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Crystal Structure of (μ -Tranis-4,4'-Dinitro-2,2'-Biimidazolato-N,N: N",N"') Bis[Bis(Triphenylphosphine Copper(I))] N,N- Dimethylformamide, [C₄₂H₃₇CuN₄O₃P₂]₂

R. G. Baughman

C. A. Hester

Harvest L. Collier

Missouri University of Science and Technology, hcollier@mst.edu

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Crystal structure of (μ -*trans*-4,4'-dinitro-2,2'-biimidazolato- $N,N':N'',N'''$)bis[bis(triphenylphosphine copper(I))] N,N -dimethylformamide, $[C_{42}H_{37}CuN_4O_3P_2]_2$

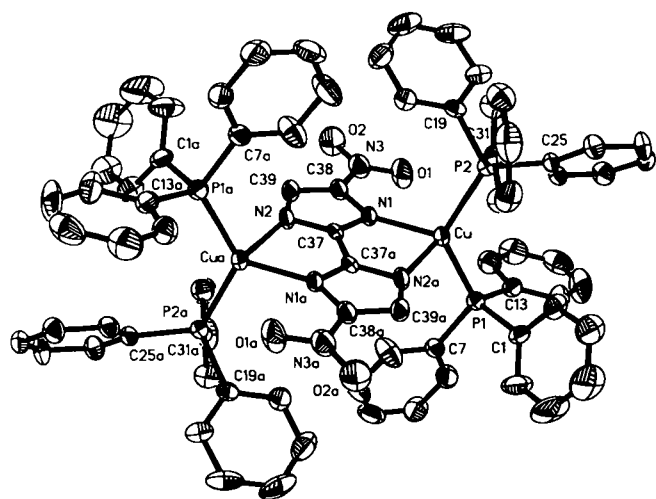
R. G. Baughman

Truman State University (formerly Northeast Missouri State U.), Division of Science, Kirksville, MO 63501-4221, U. S. A.

C. A. Hester and H. L. Collier

University of Missouri-Rolla, Department of Chemistry, Rolla, MO 65401, U. S. A.

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Source of material: The title material was prepared by a metathetical reaction between $[(Ph)_3P]_2Cu(NO_3)$ and 4,4'-dinitro-2,2'-biimidazole (see ref. 1) in N,N -dimethylformamide at room temperature. Crystals were grown by slow evaporation of the reaction mixture. The sample was sealed in a capillary with mother liquor.

