	7667(3)	4407(2)	41
H(19)	11454(6)	8853(3)	5088(2)	36
H(20)	8692(6)	7714(3)	5430(2)	39
H(1C)	-4149(5)	6759(2)	-2835(2)	26
H(4)	2515(6)	6624(24)	-1021(8)	71
H(5)	4312(7)	6577(21)	-122(7)	54
H(7)	-289(6)	5900(18)	530(7)	38
H(8)	-2088(7)	5980(16)	-358(6)	30
H(4')	2401(10)	6124(17)	-1163(5)	45
H(5')	4140(12)	5961(17)	-293(4)	48
H(7')	-185(10)	6385(15)	667(4)	37
H(8')	-1963(10)	6483(16)	-217(4)	38
H(12A)	7590(5)	5788(2)	1522(2)	38
H(13A)	9473(5)	6021(2)	2466(2)	36
H(15A)	5603(5)	7244(2)	3455(2)	36
H(16A)	3720(5)	7027(2)	2507(2)	35
H(18C)	12053(5)	7184(3)	5357(2)	63
H(21)	104(6)	11095(3)	2495(2)	41
H(22)	2544(6)	9834(3)	1805(2)	41
H(23)	1164(6)	7970(3)	1732(2)	36
H(24)	-2109(6)	8082(3)	2386(2)	36
H(25)	-2802(6)	9999(3)	2838(2)	38

H(26)	-3625(6)	10559(3)	1724(2)	46
H(27)	-333(6)	10455(3)	1082(2)	45
H(28)	312(6)	8522(3)	623(2)	45
H(29)	-2561(6)	7439(3)	981(2)	43
H(30)	-4982(6)	8695(3)	1658(2)	43
H(19C)	-3022(5)	9082(3)	692(2)	68
H(22A)	3404(5)	8991(3)	2617(2)	41
H(23A)	5262(5)	9226(3)	3569(2)	41
H(25A)	1389(6)	10479(3)	4531(2)	46
H(26A)	-442(6)	10270(3)	3583(2)	44
H(28A)	-5115(6)	8736(3)	-3131(2)	58
H(29A)	-3122(6)	7988(3)	-3789(2)	60
H(30A)	-3786(6)	6410(3)	-4334(2)	62
H(31)	-6470(6)	5590(3)	-4224(2)	54
H(32)	-8463(6)	6355(3)	-3567(2)	52
H(33)	-7809(6)	7931(3)	-3036(2)	53
H(34)	-2441(6)	11006(3)	42(2)	58
H(35)	-4490(6)	11482(3)	749(2)	58
H(36)	-7062(6)	10458(3)	714(2)	59

(') denotes second atom of a disordered group

Table 9s. Crystal data for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

Identification code	bc57
Empirical formula	$C_{32}H_{40}B_{20}$
Formula mass	640.84
Crystal size	0.06 x 0.14 x 0.28 mm
Crystal color, habit	colorless plate
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	
a = 42.1080(6) Å	α = 90°
b = 7.36570(10) Å	β = 90
c = 11.64150(10) Å	γ = 90
Volume	3610.67(8) Å^3
Z	4
Density (calculated)	1.179 Mg·m^{-3}
Absorption coefficient	0.058 mm^{-1}
F(000)	1328
Absorption correction	None

Table 10s. Data collection for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

Diffractometer	Siemens PLATFORM/SMART
Temperature	123(2) K
Radiation source	sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
Cell measurement	
Reflections used	8192
θ range	$3 < \theta < 55$
θ range, data coll'n	0.97 to 28.32
Scan type	ω scans
Index ranges	$-55 \leq h \leq 51$, $-9 \leq k \leq 9$, $-14 \leq l \leq 15$
Reflections collected	24278
Independent reflections	8717 ($R_{int} = 0.0546$)
Standard reflections	50 frames re-measured on completion
Stability of standards	no decay observed

Table 11s. Solution and refinement of phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

System for solution	Siemens SHELXTL[1,2]
Structure solution	direct
System for refinement	Siemens SHELXTL[1,2]
Hydrogen atoms	riding, with riding isotropic U
Data/ restraints/ parameters	8712 / 0 / 469
Final R indices[3] [I>2σ(I)]	R1 = 0.0610, wR2 = 0.1228
Reflections observed	7248
R indices (all data)	R1 = 0.0818, wR2 = 0.1468
Goodness-of-fit[4] on F^2	1.134
Absolute structure parameter[5]	0(3)
Largest diff. peak and hole	0.233 and -0.253 eÅ^{-3}

1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5 beta, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $$R1 = \frac{\sum ||Fo| - |Fc||}{\sum |Fo|} \; ; \quad wR2 = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2\right]}{\sum \left[w\left(Fo^2\right)^2\right]}}$$

4) $$Goodness - of - Fit = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2\right]}{(M - N)}}$$

where M is the number of reflections and N is the number of parameters refined.

5) H D Flack, Acta Cryst. A39, 876-881 (1983)

Notes on the structure determination for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

A suitable crystal was selected and mounted with silicone grease in the 123 K N_2 cold stream of a Siemens SMART 3-circle goniometer. Indexing was determined after collection of three sets of twenty 0.3°(ω) scans. Least-squares refinement of final cell dimensions was performed using all reflections harvested during data collection. A hemisphere of data was collected. Equivalent reflections were merged and all data were corrected for Lorentz and polarization effects. No merging was performed on Friedel opposites. Structure solution by direct methods in the non-centrosymmetric space group $P2_12_12_1$ revealed most of the non-hydrogen structure.

Two crystallographically independent molecules comprise the asymmetric unit. Two packing motifs are present. The phenyl groups form parallel planes with an interplanar separation of 2.62 Å. Example molecules are B(1) to C(16) and B(11) to C(32) by symmetry operator

$$\frac{1}{2}-x,1-y,-\frac{3}{2}+z\,.$$

While the planes of the phenyl rings form close separations, the ring atoms are slipped so that π-stacking does not appear to be present. Closest contact is H(16A) to H(31A) at 2.56 Å.

The second motif observed is reminiscent of the herringbone pattern of benzene. Here C(5) is 3.03 Å from H(15A) of a neighbor generated by

$$\frac{1}{2}-x,-y,\frac{1}{2}+z\,.$$

Another close approach to C(5) is made by H(23A), 2.85 Å, by

$$x,y,-1+z\,.$$

The structure determination was performed using equipment acquired under National Science Foundation grant CHE-9505926. This equipment includes a Siemens SMART CCD diffractometer system, LT-2A low-temperature apparatus and Silicon Graphics Indigo2 XL workstation.

