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THE SYNTHESIS AND CRYSTAL AND MOLECULAR STRUCTURE OF $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC_3NC_6H_5)Os_3(CO)_8$

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Summary

The complex $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC_3NC_6H_5)Os_3(CO)_8$ has been synthesized and characterized by IR, ^1H NMR and X-ray crystal structure analyses. The compound contains a dihapto-benzyne ligand bridging one edge of a triangular cluster of osmium atoms and a dihapto-formimidoyl ligand bridging a different edge on the opposite face of the cluster from the benzyne ligand.

Introduction

We are currently investigating the nature of the reactions of the cluster hydride complex $H_2Os_3(CO)_{10}$ with isocyanide molecules [1-3]. In the course of these studies we have isolated small amounts of the title compound whose ^1H NMR spectra indicated that it contained a formimidoyl, $HC{=}NC_6H_5$, ligand which was evidently formed by transfer of a hydrogen atom from the cluster to the isocyanide ligand. In hopes of more fully defining the coordinative behavior of formimidoyl ligands in cluster compounds this compound was characterized by an x-ray crystal structure analysis which is reported herein.

Experimental

Preparation of $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC{=}NC_6H_5)Os_3(CO)_8$.

0.2g of $H_2Os_3(CO)_{10}(CNC_6H_5)$ [2] in 20 ml of n-butylether was refluxed for approximately 24 hrs. The solvent was removed in vacuo. The yellow product was isolated in low yield by chromatography over $Al_2O_3\cdot6\%H_2O$ using hexanes solvent.

Crystals were grown by cooling hexanes solutions to -20°. IR:ν(CO) in hexanes: 2082m, 2048s, 2030s, 2004s, 1975s, 1965m; m.p.~195dec; ^{1}H nmr δ = 10.58s, 8.06m, 6.93m, -10.64s, +10.83s, and -12.51ppm (in d_6-acetone solvent).

Structural Analysis

All diffraction measurements were performed on an Enraf-Nonius CAD-4 fully automated four-circle diffractometer using graphite monochromatized MoK$_\alpha$-radiation. Unit cells were determined and refined using 25 randomly collected reflections obtained using the CAD-4 automatic search, center, index and least squares routines.

Structure Solution.

All calculations were performed on a Digital PDP 11/45 computer using the Enraf-Nonius SDP program library. Anomalous dispersion corrections [4a] were made for scattering [4b] by all nonhydrogen atoms. Least squares refinements minimized the function $\Sigma w(F_{obs}-F_{calc})^2$ where the weighting factor $w = 1/\sigma(F)^2$. Unweighted and weighted residuals were determined by the formulae

$$R = \frac{\Sigma\|F_{obs}|-|F_{calc}\|}{\Sigma|F_{obs}|}$$

$$R_w = \left[\frac{\Sigma w(|F_{obs}|-|F_{calc}|)^2}{\Sigma w|F_{obs}|^2}\right]^{1/2}$$

Crystal data and data collection parameters are listed in Table 1.

A crystal with dimensions 0.16mm x 0.34mm x 0.17mm was cleaved and mounted in a thin-walled glass capillary. The crystal faces were identified as $2\bar{1}\bar{1}$, $\bar{2}11$, 102, 010, $0\bar{1}0$ and $\bar{1}2\bar{9}$ with the latter being assigned to the cleavage face. ω-scan peak widths at half height lay in the range 0.15-0.25°. Of the 5413 reflections which were measured 3879 conformed to the relation $F^2 \geq 3.0\sigma(F^2)$ and were used in the subsequent structure solution and refinement. The linear absorption coefficient is 169.5 cm^{-1}. The data were corrected for absorption using the Gaussian integration method.

TABLE 1. Experimental Data for X-ray Diffraction Study of $H_3(\mu-\eta^2-C_6H_4)-(\mu-\eta^2-HC{=}NC_6H_5)Os_3(CO)_8$

(A) Crystal Parameters at 22°

Space Group: $P\bar{1}$

$a = 9.380(2)$ Å	$V = 1196.0(4)$ Å^3
$b = 9.659(2)$ Å	$Z = 2$
$c = 15.022(3)$ Å	Mol. wt. 975.9
$\alpha = 73.96(1)°$	$\rho_{calc} = 2.71\ g.cm^{-3}$
$\beta = 70.10(2)°$	
$\gamma = 72.28(2)°$	

(B) Measurement of Intensity Data

Radiation: Mo Kα; $\lambda = 0.71073$Å

Monochromator: Graphite

Takeoff Angle: 2.5°

Detector Aperture: Horizontal, A + B tan θ

A = 3.0mm; B = 1.0mm; Vertical, 4.0mm

Crystal-Detector Distance: 330mm

Crystal Orientation: b^* oriented 5.7° from Ø-axis of diffractometer

Reflections measured: $+h, \pm k, \pm \ell$

Max 2θ: 55°

Scan Type: couple θ(crystal)-2θ(counter)