$C_{42}H_{37}CuN_4O_3P_2$, monoclinic, $P12_1/n1$ (No. 14), $a = 13.400(2)$ Å, $b = 11.296(2)$ Å, $c = 25.737(4)$ Å, $\beta = 92.38(1)^\circ$, $V = 3892.4$ Å³, $Z = 4$, $R(F) = 0.059$, $R_w(F^2) = 0.093$.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow, parallelepiped, size 0.34 x 0.44 x 0.63 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	6.87 cm ⁻¹
Diffractometer:	Siemens P3
Scan mode:	θ
$T_{\text{measurement}}$:	288 K
$2\theta_{\text{max}}$:	45°
$N(hkl)_{\text{unique}}$:	4991
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	505
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	Occ.	x	y	z	U_{iso}
H(2B)	4e		0.9378(6)	0.1780(8)	0.2972(3)	0.08
H(3A)	4e		0.9271(8)	0.379(1)	0.2753(4)	0.08
H(4A)	4e		1.064(1)	0.502(1)	0.2923(5)	0.08
H(5A)	4e		1.2155(9)	0.419(1)	0.3211(6)	0.08
H(6A)	4e		1.2243(7)	0.2135(9)	0.3391(4)	0.08
H(8A)	4e		1.2741(5)	-0.0287(8)	0.2951(3)	0.08
H(9A)	4e		1.4328(6)	-0.0775(8)	0.3306(4)	0.08
H(10A)	4e		1.4662(7)	-0.0663(8)	0.4191(4)	0.08
H(11A)	4e		1.3366(7)	-0.040(1)	0.4729(4)	0.08
H(12A)	4e		1.1751(6)	0.0077(9)	0.4378(3)	0.08
H(14A)	4e		1.0711(6)	-0.2130(9)	0.3150(3)	0.08
H(15A)	4e		1.0634(7)	-0.332(1)	0.2390(5)	0.08
H(16A)	4e		1.0510(7)	-0.243(1)	0.1579(5)	0.08
H(17A)	4e		1.0686(8)	-0.046(1)	0.1507(4)	0.08
H(18A)	4e		1.0756(6)	0.0778(9)	0.2259(3)	0.08
H(20A)	4e		0.7638(6)	-0.0880(8)	0.4655(3)	0.08
H(21A)	4e		0.6652(7)	-0.242(1)	0.4979(4)	0.08
H(22A)	4e		0.5777(8)	-0.3658(9)	0.4418(6)	0.08
H(23A)	4e		0.5656(7)	-0.3209(9)	0.3534(5)	0.08
H(24A)	4e		0.6582(6)	-0.1600(7)	0.3211(3)	0.08
H(26A)	4e		0.6612(5)	0.1667(6)	0.3013(3)	0.08
H(27A)	4e		0.6254(6)	0.1712(7)	0.2116(3)	0.08
H(28A)	4e		0.7152(6)	0.0534(7)	0.1565(3)	0.08
H(29A)	4e		0.8261(5)	-0.0902(7)	0.1912(3)	0.08
H(30A)	4e		0.8597(5)	-0.0946(6)	0.2822(3)	0.08
H(32A)	4e		0.5934(6)	0.0694(8)	0.4058(3)	0.08
H(33A)	4e		0.5172(7)	0.234(1)	0.4433(3)	0.08
H(34A)	4e		0.6052(9)	0.409(1)	0.4535(3)	0.08
H(35A)	4e		0.7704(8)	0.4212(8)	0.4291(3)	0.08
H(36A)	4e		0.8475(6)	0.2507(8)	0.3940(3)	0.08
H(39A)	4e		0.9728(6)	-0.3124(7)	0.5423(3)	0.08
H(41A)	4e	0.5	0.872(2)	0.454(3)	0.539(1)	0.08
H(41B)	4e	0.5	0.873(2)	0.412(3)	0.597(1)	0.08
H(41C)	4e	0.5	0.847(2)	0.322(3)	0.552(1)	0.08
H(41D)	4e	0.5	0.839(3)	0.335(3)	0.552(2)	0.08
H(41E)	4e	0.5	0.816(3)	0.320(3)	0.610(2)	0.08
H(41F)	4e	0.5	0.743(3)	0.266(3)	0.567(2)	0.08
H(42A)	4e	0.5	0.606(5)	0.480(5)	0.535(1)	0.08
H(42B)	4e	0.5	0.656(5)	0.369(5)	0.562(1)	0.08
H(42C)	4e	0.5	0.617(5)	0.475(5)	0.595(1)	0.08
H(42D)	4e	0.5	0.624(3)	0.388(2)	0.616(1)	0.08
H(42E)	4e	0.5	0.659(3)	0.282(2)	0.582(1)	0.08
H(42F)	4e	0.5	0.732(3)	0.336(2)	0.626(1)	0.08