Table 12s. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	X	y	z	U_{eq}
B(1)	754(1)	5093(4)	1116(2)	21(1)
B(2)	663(1)	2961(4)	478(2)	20(1)
B(3)	746(1)	1224(4)	1505(2)	20(1)
B(4)	886(1)	2294(4)	2783(2)	20(1)
B(5)	889(1)	4680(4)	2543(2)	21(1)
B(6)	496(1)	5402(4)	2297(3)	22(1)
B(7)	356(1)	4340(4)	1023(3)	23(1)
B(8)	350(1)	1946(4)	1256(2)	23(1)
B(9)	488(1)	1531(4)	2683(2)	21(1)
B(10)	577(1)	3674(4)	3326(2)	21(1)
C(1)	971(1)	3177(3)	1444(2)	17(1)
C(2)	279(1)	3446(4)	2348(2)	23(1)
C(3)	1308(1)	3023(3)	1008(2)	18(1)
C(4)	1565(1)	3686(3)	1638(2)	21(1)
C(5)	1874(1)	3538(3)	1222(2)	23(1)
C(6)	1932(1)	2729(3)	160(2)	21(1)
C(7)	1676(1)	2053(3)	-464(2)	22(1)
C(8)	1370(1)	2191(3)	-46(2)	22(1)
C(9)	2248(1)	2558(3)	-298(2)	23(1)
C(10)	2503(1)	2362(3)	-736(2)	24(1)
C(11)	2808(1)	2116(3)	-1269(2)	21(1)
C(12)	3084(1)	2677(3)	-715(2)	22(1)
C(13)	3377(1)	2418(3)	-1231(2)	25(1)
C(14)	3397(1)	1627(3)	-2306(2)	27(1)
C(15)	3125(1)	1086(3)	-2870(2)	26(1)
C(16)	2830(1)	1302(3)	-2352(2)	24(1)
B(11)	863(1)	6762(4)	6205(2)	22(1)
B(12)	754(1)	6495(4)	7676(2)	21(1)
B(13)	735(1)	8686(4)	8308(2)	20(1)
B(14)	834(1)	10314(4)	7239(2)	20(1)
B(15)	910(1)	9122(4)	5943(2)	20(1)
B(16)	560(1)	8005(4)	5517(2)	23(1)
B(17)	540(1)	10203(4)	6153(3)	22(1)
B(18)	434(1)	9933(4)	7622(3)	23(1)
B(19)	384(1)	7570(4)	7893(2)	23(1)
B(20)	461(1)	6374(4)	6590(3)	24(1)
C(17)	1009(1)	8202(3)	7254(2)	17(1)
C(18)	297(1)	8495(4)	6586(2)	23(1)
C(19)	1351(1)	8060(3)	7640(2)	18(1)
C(20)	1601(1)	8705(3)	6972(2)	21(1)

C(21)	1913(1)	8594(3)	7362(2)	23(1)
C(22)	1980(1)	7833(3)	8432(2)	22(1)
C(23)	1729(1)	7190(3)	9100(2)	24(1)
C(24)	1420(1)	7293(3)	8707(2)	21(1)
C(25)	2297(1)	7672(3)	8880(2)	25(1)
C(26)	2546(1)	7461(3)	9355(2)	25(1)
C(27)	2830(1)	7158(3)	10010(2)	21(1)
C(28)	3131(1)	7530(3)	9564(2)	23(1)
C(29)	3399(1)	7173(4)	10214(2)	26(1)
C(30)	3370(1)	6496(4)	11320(2)	27(1)
C(31)	3073(1)	6152(3)	11780(2)	25(1)
C(32)	2804(1)	6465(3)	11126(2)	23(1)

Table 13s. Bond lengths [Å] for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

B(1)-C(1)	1.725(4)	B(1)-B(6)	1.767(4)
B(1)-B(7)	1.768(4)	B(1)-B(2)	1.779(4)
B(1)-B(5)	1.782(4)	B(2)-C(1)	1.724(3)
B(2)-B(7)	1.762(4)	B(2)-B(8)	1.766(4)
B(2)-B(3)	1.786(4)	B(3)-C(1)	1.723(4)
B(3)-B(9)	1.767(4)	B(3)-B(8)	1.776(4)
B(3)-B(4)	1.784(4)	B(4)-C(1)	1.727(3)
B(4)-B(10)	1.769(4)	B(4)-B(9)	1.773(4)
B(4)-B(5)	1.779(4)	B(5)-C(1)	1.727(4)
B(5)-B(6)	1.759(4)	B(5)-B(10)	1.761(4)
B(6)-C(2)	1.708(4)	B(6)-B(7)	1.778(4)
B(6)-B(10)	1.780(4)	B(7)-C(2)	1.708(4)
B(7)-B(8)	1.784(4)	B(8)-C(2)	1.711(4)
B(8)-B(9)	1.786(4)	B(9)-C(2)	1.708(4)
B(9)-B(10)	1.787(4)	B(10)-C(2)	1.703(4)
C(1)-C(3)	1.510(3)	C(3)-C(4)	1.396(3)
C(3)-C(8)	1.396(3)	C(4)-C(5)	1.391(3)
C(5)-C(6)	1.394(3)	C(6)-C(7)	1.393(3)
C(6)-C(9)	1.439(3)	C(7)-C(8)	1.384(3)
C(9)-C(10)	1.195(3)	C(10)-C(11)	1.440(3)
C(11)-C(12)	1.391(3)	C(11)-C(16)	1.399(4)
C(12)-C(13)	1.388(3)	C(13)-C(14)	1.383(4)
C(14)-C(15)	1.381(4)	C(15)-C(16)	1.391(4)
B(11)-C(17)	1.730(4)	B(11)-B(16)	1.765(4)
B(11)-B(20)	1.775(4)	B(11)-B(15)	1.776(4)
B(11)-B(12)	1.783(4)	B(12)-C(17)	1.723(4)
B(12)-B(19)	1.767(4)	B(12)-B(20)	1.769(4)
B(12)-B(13)	1.776(4)	B(13)-C(17)	1.720(4)
B(13)-B(18)	1.759(4)	B(13)-B(19)	1.760(4)
B(13)-B(14)	1.778(4)	B(14)-C(17)	1.722(4)
B(14)-B(18)	1.766(4)	B(14)-B(17)	1.771(4)
B(14)-B(15)	1.775(4)	B(15)-C(17)	1.722(4)
B(15)-B(16)	1.761(4)	B(15)-B(17)	1.767(4)
B(16)-C(18)	1.703(4)	B(16)-B(17)	1.782(4)
B(16)-B(20)	1.783(4)	B(17)-C(18)	1.698(4)
B(17)-B(18)	1.780(4)	B(18)-C(18)	1.706(4)
B(18)-B(19)	1.781(4)	B(19)-C(18)	1.707(4)
B(19)-B(20)	1.784(4)	B(20)-C(18)	1.708(4)
C(17)-C(19)	1.512(3)	C(19)-C(20)	1.391(3)
C(19)-C(24)	1.395(3)	C(20)-C(21)	1.393(3)
C(21)-C(22)	1.395(3)	C(22)-C(23)	1.396(3)
C(22)-C(25)	1.439(3)	C(23)-C(24)	1.381(3)
C(25)-C(26)	1.197(3)	C(26)-C(27)	1.435(3)

