trans ligand, and the W=O$_t$ distance is longer (1.712 (7) Å) than those observed (1.66 (1) Å) in structures with weakly bound μ-Cl ligands in the trans position, as found[13] in the ions [Cl$_2$OW(μ-Cl)(μ-SR)$_2$WCl$_2$O]$^-$. The oxo ligand nevertheless causes an apparent weakening of the W–O(PPh$_3$) bond, which is longer (2.124 (7) Å) than that observed in WOCl$_3$(Ph$_3$PO)$_2$ (2.088 (11) Å)[14] and in WSCl$_3$(Ph$_3$PO)$_2$ (2.06 (1) Å).[15] The variation of Mo=O bond lengths found in MoOCl$_3$(Ph$_3$PO)$_2$ is compatible with an interpretation of a trans influence of the oxo ligand in **1**, since Mo—O(PPh$_3$) trans to Mo=O is 2.136 (11) Å, while that trans to a terminal Cl is much shorter (2.065 (10) Å).[16] The geometry of the Ph$_3$PO ligand is normal and has dimensions P–O = 1.518 (7) Å, P–C = 1.79 Å (mean), and O–P–C = 107–112°. The W–O–P angle is 155.8 (4)°, and the complete set of data is consistant with those previously reported by Mabbs and co-workers[14] and by Garner and co-workers.[16]

The Cl$_2$S$_2$ unit is planar to within 0.03 Å, with the W atom lying 0.13 Å out of this plane, toward O(1). In the triply bridged anionic complexes [Cl$_2$OW(μ-Cl)(μ-SR)$_2$WOCl$_2$]$^-$ we observed a much greater deviation (0.38 Å),[13] which is indicative of weaker W=O$_t$ bonding in **1** and consistent with the comparative W=O bond lengths described above.

Origin of 1. The isolation of **1** in the reaction described above is in itself of some interest, since the Ph$_3$PO must have originated from Ph$_3$P coordinated to a Cu^I center. The abstraction of oxygen from metal centers by Ph$_3$P is well documented,[17] and it seems likely that the Ph$_3$PO arose in this way. It requires only very minute quantities of adventitious oxygen to yield oxotungsten complexes, and these tend to crystallize from solution much more quickly than the target complexes. Hence, the likely pathway here was the oxidation of W^{IV} to a W^{VI} dioxo species, followed by reaction with free Ph$_3$P (derived from the dissociation of [CuCl(Ph$_3$P)]$_4$). The catalytic oxidation of Ph$_3$P at the copper center cannot be excluded as another possible mechanism. The dimerization of W(SR)$_n$ complexes is a facile reaction, and indeed isolation of terminal thiolato–tungsten complexes has been shown to be very difficult, unless hindered thiols are used.

Anti (O)W(μ-SR)$_2$W(O) Stereochemistry. There seems to be general agreement in the literature that syn [Mo$_2$O$_4$]$^{2+}$ and [Mo$_2$S$_4$]$^{2+}$ cores are intrinsically more stable than their anti isomers.[3] Factors such as enhanced Mo–Mo bonding interactions[18,19] and diminished O$_t$···O$_b$ interactions[20] have been cited to explain this apparent preference for the syn isomer. Hence, the anti geometry of **1**, which has a OM(μ-S)$_2$MO core, would not be expected to be stable. The most likely reason for the centrosymmetric anti structure being found for **1** would seem to be steric crowding, which the two Ph$_3$PO ligands would generate if they were mutually syn. The crowding is accentuated by the *i*-Bu groups of the bridging thiolates, and as Figure 1 shows, the anti configurations of these two groups interact minimally with the phenyl groups of the mutually anti Ph$_3$PO ligands. Steric factors of this type have been invoked previously to account for structural stabilities in [L$_2$Mo$_2$O$_4$]$^{2+}$ and related oxomolybdenum cores.[21,22]

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X-ray Crystal Structure of Pd₂Cl₂(2,6-Me₂C₆H₃NC)₂(py)₂. Unusual C-N-C Bond Angles and Infrared Spectrum in Bridging Isocyanide Groups[1]

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In the infrared spectrum of the transitional-metal complexes of isocyanides, the terminal NC stretching frequencies generally appear above 1900 cm^{-1},[2] but in some complexes the NC absorption occurs at ca. 1820 cm^{-1}, Ru(*t*-BuNC)$_5$ (1815 cm^{-1})[3] and Fe(*t*-BuNC)$_5$ (1830 cm^{-1}).[3] The low frequencies result from the bending of the NC bond, which is a reflection of a higher backbonding. For example, the solid-state structure of Fe(*t*-BuNC)$_5$ shows substantial bending at the nitrogen atoms (mean value 134 (2)°). For a bridging isocyanide coordinated to two or more metals, the NC stretching frequencies of the M–M bridging ligand range from 1880 to 1580 cm^{-1}.[2]

We report the synthesis and X-ray crystal structure of Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_2$(py)$_2$. As described below, this presents an interesting structural feature, including a unique linear bridging C–N–C bond.