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	Occ.	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cu	4e		0.95472(6)	-0.0003(1)	0.39297(3)	0.0430(5)	0.0731(7)	0.0402(5)	-0.0015(6)	-0.0048(3)	0.0150(6)
P(1)	4e		1.0806(1)	0.0236(2)	0.33876(7)	0.040(1)	0.058(2)	0.049(1)	0.001(1)	-0.0009(8)	0.012(1)
P(2)	4e		0.7911(1)	0.0184(2)	0.36999(6)	0.039(1)	0.053(1)	0.040(1)	-0.002(1)	-0.0042(8)	0.007(1)
O(1)	4e		0.9308(5)	-0.2987(5)	0.3867(2)	0.144(6)	0.071(4)	0.064(4)	-0.020(4)	-0.033(4)	-0.012(4)
O(2)	4e		0.9181(5)	-0.4232(6)	0.4512(2)	0.159(7)	0.057(4)	0.099(5)	-0.031(5)	-0.032(4)	0.001(4)
N(1)	4e		0.9703(4)	-0.1186(6)	0.4537(2)	0.046(4)	0.050(5)	0.032(4)	-0.001(3)	-0.008(3)	0.002(3)
N(2)	4e		0.9986(4)	-0.1307(6)	0.5414(2)	0.060(4)	0.057(5)	0.031(4)	0.001(4)	-0.011(3)	0.006(4)
N(3)	4e		0.9344(5)	-0.3237(7)	0.4333(3)	0.090(6)	0.067(6)	0.071(5)	-0.010(5)	-0.020(5)	0.003(5)
C(1)	4e		1.0824(6)	0.1780(7)	0.3202(3)	0.043(5)	0.057(6)	0.073(6)	-0.006(5)	0.009(4)	0.019(5)
C(2)	4e		0.9945(6)	0.2294(8)	0.3023(3)	0.064(6)	0.051(6)	0.097(7)	0.014(5)	0.010(5)	0.021(5)
C(3)	4e		0.9878(8)	0.347(1)	0.2907(4)	0.086(8)	0.084(9)	0.127(9)	0.028(7)	0.013(7)	0.031(7)
C(4)	4e		1.070(1)	0.418(1)	0.2979(5)	0.16(1)	0.055(8)	0.24(2)	0.012(9)	-0.01(1)	0.058(9)
C(5)	4e		1.1576(9)	0.370(1)	0.3152(6)	0.12(1)	0.07(1)	0.31(2)	-0.037(8)	-0.01(1)	0.08(1)
C(6)	4e		1.1634(7)	0.2503(9)	0.3264(4)	0.061(7)	0.076(8)	0.19(1)	-0.013(6)	-0.001(7)	0.052(8)
C(7)	4e		1.2081(5)	-0.0068(7)	0.3631(3)	0.047(4)	0.053(5)	0.059(5)	-0.007(5)	-0.007(4)	0.017(5)
C(8)	4e		1.2863(5)	-0.0320(8)	0.3321(3)	0.048(5)	0.14(1)	0.079(6)	0.010(6)	0.009(4)	0.038(7)
C(9)	4e		1.3808(6)	-0.0561(8)	0.3534(4)	0.043(6)	0.121(9)	0.125(9)	0.023(5)	0.017(6)	0.040(7)
C(10)	4e		1.3986(7)	-0.0574(8)	0.4056(4)	0.052(6)	0.094(8)	0.115(9)	-0.013(6)	-0.026(6)	0.007(7)
C(11)	4e		1.3240(7)	-0.033(1)	0.4360(4)	0.072(6)	0.18(1)	0.081(7)	0.019(8)	-0.025(6)	-0.012(8)
C(12)	4e		1.2282(6)	-0.0105(9)	0.4151(3)	0.061(5)	0.133(9)	0.079(6)	0.042(7)	-0.013(4)	-0.038(7)
C(13)	4e		1.0755(5)	-0.0574(8)	0.2778(3)	0.048(5)	0.063(6)	0.055(5)	0.000(4)	0.002(4)	0.009(4)
C(14)	4e		1.0690(6)	-0.1777(9)	0.2810(3)	0.075(7)	0.096(9)	0.061(6)	-0.005(6)	0.007(5)	-0.011(6)
C(15)	4e		1.0646(7)	-0.247(1)	0.2366(5)	0.103(8)	0.093(9)	0.108(9)	-0.006(7)	0.017(7)	-0.011(8)
C(16)	4e		1.0618(7)	-0.195(1)	0.1886(5)	0.079(7)	0.16(1)	0.089(9)	-0.012(9)	0.004(7)	-0.05(1)
C(17)	4e		1.0664(8)	-0.079(1)	0.1850(4)	0.14(1)	0.17(1)	0.037(6)	0.03(1)	0.005(6)	-0.005(8)
C(18)	4e		1.0732(6)	-0.0069(9)	0.2291(3)	0.098(6)	0.108(8)	0.053(5)	0.031(7)	0.009(4)	0.010(7)
C(19)	4e		0.7176(5)	-0.1067(7)	0.3906(3)	0.032(5)	0.053(6)	0.057(5)	0.001(4)	0.001(4)	0.004(5)