C(27)-C(28)	1.394(3)	C(27)-C(32)	1.400(4)
C(28)-C(29)	1.386(3)	C(29)-C(30)	1.385(4)
C(30)-C(31)	1.386(4)	C(31)-C(32)	1.382(3)

Table 14s. Bond angles [°] for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

C(1)-B(1)-B(6)	105.0(2)	C(1)-B(1)-B(7)	105.0(2)
B(6)-B(1)-B(7)	60.4(2)	C(1)-B(1)-B(2)	58.9(2)
B(6)-B(1)-B(2)	107.8(2)	B(7)-B(1)-B(2)	59.6(2)
C(1)-B(1)-B(5)	59.0(2)	B(6)-B(1)-B(5)	59.4(2)
B(7)-B(1)-B(5)	107.7(2)	B(2)-B(1)-B(5)	107.8(2)
C(1)-B(2)-B(7)	105.3(2)	C(1)-B(2)-B(8)	105.4(2)
B(7)-B(2)-B(8)	60.8(2)	C(1)-B(2)-B(1)	59.0(2)
B(7)-B(2)-B(1)	59.9(2)	B(8)-B(2)-B(1)	108.7(2)
C(1)-B(2)-B(3)	58.8(2)	B(7)-B(2)-B(3)	108.4(2)
B(8)-B(2)-B(3)	60.0(2)	B(1)-B(2)-B(3)	108.1(2)
C(1)-B(3)-B(9)	105.3(2)	C(1)-B(3)-B(8)	105.1(2)
B(9)-B(3)-B(8)	60.5(2)	C(1)-B(3)-B(4)	59.0(2)
B(9)-B(3)-B(4)	59.9(2)	B(8)-B(3)-B(4)	108.3(2)
C(1)-B(3)-B(2)	58.83(14)	B(9)-B(3)-B(2)	107.9(2)
B(8)-B(3)-B(2)	59.5(2)	B(4)-B(3)-B(2)	107.9(2)
C(1)-B(4)-B(10)	105.0(2)	C(1)-B(4)-B(9)	104.9(2)
B(10)-B(4)-B(9)	60.6(2)	C(1)-B(4)-B(5)	59.0(2)
B(10)-B(4)-B(5)	59.5(2)	B(9)-B(4)-B(5)	108.0(2)
C(1)-B(4)-B(3)	58.77(14)	B(10)-B(4)-B(3)	108.0(2)
B(9)-B(4)-B(3)	59.6(2)	B(5)-B(4)-B(3)	107.9(2)
C(1)-B(5)-B(6)	105.2(2)	C(1)-B(5)-B(10)	105.3(2)
B(6)-B(5)-B(10)	60.7(2)	C(1)-B(5)-B(4)	59.0(2)
B(6)-B(5)-B(4)	108.6(2)	B(10)-B(5)-B(4)	59.9(2)
C(1)-B(5)-B(1)	58.9(2)	B(6)-B(5)-B(1)	59.9(2)
B(10)-B(5)-B(1)	108.5(2)	B(4)-B(5)-B(1)	108.3(2)
C(2)-B(6)-B(5)	104.1(2)	C(2)-B(6)-B(1)	104.3(2)
B(5)-B(6)-B(1)	60.7(2)	C(2)-B(6)-B(7)	58.6(2)
B(5)-B(6)-B(7)	108.3(2)	B(1)-B(6)-B(7)	59.8(2)
C(2)-B(6)-B(10)	58.4(2)	B(5)-B(6)-B(10)	59.7(2)
B(1)-B(6)-B(10)	108.3(2)	B(7)-B(6)-B(10)	108.0(2)
C(2)-B(7)-B(2)	104.1(2)	C(2)-B(7)-B(1)	104.3(2)
B(2)-B(7)-B(1)	60.5(2)	C(2)-B(7)-B(6)	58.6(2)
B(2)-B(7)-B(6)	108.1(2)	B(1)-B(7)-B(6)	59.8(2)
C(2)-B(7)-B(8)	58.6(2)	B(2)-B(7)-B(8)	59.7(2)
B(1)-B(7)-B(8)	108.3(2)	B(6)-B(7)-B(8)	108.2(2)
C(2)-B(8)-B(2)	103.8(2)	C(2)-B(8)-B(3)	103.7(2)
B(2)-B(8)-B(3)	60.5(2)	C(2)-B(8)-B(7)	58.5(2)
B(2)-B(8)-B(7)	59.5(2)	B(3)-B(8)-B(7)	107.9(2)
C(2)-B(8)-B(9)	58.4(2)	B(2)-B(8)-B(9)	107.9(2)
B(3)-B(8)-B(9)	59.5(2)	B(7)-B(8)-B(9)	107.8(2)
C(2)-B(9)-B(3)	104.2(2)	C(2)-B(9)-B(4)	103.9(2)
B(3)-B(9)-B(4)	60.5(2)	C(2)-B(9)-B(8)	58.6(2)
B(3)-B(9)-B(8)	60.0(2)	B(4)-B(9)-B(8)	108.3(2)