The reaction of Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_4$ (**1**)[4] with pyridine (py) gave orange crystals, formulated as Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_2$(py)$_2$ (**2**). The infrared spectrum of **2** in KBr shows two absorption peaks at 2056 (s) and 1976 cm^{-1}, which are lower in energy by ca. 200–130 cm^{-1} from those for **1**. The ^{1}H NMR spectrum shows a peak at δ 2.52 due to *o*-methyl groups, compared with that (δ 2.53) of **1**.

Although the infrared and ^{1}H NMR spectroscopic data indicate the presence of terminal isocyanide groups, an X-ray analysis of **2** confirms the presence of two μ-bridging isocyanide ligands. A metal–metal bond joins the two palladium atoms and is bridged by two isocyanide ligands (Figure 1). The palladium geometry (ignoring the metal–metal bond) may be apparently described as square planar. A dihedral angle between the two planes consisting of the metal and two bridging carbons is ca. 129.7 (5)°, compared with the corresponding bridge plane–bridge plane angle (127.5°) in Co$_2$(CO)$_8$[5] and being smaller than that found in Co$_2$(*t*-BuNC)$_8$.[6] The Pd–Pd bond length is 2.662 (1) Å, longer than those found in the unbridging complexes [Pd$_2$(MeNC)$_6$]$^{2+}$ (2.5310 (9) Å),[7] Pd$_2$Cl$_2$(*t*-BuNC)$_4$ (2.532 (2) Å,[4] and Pd$_2$I$_2$(MeNC)$_4$ (2.533 (1) Å)[8] and shorter than the Pd–Pd bond distances (2.734 Å) found

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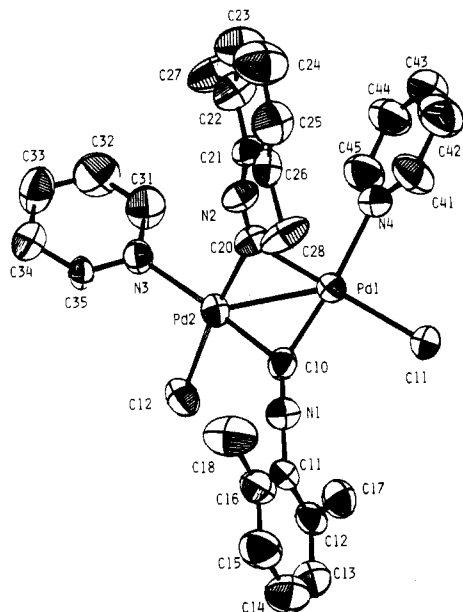(8) Rutherford, N. M.; Olmstead, M. M.; Balch, A. L. *Inorg. Chem.* **1984,** *22,* 2833.

Figure 1. Structure of Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_2$(py)$_2$ (**2**).

Table I. Selected Bond Distances (Å) and Angles (deg)

Pd(1)–Pd(2)	2.662 (1)	Pd(1)–Cl(1)	2.387 (3)
Pd(1)–Cl(10)	1.965 (13)	Pd(1)–C(20)	2.054 (13)
Pd(1)–N(4)	2.144 (11)	Pd(2)–Cl(2)	2.392 (4)
Pd(2)–C(10)	2.062 (10)	Pd(2)–C(20)	1.963 (14)
Pd(3)–N(3)	2.144 (9)	C(10)–N(1)	1.185 (17)
C(20)–N(2)	1.181 (20)		