C(20)	4e		0.7209(6)	-0.1353(8)	0.4431(3)	0.055(5)	0.085(7)	0.074(7)	-0.002(5)	-0.001(5)	0.020(5)
C(21)	4e		0.6662(7)	-0.231(1)	0.4609(4)	0.085(8)	0.10(1)	0.101(8)	0.007(7)	0.028(7)	0.047(8)
C(22)	4e		0.6103(8)	-0.2973(9)	0.4282(6)	0.088(9)	0.044(7)	0.19(2)	-0.001(6)	0.05(1)	0.034(9)
C(23)	4e		0.6072(7)	-0.2724(9)	0.3760(5)	0.071(7)	0.054(7)	0.15(1)	-0.025(6)	0.028(7)	-0.029(7)
C(24)	4e		0.6596(6)	-0.1753(7)	0.3578(3)	0.055(5)	0.056(6)	0.081(6)	-0.004(5)	0.017(5)	-0.007(5)
C(25)	4e		0.7610(5)	0.0320(6)	0.3005(2)	0.042(4)	0.047(5)	0.040(4)	-0.001(4)	-0.005(3)	0.006(4)
C(26)	4e		0.6934(5)	0.1116(6)	0.2790(3)	0.065(5)	0.049(5)	0.045(5)	0.010(5)	-0.002(4)	-0.009(4)
C(27)	4e		0.6763(6)	0.1197(7)	0.2260(3)	0.082(6)	0.065(6)	0.042(5)	0.021(5)	-0.018(5)	0.005(4)
C(28)	4e		0.7262(6)	0.0464(7)	0.1935(3)	0.076(6)	0.067(6)	0.041(5)	-0.018(5)	-0.012(5)	0.012(5)
C(29)	4e		0.7929(5)	-0.0366(7)	0.2138(3)	0.063(5)	0.082(7)	0.042(5)	0.005(5)	0.007(4)	-0.009(4)
C(30)	4e		0.8106(5)	-0.0412(6)	0.2674(3)	0.041(4)	0.059(6)	0.052(5)	0.003(4)	-0.008(4)	0.004(4)
C(31)	4e		0.7272(6)	0.1441(7)	0.3981(3)	0.042(5)	0.059(6)	0.037(5)	-0.006(5)	-0.006(4)	0.007(4)
C(32)	4e		0.6298(6)	0.1416(8)	0.4120(3)	0.065(6)	0.060(6)	0.076(6)	0.004(5)	0.008(5)	-0.015(5)
C(33)	4e		0.5849(7)	0.239(1)	0.4324(3)	0.075(7)	0.091(8)	0.072(6)	0.014(7)	0.002(5)	-0.008(6)
C(34)	4e		0.6371(9)	0.341(1)	0.4389(3)	0.14(1)	0.073(8)	0.053(6)	0.035(8)	0.000(7)	-0.023(6)
C(35)	4e		0.7353(8)	0.3474(8)	0.4251(3)	0.126(9)	0.052(7)	0.071(7)	-0.020(7)	-0.001(6)	0.000(5)
C(36)	4e		0.7796(6)	0.2477(8)	0.4047(3)	0.067(6)	0.066(7)	0.059(5)	-0.008(6)	0.001(4)	-0.013(5)
C(37)	4e		0.9915(6)	-0.0621(5)	0.4987(3)	0.039(4)	0.045(4)	0.033(3)	-0.005(5)	-0.010(3)	0.001(5)
C(38)	4e		0.9596(5)	-0.2316(7)	0.4699(3)	0.063(5)	0.044(6)	0.047(5)	-0.005(5)	-0.012(4)	0.003(4)
C(39)	4e		0.9775(6)	-0.2408(7)	0.5225(3)	0.073(6)	0.046(6)	0.054(5)	-0.011(5)	-0.012(4)	0.016(4)
O(3A)	4e	0.5	0.602(3)	0.543(6)	0.554(1)	0.11(2)	0.24(5)	0.07(1)	0.12(2)	-0.02(1)	-0.05(2)
O(3B)	4e	0.5	0.632(5)	0.568(5)	0.561(2)	0.18(4)	0.22(4)	0.13(3)	0.05(3)	0.05(3)	0.08(3)
N(4)	4e		0.742(1)	0.436(1)	0.5706(4)	0.10(1)	0.10(1)	0.123(9)	0.025(9)	0.026(8)	0.004(7)
C(40A)	4e	0.5	0.717(3)	0.539(4)	0.552(1)	0.10(2)	0.21(4)	0.09(2)	0.12(3)	0.06(2)	0.05(2)
C(40B)	4e	0.5	0.808(3)	0.530(3)	0.553(1)	0.21(4)	0.12(3)	0.28(4)	-0.07(3)	0.11(3)	-0.04(3)
C(41A)	4e	0.5	0.841(2)	0.403(3)	0.564(1)	0.13(3)	0.10(3)	0.17(2)	0.05(2)	0.07(2)	0.03(2)
C(41B)	4e	0.5	0.787(3)	0.331(3)	0.576(2)	0.18(4)	0.19(5)	0.39(6)	-0.03(4)	0.08(4)	0.06(4)
C(42A)	4e	0.5	0.680(3)	0.354(2)	0.600(1)	0.19(3)	0.07(2)	0.29(4)	0.02(2)	0.12(4)	0.04(2)
C(42B)	4e	0.5	0.648(5)	0.454(5)	0.564(1)	0.22(6)	0.4(1)	0.06(2)	0.15(7)	0.02(3)	-0.04(4)

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