C(2)-B(9)-B(10)	58.3(2)	B(3)-B(9)-B(10)	108.0(2)
B(4)-B(9)-B(10)	59.6(2)	B(8)-B(9)-B(10)	107.8(2)
C(2)-B(10)-B(5)	104.2(2)	C(2)-B(10)-B(4)	104.3(2)
B(5)-B(10)-B(4)	60.5(2)	C(2)-B(10)-B(6)	58.7(2)
B(5)-B(10)-B(6)	59.6(2)	B(4)-B(10)-B(6)	108.1(2)
C(2)-B(10)-B(9)	58.6(2)	B(5)-B(10)-B(9)	108.2(2)
B(4)-B(10)-B(9)	59.8(2)	B(6)-B(10)-B(9)	108.1(2)
C(3)-C(1)-B(3)	117.8(2)	C(3)-C(1)-B(2)	118.7(2)
B(3)-C(1)-B(2)	62.4(2)	C(3)-C(1)-B(1)	119.0(2)
B(3)-C(1)-B(1)	113.6(2)	B(2)-C(1)-B(1)	62.1(2)
C(3)-C(1)-B(4)	118.1(2)	B(3)-C(1)-B(4)	62.3(2)
B(2)-C(1)-B(4)	113.4(2)	B(1)-C(1)-B(4)	113.5(2)
C(3)-C(1)-B(5)	119.1(2)	B(3)-C(1)-B(5)	113.2(2)
B(2)-C(1)-B(5)	113.0(2)	B(1)-C(1)-B(5)	62.2(2)
B(4)-C(1)-B(5)	62.0(2)	B(10)-C(2)-B(7)	115.1(2)
B(10)-C(2)-B(6)	62.9(2)	B(7)-C(2)-B(6)	62.7(2)
B(10)-C(2)-B(9)	63.2(2)	B(7)-C(2)-B(9)	115.2(2)
B(6)-C(2)-B(9)	115.4(2)	B(10)-C(2)-B(8)	115.5(2)
B(7)-C(2)-B(8)	62.9(2)	B(6)-C(2)-B(8)	115.2(2)
B(9)-C(2)-B(8)	63.0(2)	C(4)-C(3)-C(8)	118.1(2)
C(4)-C(3)-C(1)	121.7(2)	C(8)-C(3)-C(1)	120.2(2)
C(5)-C(4)-C(3)	121.0(2)	C(4)-C(5)-C(6)	120.5(2)
C(7)-C(6)-C(5)	118.6(2)	C(7)-C(6)-C(9)	119.4(2)
C(5)-C(6)-C(9)	122.0(2)	C(8)-C(7)-C(6)	120.8(2)
C(7)-C(8)-C(3)	121.0(2)	C(10)-C(9)-C(6)	175.9(3)
C(9)-C(10)-C(11)	179.5(3)	C(12)-C(11)-C(16)	119.4(2)
C(12)-C(11)-C(10)	120.5(2)	C(16)-C(11)-C(10)	120.0(2)
C(13)-C(12)-C(11)	120.1(2)	C(14)-C(13)-C(12)	120.3(2)
C(15)-C(14)-C(13)	120.1(2)	C(14)-C(15)-C(16)	120.2(2)
C(15)-C(16)-C(11)	119.8(2)	C(17)-B(11)-B(16)	105.0(2)
C(17)-B(11)-B(20)	105.0(2)	B(16)-B(11)-B(20)	60.5(2)
C(17)-B(11)-B(15)	58.8(2)	B(16)-B(11)-B(15)	59.6(2)
B(20)-B(11)-B(15)	107.9(2)	C(17)-B(11)-B(12)	58.7(2)
B(16)-B(11)-B(12)	107.9(2)	B(20)-B(11)-B(12)	59.6(2)
B(15)-B(11)-B(12)	107.6(2)	C(17)-B(12)-B(19)	105.2(2)
C(17)-B(12)-B(20)	105.5(2)	B(19)-B(12)-B(20)	60.6(2)
C(17)-B(12)-B(13)	58.9(2)	B(19)-B(12)-B(13)	59.6(2)
B(20)-B(12)-B(13)	108.1(2)	C(17)-B(12)-B(11)	59.1(2)
B(19)-B(12)-B(11)	108.4(2)	B(20)-B(12)-B(11)	60.0(2)
B(13)-B(12)-B(11)	108.0(2)	C(17)-B(13)-B(18)	105.6(2)
C(17)-B(13)-B(19)	105.7(2)	B(18)-B(13)-B(19)	60.8(2)
C(17)-B(13)-B(12)	59.04(14)	B(18)-B(13)-B(12)	108.6(2)
B(19)-B(13)-B(12)	60.0(2)	C(17)-B(13)-B(14)	59.0(2)
B(18)-B(13)-B(14)	59.9(2)	B(19)-B(13)-B(14)	108.6(2)
B(12)-B(13)-B(14)	108.2(2)	C(17)-B(14)-B(18)	105.2(2)
C(17)-B(14)-B(17)	105.4(2)	B(18)-B(14)-B(17)	60.4(2)
C(17)-B(14)-B(15)	59.0(2)	B(18)-B(14)-B(15)	108.0(2)