Pd(2)–Pd(1)–Cl(1)	138.2 (1)	Pd(2)–Pd(1)–C(10)	50.9 (3)
Pd(2)–Pd(1)–C(20)	47.1 (4)	Pd(2)–Pd(1)–N(4)	122.9 (2)
Cl(1)–Pd(1)–C(10)	93.0 (4)	Cl(1)–Pd(1)–C(20)	168.3 (3)
Cl(1)–Pd(1)–N(4)	172.9 (3)	C(20)–Pd(1)–N(4)	89.0 (5)
Pd(1)–Pd(2)–Cl(2)	123.7 (1)	Pd(1)–Pd(2)–C(10)	47.1 (4)
Pd(1)–Pd(2)–C(20)	50.0 (4)	Cl(2)–Pd(2)–C(20)	50.0 (4)
Pd(1)–Pd(2)–N(3)	136.2 (3)	Cl(2)–Pd(2)–C(10)	89.8 (4)
Cl(2)–Pd(2)–N(3)	91.9 (3)	C(10)–Pd(2)–C(20)	173.4 (4)
C(10)–Pd(2)–N(3)	172.1 (4)	C(20)–Pd(2)–N(3)	93.0 (4)
C(10)–N(1)–C(11)	175.2 (13)	Pd(1)–C(10)–Pd(2)	82.7 (5)
Pd(1)–C(10)–N(1)	143.2 (8)	Pd(2)–C(10)–N(1)	133.8 (9)
C(20)–N(2)–C(21)	157.6 (9)	Pd(1)–C(20)–Pd(2)	83.0 (6)
Pd(1)–C(20)–N(2)	133.0 (8)	Pd(2)–C(20)–N(2)	143.8 (9)

in triangular Pd$_3$(μ-SO$_2$)$_2$(t-BuNC)$_5$ with the SO$_2$ bridging ligands.[9]

The most salient feature is the C–N–C bond angles of the bridging isocyanide groups. The bond angles are 175.2 (13)° for C(10)–N(1)–C(11) and 157.6 (9)° for C(20)–N(2)–C(21). The former is almost linear, and the latter is larger by ca. 20 than those (~125°) in usual bridging isocyanide ligands and those (123–140°) of the great bent terminal isocyanide ligands in Fe-(t-BuNC)$_5$. The linearity in bridging isocyanide ligands led to the high C–N stretching frequencies in the infrared spectrum. The C–N bond lengths are relatively shorter by ca. 0.04–0.05 Å than those found in usual bridging structure, likely arising from the linearity. The close nonbonded distances in the molecule are 2.75 Å for C(10)⋯C(20) and 3.63 (2) Å for Cl(2)⋯C(35). The shortest intermolecular distance is 3.44 (2) Å for C(28)⋯C(28) (−x, −y, z), within the sum of the van der Waals distance.

The electronic spectra of **1**, **2**, and PdCl$_2$(2,6-Me$_2$C$_6$H$_3$NC)(py) are illustrated in Figure 2. The lowest energy band in **2** appeared at 377 nm, assignable to the σ–σ* transition, indicating a ba-
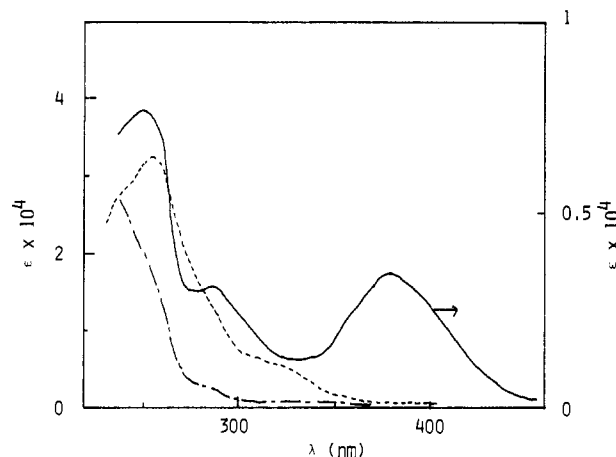
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Figure 2. Electronic spectra in CH$_2$Cl$_2$: Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_2$(py)$_2$ (—); Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_4$ (---); PdCl$_2$(2,6-Me$_2$C$_6$H$_3$NC)(py) (−·−).

thochromic shift in comparison with those of **1** and its related complexes.[12] Replacement of isocyanide by pyridine results in increased localization of electron density on the palladium atoms, which would increase dπ–dπ repulsive interactions on the metal–metal bond. This effect was likely observed as the bathochromic shift. The red shift may be related with the longer metal–metal bond distance in **2** than those of nonbridging complexes.

In the present reaction, the driving force of rearrangement of a terminal isocyanide to a bridging one may result in dispersing increased electron density on metals introduced by the N donor of pyridine.