B(17)-B(14)-B(15)	59.8(2)	C(17)-B(14)-B(13)	58.9(2)
B(18)-B(14)-B(13)	59.5(2)	B(17)-B(14)-B(13)	107.8(2)
B(15)-B(14)-B(13)	107.7(2)	C(17)-B(15)-B(16)	105.6(2)
C(17)-B(15)-B(17)	105.5(2)	B(16)-B(15)-B(17)	60.7(2)
C(17)-B(15)-B(14)	59.0(2)	B(16)-B(15)-B(14)	108.6(2)
B(17)-B(15)-B(14)	60.0(2)	C(17)-B(15)-B(11)	59.3(2)
B(16)-B(15)-B(11)	59.9(2)	B(17)-B(15)-B(11)	108.6(2)
B(14)-B(15)-B(11)	108.5(2)	C(18)-B(16)-B(15)	103.8(2)
C(18)-B(16)-B(11)	104.4(2)	B(15)-B(16)-B(11)	60.5(2)
C(18)-B(16)-B(17)	58.3(2)	B(15)-B(16)-B(17)	59.8(2)
B(11)-B(16)-B(17)	108.4(2)	C(18)-B(16)-B(20)	58.6(2)
B(15)-B(16)-B(20)	108.2(2)	B(11)-B(16)-B(20)	60.0(2)
B(17)-B(16)-B(20)	108.1(2)	C(18)-B(17)-B(15)	103.8(2)
C(18)-B(17)-B(14)	104.1(2)	B(15)-B(17)-B(14)	60.2(2)
C(18)-B(17)-B(18)	58.7(2)	B(15)-B(17)-B(18)	107.7(2)
B(14)-B(17)-B(18)	59.6(2)	C(18)-B(17)-B(16)	58.5(2)
B(15)-B(17)-B(16)	59.5(2)	B(14)-B(17)-B(16)	107.8(2)
B(18)-B(17)-B(16)	108.0(2)	C(18)-B(18)-B(13)	103.9(2)
C(18)-B(18)-B(14)	104.0(2)	B(13)-B(18)-B(14)	60.6(2)
C(18)-B(18)-B(17)	58.3(2)	B(13)-B(18)-B(17)	108.2(2)
B(14)-B(18)-B(17)	59.9(2)	C(18)-B(18)-B(19)	58.6(2)
B(13)-B(18)-B(19)	59.6(2)	B(14)-B(18)-B(19)	108.2(2)
B(17)-B(18)-B(19)	108.0(2)	C(18)-B(19)-B(13)	103.8(2)
C(18)-B(19)-B(12)	103.9(2)	B(13)-B(19)-B(12)	60.5(2)
C(18)-B(19)-B(18)	58.5(2)	B(13)-B(19)-B(18)	59.6(2)
B(12)-B(19)-B(18)	108.0(2)	C(18)-B(19)-B(20)	58.6(2)
B(13)-B(19)-B(20)	108.1(2)	B(12)-B(19)-B(20)	59.7(2)
B(18)-B(19)-B(20)	108.1(2)	C(18)-B(20)-B(12)	103.8(2)
C(18)-B(20)-B(11)	103.8(2)	B(12)-B(20)-B(11)	60.4(2)
C(18)-B(20)-B(16)	58.4(2)	B(12)-B(20)-B(16)	107.7(2)
B(11)-B(20)-B(16)	59.5(2)	C(18)-B(20)-B(19)	58.5(2)
B(12)-B(20)-B(19)	59.7(2)	B(11)-B(20)-B(19)	108.0(2)
B(16)-B(20)-B(19)	107.8(2)	C(19)-C(17)-B(13)	116.2(2)
C(19)-C(17)-B(15)	121.3(2)	B(13)-C(17)-B(15)	112.9(2)
C(19)-C(17)-B(14)	118.2(2)	B(13)-C(17)-B(14)	62.2(2)
B(15)-C(17)-B(14)	62.1(2)	C(19)-C(17)-B(12)	117.2(2)
B(13)-C(17)-B(12)	62.1(2)	B(15)-C(17)-B(12)	112.9(2)
B(14)-C(17)-B(12)	113.3(2)	C(19)-C(17)-B(11)	120.3(2)
B(13)-C(17)-B(11)	113.2(2)	B(15)-C(17)-B(11)	61.9(2)
B(14)-C(17)-B(11)	113.3(2)	B(12)-C(17)-B(11)	62.2(2)
B(17)-C(18)-B(16)	63.2(2)	B(17)-C(18)-B(18)	63.1(2)
B(16)-C(18)-B(18)	115.4(2)	B(17)-C(18)-B(19)	115.5(2)
B(16)-C(18)-B(19)	115.3(2)	B(18)-C(18)-B(19)	62.9(2)
B(17)-C(18)-B(20)	115.8(2)	B(16)-C(18)-B(20)	63.0(2)
B(18)-C(18)-B(20)	115.4(2)	B(19)-C(18)-B(20)	63.0(2)
C(20)-C(19)-C(24)	118.6(2)	C(20)-C(19)-C(17)	122.1(2)
C(24)-C(19)-C(17)	119.3(2)	C(19)-C(20)-C(21)	120.8(2)

C(20)-C(21)-C(22)	120.4(2)	C(21)-C(22)-C(23)	118.7(2)
C(21)-C(22)-C(25)	123.0(2)	C(23)-C(22)-C(25)	118.3(2)
C(24)-C(23)-C(22)	120.7(2)	C(23)-C(24)-C(19)	120.9(2)
C(26)-C(25)-C(22)	173.0(3)	C(25)-C(26)-C(27)	175.1(3)
C(28)-C(27)-C(32)	119.2(2)	C(28)-C(27)-C(26)	121.8(2)
C(32)-C(27)-C(26)	118.9(2)	C(29)-C(28)-C(27)	119.9(2)
C(30)-C(29)-C(28)	120.2(2)	C(29)-C(30)-C(31)	120.3(2)
C(32)-C(31)-C(30)	119.7(2)	C(31)-C(32)-C(27)	120.5(2)

Table 15s. Anisotropic displacement parameters [Å^2 x 10^3] for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B(1)	21(1)	24(1)	19(1)	1(1)	2(1)	2(1)
B(2)	20(1)	24(1)	17(1)	1(1)	-2(1)	-1(1)
B(3)	21(1)	19(1)	19(1)	0(1)	-1(1)	-1(1)
B(4)	26(1)	21(1)	13(1)	0(1)	0(1)	-2(1)
B(5)	19(1)	22(1)	20(1)	-3(1)	2(1)	1(1)
B(6)	22(1)	22(1)	22(1)	-1(1)	4(1)	0(1)
B(7)	16(1)	32(2)	22(1)	2(1)	1(1)	2(1)
B(8)	22(1)	28(2)	19(1)	-2(1)	1(1)	-4(1)
B(9)	22(1)	21(1)	20(1)	-2(1)	4(1)	-2(1)
B(10)	21(1)	25(2)	18(1)	-3(1)	3(1)	0(1)
C(1)	16(1)	18(1)	16(1)	-1(1)	1(1)	-2(1)
C(2)	17(1)	29(1)	23(1)	-2(1)	2(1)	0(1)
C(3)	18(1)	17(1)	19(1)	2(1)	3(1)	1(1)
C(4)	22(1)	20(1)	19(1)	-1(1)	1(1)	1(1)
C(5)	20(1)	21(1)	29(1)	-1(1)	-1(1)	-2(1)
C(6)	21(1)	16(1)	27(1)	4(1)	4(1)	2(1)
C(7)	23(1)	21(1)	22(1)	-2(1)	4(1)	2(1)
C(8)	19(1)	23(1)	23(1)	-2(1)	2(1)	-3(1)
C(9)	22(1)	19(1)	27(1)	2(1)	2(1)	1(1)
C(10)	22(1)	21(1)	30(1)	1(1)	1(1)	-1(1)
C(11)	18(1)	17(1)	26(1)	4(1)	2(1)	1(1)
C(12)	25(1)	22(1)	20(1)	0(1)	3(1)	1(1)
C(13)	18(1)	25(1)	32(1)	6(1)	-1(1)	-1(1)
C(14)	20(1)	24(1)	37(2)	6(1)	10(1)	2(1)
C(15)	37(2)	19(1)	22(1)	-1(1)	8(1)	1(1)
C(16)	24(1)	21(1)	27(1)	2(1)	-3(1)	-2(1)
B(11)	22(1)	23(1)	20(1)	-5(1)	-1(1)	2(1)
B(12)	21(1)	20(1)	22(1)	3(1)	0(1)	-2(1)
B(13)	17(1)	23(1)	21(1)	0(1)	1(1)	0(1)
B(14)	20(1)	19(1)	20(1)	2(1)	-1(1)	2(1)
B(15)	21(1)	23(1)	16(1)	2(1)	-1(1)	1(1)
B(16)	22(1)	27(2)	19(1)	-2(1)	-3(1)	0(1)
B(17)	18(1)	26(1)	22(1)	3(1)	-5(1)	1(1)
B(18)	21(1)	26(1)	23(1)	-3(1)	-2(1)	3(1)
B(19)	19(1)	30(2)	21(1)	1(1)	1(1)	-2(1)
B(20)	23(1)	24(1)	25(2)	1(1)	-2(1)	-1(1)
C(17)	18(1)	17(1)	16(1)	2(1)	0(1)	2(1)
C(18)	16(1)	27(1)	25(1)	-1(1)	-2(1)	-1(1)
C(19)	19(1)	17(1)	19(1)	-2(1)	-1(1)	0(1)

C(20)	24(1)	21(1)	17(1)	1(1)	-1(1)	1(1)
C(21)	21(1)	21(1)	28(1)	0(1)	0(1)	-2(1)
C(22)	20(1)	17(1)	29(1)	-2(1)	-4(1)	2(1)
C(23)	28(1)	21(1)	22(1)	3(1)	-5(1)	2(1)
C(24)	22(1)	23(1)	20(1)	3(1)	2(1)	0(1)
C(25)	24(1)	20(1)	30(1)	0(1)	-2(1)	1(1)
C(26)	22(1)	21(1)	32(1)	-2(1)	-1(1)	0(1)
C(27)	19(1)	17(1)	26(1)	-1(1)	-3(1)	3(1)
C(28)	25(1)	21(1)	22(1)	0(1)	1(1)	0(1)
C(29)	17(1)	25(1)	34(1)	-5(1)	2(1)	-2(1)
C(30)	25(1)	24(1)	32(2)	-5(1)	-11(1)	4(1)
C(31)	32(1)	21(1)	22(1)	0(1)	-3(1)	3(1)
C(32)	20(1)	20(1)	29(1)	-1(1)	5(1)	-1(1)

Table 16s. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for phenyl[4-(1,12-dicarba-*closo*-dodecaboran-1-yl)phenyl]acetylene, 6

	x	y	z	U_{eq}
H(1)	846(1)	6259(4)	595(2)	25
H(2)	695(1)	2726(4)	-465(2)	24
H(3)	833(1)	-150(4)	1240(2)	23
H(4)	1064(1)	1625(4)	3358(2)	24
H(5)	1069(1)	5579(4)	2963(2)	25
H(6)	409(1)	6777(4)	2563(3)	27
H(7)	177(1)	5016(4)	454(3)	28
H(8)	168(1)	1053(4)	840(2)	28
H(9)	396(1)	363(4)	3202(2)	26
H(10)	543(1)	3913(4)	4268(2)	25
H(2C)	63(1)	3590(4)	2618(2)	28
H(4A)	1529(1)	4247(3)	2361(2)	25
H(5A)	2046(1)	3992(3)	1665(2)	28
H(7A)	1712(1)	1490(3)	-1187(2)	27
H(8A)	1198(1)	1711(3)	-482(2)	26
H(12A)	3071(1)	3238(3)	18(2)	27
H(13A)	3565(1)	2786(3)	-845(2)	30
H(14A)	3599(1)	1456(3)	-2656(2)	32
H(15A)	3139(1)	564(3)	-3615(2)	31
H(16A)	2643(1)	899(3)	-2733(2)	29
H(11)	1009(1)	5721(4)	5742(2)	26
H(12)	829(1)	5273(4)	8181(2)	25
H(13)	797(1)	8907(4)	9234(2)	24
H(14)	960(1)	11607(4)	7454(2)	24
H(15)	1087(1)	9634(4)	5303(2)	24
H(16)	497(1)	7782(4)	4592(2)	27
H(17)	464(1)	11422(4)	5647(3)	26
H(18)	288(1)	10977(4)	8083(3)	28
H(19)	206(1)	7062(4)	8530(2)	28
H(20)	333(1)	5084(4)	6374(3)	29
H(18C)	67(1)	8627(4)	6425(2)	27
H(20A)	1558(1)	9226(3)	6242(2)	25
H(21A)	2081(1)	9040(3)	6897(2)	28
H(23A)	1770(1)	6676(3)	9833(2)	28
H(24A)	1252(1)	6836(3)	9169(2)	26
H(28A)	3151(1)	8028(3)	8815(2)	27
H(29A)	3604(1)	7392(4)	9901(2)	31
H(30A)	3555(1)	6267(4)	11764(2)	32
H(31A)	3053(1)	5702(3)	12542(2)	30
H(32A)	2601(1)	6208(3)	11436(2)	28

Table 17s. Crystal data for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

Identification code	bc91
Empirical formula	$C_{29}H_{21}CoN_4$
Formula mass	484.43
Crystal size, mm	0.165 × 0.165 × 0.22
Crystal color, habit	orange block
Crystal system	Tetragonal
Space group	*I*4
a, Å	13.2063(2)
b, Å	13.2063(2)
c, Å	6.8998(2)
α, °	90
β, °	90
γ, °	90
Volume, $Å^3$	1203.37(4)
Z, formula units/cell	2
Density (calculated), $Mg{\cdot}m^{-3}$	1.337
Absorption coefficient, mm^{-1}	0.737
F(000)	500
Absorption correction	Semi-empirical
Range Transmission Coefficients	0.913 to 0.762