Experimental Section

Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_2$(py)$_2$ (2). Pyridine (2 mL) was added to a solution of Pd$_2$Cl$_2$(2,6-Me$_2$C$_6$H$_3$NC)$_4$[4] (0.2 g, 0.25 mmol) in CH$_2$Cl$_2$ (20 mL). After 1 h, the solvent was removed to ca. 5 mL and benzene was added to the orange solution. The very pale yellow crystals (0.03 g) of PdCl$_2$(py)$_2$ were filtered. The orange-yellow crystals (0.11 g, 62.5%) of **2** were crystallized from the mother liquor. IR (Nujol): 2056, 1976 cm^{-1} (C≡N). ^{1}H NMR (CDCl$_3$): δ 2.52 (o-Me), 7.3 (aromatic and pyridine protons). Electronic spectrum (CH$_2$Cl$_2$)[8] λ_{max} (ϵ, M^{-1} cm^{-1}): 378 (3500), 288 (3200), 251 (7750) nm. Anal. Calcd for C$_{28}$H$_{28}$N$_4$Cl$_2$Pd$_2$: C, 47.75; H, 4.01; N, 7.96. Found: C, 47.68; H, 3.97; N, 7.90.

Reaction of 2 with 2,6-Xylyl Isocyanide. A mixture of **2** (0.07 g, 0.1 mmol) and 2,6-xylyl isocyanide (0.1 g, 0.75 mmol) was stirred in CH$_2$Cl$_2$ (15 mL) at room temperature. After 0.5 h, the solvent was removed to ca. 3 mL and hexane was added to the solution to give **1** (0.06 g, 74%).

Structure Determination. Orange crystals of **2** were obtained from a mixture of pyridine and benzene. X-ray photographic data from Weissenberg photographs showed the crystal to be monoclinic, with systematic extinctions (*h0l*, *h* = 2*n*; 0*k*0, *k* = 2*n*) consistent with the space group $P2_1/a$. Crystal data for C$_{28}$H$_{28}$N$_4$Cl$_2$Pd$_2$, mol wt 704.3, are a = 22.378 (6) Å, b = 9.485 (4) Å, c = 16.024 (4) Å, β = 121.22 (2)°, V = 2909 (2) Å^3, Z = 4, and $F(000)$ = 1032. Data collection was carried out on a Rigaku four-circle diffractometer using graphite-monochromated Mo Kα (λ = 0.7107 Å) radiation with 2θ < 45 and the ω–2θ ($\leq$30°) and ω (>30°) scan techniques with scan rate 4°min^{-1}. A total of 3036 reflections were measured. The 2800 reflections for which $F_o \geq 3\sigma(F_o)$ were used in the calcns. Intensities were corrected for Lorentz and polarization effects. The linear absorption coefficient is 14.3 cm^{-1}, and no absorption correction was made. The positions of the two Pd atoms were determined by a Patterson map using the UNICS III program system.[12] The remaining atoms were located in succeeding different Fourier syntheses. The positions of the atoms were refined anisotropically by using block-diagonal least-squares methods, minimizing $\sum o|F_o| - |F_c|)^2$. The final $R[=\sum||F_r| - |F_c||/\sum F_o|]$ and R_w [$=\sum w(|F_o| - |F_c|)^2/\sum F_o^2)^{1/2}$] values were 0.056 and 0.045, respectively, adopting $1/\sigma(F_j)^2$. The standard deviation was 2.7, in which deviation of an observation, [$\sum w(|F_o| - |F_c|)^2/(m - n)]^{1/2}$, was 1.45, where the numbers of reflections (*m*) and refined parameters (*n*) were 2800 and 326, respectively. A final difference Fourier map showed smaller residual peaks than 0.6 e Å^{-3}. No attempt was made to

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Table II. Positional Parameters (×10⁴)

atom	x	y	z
Pd(1)	879 (0.5)	2003 (1)	2348 (1)
Pd(2)	1789 (0.5)	305 (1)	3759 (1)
Cl1	-258 (1)	2941 (4)	1779 (2)
Cl2	1738 (2)	-285 (4)	5171 (2)
N1	269 (4)	-414 (10)	2867 (6)
C10	713 (5)	346 (11)	2935 (7)
C11	-248 (6)	-1260 (12)	2857 (8)
C12	-576 (6)	-732 (12)	3342 (7)
C13	-1089 (6)	-1607 (14)	3329 (9)
C14	-1253 (7)	-2903 (16)	2844 (10)
C15	-905 (7)	-3409 (15)	2372 (10)
C16	-372 (6)	-2571 (13)	2386 (9)
C17	-387 (6)	699 (12)	3819 (8)
C18	17 (8)	-3025 (16)	1879 (11)
N2	2018 (5)	838 (10)	2101 (7)
C20	1758 (5)	967 (12)	2576 (8)
C21	2059 (5)	816 (12)	1269 (8)
C22	2652 (6)	1423 (15)	1332 (9)
C23	2686 (8)	1302 (16)	471 (10)
C24	2134 (8)	702 (19)	-382 (10)
C25	1569 (6)	118 (16)	-391 (8)
C26	1510 (6)	191 (13)	423 (8)
C27	3219 (6)	2117 (17)	2254 (10)
C28	863 (6)	-355 (16)	404 (9)
N3	2898 (4)	-18 (10)	4527 (6)
C31	3331 (6)	1096 (14)	4723 (10)
C32	4047 (7)	922 (16)	5266 (10)
C33	4340 (6)	-436 (16)	5593 (9)
C34	3883 (6)	-1561 (14)	5371 (9)
C35	3162 (6)	-1304 (12)	4838 (8)
N4	1191 (5)	3803 (10)	1858 (7)
C41	882 (7)	4148 (15)	904 (9)
C42	1118 (8)	5361 (17)	613 (10)
C43	1665 (8)	6171 (15)	1332 (11)
C44	1963 (7)	5820 (15)	2305 (11)
C45	1721 (7)	4628 (15)	2540 (10)