Table 18s. Data collection parameters for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

Diffractometer	Siemens SMART CCD
Temperature, K	157(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 (MoKα)
Monochromator	graphite
Cell measurement	
Reflections used	4087
θ range	$2.18 < \theta < 27.91$
θ range, data collection	$2.18 < \theta < 27.91$
Scan type	0.3° ω scans
Index ranges	$-13 \leq h \leq 17$,
	$-17 \leq k \leq 17$,
	$-9 \leq l \leq 8$
Reflections collected	4146
Independent reflections	1408 ($R_{int} = 0.0199$)
Standard reflections	50 frames re-measured on completion
Stability of standards	no decay observed

Table 19s. Structure Solution and Refinement for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

System used[1,2]	Siemens SHELXTL
Structure solution	direct
Data/ restraints/ parameters	1408 / 1/ 81
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	$w^{-1} = [\sigma^2(Fo^2)+(0.0356P)^2+0.3481P]$ where $P=(Fo^2+2Fc^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0230, wR2 = 0.0587
Reflections observed	1399
R indices (all data)	R1 = 0.0232, wR2 = 0.0588
Goodness-of-fit[4] on F^2	1.093
Absolute structure parameter	-0.019(14)
Largest diff. peak and hole	0.296 and -0.315

1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $$R1 = \frac{\sum \| |Fo| - |Fc| \|}{\sum |Fo|} \; ; \quad wR2 = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{\sum \left[w\left(Fo^2\right)^2 \right]}}$$

4) $$Goodness - of - Fit = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{(M - N)}}$$

where M is the number of reflections and N is the number of parameters refined.

5) Flack, H. D. *Acta Cryst.* (1983). **A39.** 876-881.

Table 20s. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co	0	0	4307(1)	13(1)
N	-1732(1)	3634(1)	7337(3)	34(1)
C(1)	-333(1)	713(1)	6768(2)	15(1)
C(2)	-806(1)	1713(1)	6954(2)	17(1)
C(3)	-1695(1)	1841(1)	8030(2)	21(1)
C(4)	-2122(1)	2800(1)	8169(3)	29(1)
C(5)	-878(1)	3502(1)	6327(3)	32(1)
C(6)	-390(1)	2577(1)	6084(2)	24(1)
C(7)	325(20)	808(7)	1885(8)	18(1)
C(8)	882(8)	-111(23)	1850(7)	18(1)
C(9)	180(32)	-926(3)	1866(9)	18(1)
C(10)	-811(20)	-510(27)	1912(9)	18(1)
C(11)	-722(12)	562(24)	1924(7)	18(1)
Co(2)	0	0	-93(17)	13(1)

Table 21s. Bond lengths (Å) for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

Co-C(1)	1.9909(14)	Co-C(7)	2.028(5)
Co-C(8)	2.062(6)	Co-C(9)	2.094(6)
Co-C(10)	2.081(5)	Co-C(11)	2.040(6)
N-C(5)	1.337(2)	N-C(4)	1.345(2)
C(1)-C(2)	1.467(2)	C(1)-C(1)#1	1.469(2)
C(2)-C(3)	1.399(2)	C(2)-C(6)	1.402(2)
C(3)-C(4)	1.390(2)	C(5)-C(6)	1.391(2)
C(7)-C(8)	1.42	C(7)-C(11)	1.42
C(7)-Co(2)	1.785(10)	C(8)-C(9)	1.42
C(8)-Co(2)	1.782(10)	C(9)-C(10)	1.42
C(9)-Co(2)	1.838(11)	C(10)-C(11)	1.42
C(10)-Co(2)	1.874(10)	C(11)-Co(2)	1.842(11)
Co(2)-C(1)#2	2.402(11)		

Symmetry transformations used to generate equivalent atoms:
#1 y,-x,z #2 -x,-y,z-1

Table 22s. Bond angles(°)for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

C(1)#1-Co-C(1)	62.88(8)	C(1)#2-Co-C(1)	43.29(5)
C(1)-Co-C(1)#3	43.28(5)	C(1)-Co-C(7)#2	156.8(7)
C(1)-Co-C(7)#1	154.8(7)	C(1)-Co-C(7)#3	119.1(4)
C(1)#1-Co-C(7)	154.8(7)	C(1)#2-Co-C(7)	119.1(4)
C(1)-Co-C(7)	120.1(3)	C(1)#3-Co-C(7)	156.8(7)
C(7)#2-Co-C(7)	47.3(2)	C(7)#1-Co-C(7)	69.1(3)
C(7)#3-Co-C(7)	47.3(2)	C(1)-Co-C(11)#1	164.3(10)
C(7)-Co-C(11)#1	55.2(10)	C(1)-Co-C(11)#3	145.9(5)
C(7)-Co-C(11)#3	70.1(11)	C(1)-Co-C(11)#2	123.2(5)
C(1)#1-Co-C(11)	164.3(8)	C(1)#2-Co-C(11)	145.9(9)
C(1)-Co-C(11)	114.4(4)	C(1)#3-Co-C(11)	123.2(4)
C(7)#2-Co-C(11)	70.1(3)	C(7)#1-Co-C(11)	55.2(4)
C(7)#3-Co-C(11)	9.4(3)	C(7)-Co-C(11)	40.86(8)
C(11)#1-Co-C(11)	72.6(4)	C(11)#3-Co-C(11)	50(2)
C(11)#2-Co-C(11)	49.5(10)	C(5)-N-C(4)	115.97(14)
C(2)-C(1)-C(1)#3	134.5(2)	C(2)-C(1)-C(1)#2	135.1(2)
C(2)-C(1)-Co	126.45(11)	C(1)#3-C(1)-Co	68.36(3)
C(1)#2-C(1)-Co	68.36(3)	C(2)-C(1)-Co(2)#4	110.6(2)
Co-C(1)-Co(2)#4	122.95(13)	C(3)-C(2)-C(6)	117.23(13)
C(3)-C(2)-C(1)	120.84(14)	C(6)-C(2)-C(1)	121.92(14)
C(4)-C(3)-C(2)	119.13(14)	N-C(4)-C(3)	124.2(2)
N-C(5)-C(6)	124.6(2)	C(5)-C(6)-C(2)	118.8(2)
C(8)-C(7)-C(11)	108.0	C(8)-C(7)-Co(2)	66.4(3)
C(11)-C(7)-Co(2)	69.1(3)	C(8)-C(7)-Co	71.0(2)
C(11)-C(7)-Co	70.0(3)	Co(2)-C(7)-Co	105.3(3)
C(7)-C(8)-C(9)	108.0	C(7)-C(8)-Co(2)	66.6(3)
C(9)-C(8)-Co(2)	69.0(3)	C(7)-C(8)-Co	68.4(2)
C(9)-C(8)-Co	71.2(2)	Co(2)-C(8)-Co	104.1(4)
C(10)-C(9)-C(8)	108.0	C(10)-C(9)-Co(2)	68.9(3)
C(8)-C(9)-Co(2)	64.8(2)	C(10)-C(9)-Co	69.6(3)
C(8)-C(9)-Co	68.8(3)	Co(2)-C(9)-Co	100.8(3)
C(9)-C(10)-C(11)	108.0	C(9)-C(10)-Co(2)	66.2(3)
C(11)-C(10)-Co(2)	66.3(3)	C(9)-C(10)-Co	70.6(3)
C(11)-C(10)-Co	68.3(2)	Co(2)-C(10)-Co	100.1(3)
C(7)-C(11)-C(10)	108.0	C(7)-C(11)-Co(2)	64.8(2)
C(10)-C(11)-Co(2)	68.7(3)	C(7)-C(11)-Co	69.1(3)
C(10)-C(11)-Co	71.4(2)	Co(2)-C(11)-Co	102.7(4)
C(8)-Co(2)-C(7)	46.9(3)	C(8)-Co(2)-C(9)	46.2(3)
C(7)-Co(2)-C(9)	78.7(5)	C(8)-Co(2)-C(11)	78.7(5)
C(7)-Co(2)-C(11)	46.1(3)	C(9)-Co(2)-C(11)	77.3(4)
C(8)-Co(2)-C(10)	77.8(5)	C(7)-Co(2)-C(10)	77.8(5)