locate the hydrogen atoms. The positional parameters are given in Table II. Anomalous dispersion effects and atomic scattering factors were taken from the usual tabulation.[13]

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Supplementary Material Available: Listings of nonbonded distances (SM Table I), least-squares planes and interplanar angles (SM Table II), and anisotropic thermal parameters (SM Table III) (3 pages). Ordering information is given on any current masthead page.

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Can F₂H⁺ Exist in the Topological Form FHF⁺?

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Although the anion[1] F_2H^- and the neutral radical[2] F_2H have been studied extensively, the cation analogue, F_2H^+, has only oblique literature references.[3] The potential energy surface of the cation is of interest in its own right. Futher, the development

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Table I. Energies and Structures of FHF⁺

struct	method	r(FF), Å	r(FH), Å	angle, deg	energy, hartrees
$D_{\infty h}{}^a$	HF	2.108	1.054		-198.690 15
	MP2	2.144	1.072		-199.177 49
	MP3	2.160	1.080		-199.146 21
C_{2v}	HF	1.394	1.183	72.2ᵇ	-198.800 33
	MP2	1.487	1.200	76.6	-199.296 87
	MP3	1.477	1.186	77.0	-199.248 39
C_s	HF	1.375	0.953	109.0ᶜ	-198.875 90
	MP2	1.427	0.984	102.6	-199.338 92
	MP3	1.416	0.972	104.4	-199.300 79
$C_{\infty v}$	HF	1.413	0.972		-198.825 59
	MP2	1.403	1.006		-199.268 66
	MP3	1.404	0.995		-199.232 94

^{a} A $C_{\infty v}$ structure of this topology with FH bond lengths of 1.200 and 1.054 Å gave a HF energy of -198.685 24 hartrees and optimized to $D_{\infty h}$. ^{b} Measure of angle F–H–F. ^{c} Measure of angle F–F–H.
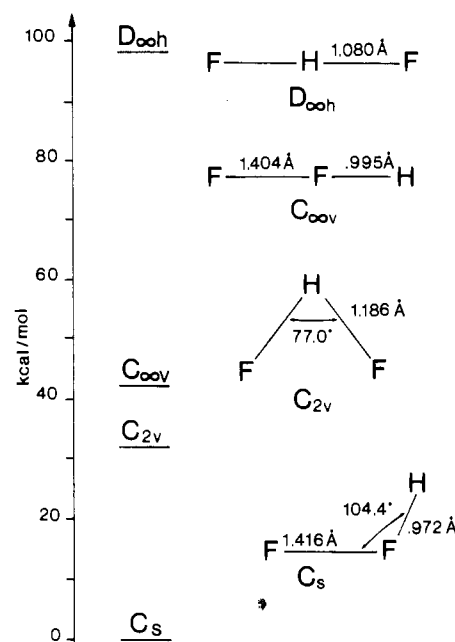

Figure 1. MP3 structures and relative energies of F₂H⁺.

of the charge reversal experiment[4] and multiphoton laser techniques makes this cation accessible in the topology FHF⁺ from the linear FHF⁻ anion. In this work we have completed ab initio calculations on both topologies FFH⁺ and FHF⁺ in order to ascertain whether or not the latter could have an independent existence, even if metastable. We also have calculated the proton affinity of F_2 and transition-state energies and harmonic vibrational frequencies for F_2H^+.

The GAUSSIAN 82 program package was employed for this study.[5] All calculations were executed by using the 6-311G(d,p) (also denoted 6-311G**) basis set.[6] To determine unambiguously

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