C(9)-Co(2)-C(10)	45.0(3)	C(11)-Co(2)-C(10)	44.9(3)
C(8)-Co(2)-C(1)#5	121.8(3)	C(7)-Co(2)-C(1)#5	151.6(6)
C(9)-Co(2)-C(1)#5	112.3(3)	C(11)-Co(2)-C(1)#5	159.0(5)
C(10)-Co(2)-C(1)#5	129.0(7)	C(8)-Co(2)-C(1)#6	115.9(5)
C(7)-Co(2)-C(1)#6	119.1(3)	C(9)-Co(2)-C(1)#6	137.2(9)
C(11)-Co(2)-C(1)#6	144.1(9)	C(10)-Co(2)-C(1)#6	162.7(4)
C(8)-Co(2)-C(1)#7	156.8(5)	C(7)-Co(2)-C(1)#7	153.3(6)
C(9)-Co(2)-C(1)#7	126.3(7)	C(11)-Co(2)-C(1)#7	123.5(4)
C(10)-Co(2)-C(1)#7	112.1(3)	C(8)-Co(2)-C(1)#8	146.1(8)
C(7)-Co(2)-C(1)#8	120.0(4)	C(9)-Co(2)-C(1)#8	161.3(5)
C(11)-Co(2)-C(1)#8	115.4(4)	C(10)-Co(2)-C(1)#8	134.6(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,z #2 y,-x,z #3 -y,x,z #4 x,y,z+1
#5 -x,-y,z-1 #6 y,-x,z-1 #7 -y,x,z-1
#8 x,y,z-1

Table 23s. Anisotropic displacement parameters ($Å^2 \times 10^3$) for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co	15(1)	15(1)	11(1)	0	0	0
N	38(1)	22(1)	43(1)	-4(1)	5(1)	9(1)
C(1)	15(1)	16(1)	16(1)	-2(1)	1(1)	0(1)
C(2)	17(1)	16(1)	17(1)	-3(1)	-1(1)	2(1)
C(3)	23(1)	24(1)	16(1)	0(1)	2(1)	3(1)
C(4)	29(1)	31(1)	26(1)	-4(1)	6(1)	10(1)
C(5)	34(1)	17(1)	44(1)	0(1)	3(1)	1(1)
C(6)	22(1)	18(1)	31(1)	-1(1)	4(1)	0(1)
C(7)	24(2)	15(2)	15(1)	0(1)	1(1)	-1(2)
C(8)	24(2)	15(2)	15(1)	0(1)	1(1)	-1(2)
C(9)	24(2)	15(2)	15(1)	0(1)	1(1)	-1(2)
C(10)	24(2)	15(2)	15(1)	0(1)	1(1)	-1(2)
C(11)	24(2)	15(2)	15(1)	0(1)	1(1)	-1(2)
Co(2)	15(1)	15(1)	11(1)	0	0	0

Table 24s. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for tetra(4-pyridyl)cyclobutadienecyclopentadienylcobalt, 7

	x	y	z	U_{eq}
H(3A)	-2003(1)	1279(1)	8658(2)	25
H(4A)	-2728(1)	2871(1)	8898(3)	34
H(5A)	-584(1)	4080(1)	5733(3)	38
H(6A)	214(1)	2532(1)	5343(2)	29
H(7A)	603(20)	1471(7)	1884(8)	21
H(8A)	1599(10)	-171(44)	1820(13)	21
H(9A)	345(53)	-1626(7)	1849(15)	21
H(10A)	-1426(31)	-883(45)	1932(16)	21
H(11A)	-1266(26)	1031(41)	1953(13)	21

Table 25s. Crystal data for tetra(4-ethoxycarbonylphenyl) cyclobutadienecyclopentadienylcobalt, 10

Identification code	bc66
Empirical formula	$C_{45}H_{41}CoO_8$
Formula mass	768.71
Crystal size, mm	0.04 x 0.08 x 0.08
Crystal color, habit	orange needle
Crystal system	Tetragonal
Space group	*I*4
a, Å	16.233(2)
b, Å	16.233(2)
c, Å	7.0765(8)
α, °	90
β, °	90
γ, °	90
Volume, $Å^3$	1864.8(4)
Z, formula units/cell	2
Density (calculated), $Mg{\cdot}m^{-3}$	1.369
Absorption coefficient, mm^{-1}	0.516
F(000)	804
Absorption correction	semi-empirical
Range Transmission Coefficients	0.984 to 0.966