Scan Speed: variable max θ = 10.00 min^{-1}

min θ = 1.25° min^{-1}

θ Scan Width = 0.80 + 0.347 tanθ ° on each side of calc. position

Background: moving crystal-moving counter

1/4 additional scan at each end of scan

Std. Reflections: 3 measured after approx. each

100 data reflections showed only random fluctuation of + 3%

Reflections measured: 5413

Data used ($F^2 > 3.0\ \sigma(F^2)$): 3379 reflections

(C) Treatment of Data

Absorption coeff: $\mu = 169.5\ cm^{-1}$

Grid: 10x8x10

Transmission factors: max. 0.141; min. 0.037

Ignorance factor: p = 0.05

Decay correction: min. 0.99; max. 1.04

The structure was solved by a combination of Patterson and difference Fourier techniques. Full matrix least squares refinement using anisotropic thermal parameters for all nonhydrogen atoms converged to the final residuals R = 0.067 and R_w = 0.088. Although many hydrogen atoms were observed in differenc Fourier syntheses, all hydrogen positions were calculated using idealized geometry. Hydrogen atoms were included in structure factor calculations using isotropic temperature factors of 5.0, but they were not refined. The largest peaks in a final difference Fourier synthesis were 4.1-4.4 $e^-/\mathring{A}^3$ and were clustered about the metal atoms. The largest value of the shift/error parameter on the final cycle of refinement was 0.13. The error in an observation of unit weight was 2.91. Final fractional atomic coordinates are listed in Table 2.

Table 2. Final Fractional Atomic Coordinates with Esds for $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC{=}NC_6H_5)Os_3(CO)_8$

Atoms	x/a	y/b	z/c	Atoms	x/a	y/b	z/c
OS1	0.34074(7)	0.12678(7)	0.35575(5)	C5	0.554(2)	0.296(2)	0.014(1)
OS2	0.47078(8)	0.20189(7)	0.15113(4)	C6	0.261(2)	0.308(2)	0.152(1)
OS3	0.56400(7)	0.31794(7)	0.27932(5)	C7	0.648(2)	0.305(2)	0.381(1)
O1	0.231(2)	0.073(2)	0.577(1)	C8	0.654(1)	0.484(2)	0.200(2)
O2	0.548(2)	-0.188(1)	0.338(1)	C11	0.329(2)	0.445(1)	0.333(1)
O3	0.056(2)	0.070(2)	0.329(1)	C12	0.230(2)	0.352(2)	0.358(1)
O4	0.410(2)	-0.075(2)	0.127(1)	C13	0.072(2)	0.426(2)	0.378(1)
O5	0.587(2)	0.351(2)	-0.060(1)	C14	0.019(2)	0.572(3)	0.379(2)
O6	0.139(2)	0.369(2)	0.150(1)	C15	0.119(3)	0.656(2)	0.359(2)
O7	0.705(2)	0.303(2)	0.438(1)	C16	0.280(2)	0.593(2)	0.332(1)
O8	0.711(2)	0.570(2)	0.156(2)	C21	0.808(2)	-0.032(2)	0.126(1)
N	0.705(2)	0.095(1)	0.1661(9)	C22	0.813(2)	-0.048(2)	0.034(1)
C1	0.271(2)	0.091(2)	0.496(2)	C23	0.912(2)	-0.164(2)	-0.008(1)
C2	0.475(2)	-0.071(2)	0.342(1)	C24	1.011(3)	-0.269(2)	0.041(2)
C3	0.167(2)	0.090(2)	0.337(1)	C25	1.004(3)	-0.258(3)	0.134(2)
C4	0.433(2)	0.025(2)	0.137(1)	C26	0.904(3)	-0.138(2)	0.172(1)
				C27	0.745(2)	0.156(2)	0.216(1)

Anisotropic thermal parameters are listed in Table 3. Bond distances and angles with estimated standard deviations determined from the inverse matrix obtained on the final cycle of refinement are listed in Tables 3 and 4.*

Results and Discussion

The molecular structure of $H_3(\mu\text{-}\eta^2\text{-}C_6H_4)(\mu\text{-}\eta^2\text{-}HC{=}NC_6H_5)Os_3(CO)_8$ is shown in the Figure. The complex consists of a triangular cluster of osmium atoms. There are eight normal linear carbonyl groups in addition a C_6H_4, benzyne, and a $HC{=}NC_6H_5$, N-phenylformimidoyl,ligand.

The benzyne ligand bridges the one edge of the cluster along the Os(1)-Os(3) bond. The carbon atom C(11) is bonded solely to osmium atom Os(3), Os(3)-C(11) = 2.165(9)Å and carbon atom C(12) is bonded solely to Os(1), Os(1)-C(12) = 2.107(10)Å. These distances are very similar to the osmium-carbon distances found in three other triosmium-benzyne complexes even though the benzyne ligands in each of these latter complexes bridged the face of Os_3 cluster [5,6]. The average carbon-carbon bond distance around the benzyne ring is 1.37Å and within the precision of determinations there do not appear to be any significant (greater than 3σ) deviations from that value. The identification of the benzyne ring in this complex was a complete surprise. Its origin must have been an isocyanide ligand but mechanistic details are not presently known. Interestingly, the preparation of several benzyne-triosmium complexes through the activation of triphenylphosphine ligands have been reported [5-7].

The phenylformimidoyl ligand bridges the Os(2)-Os(3) edge of the cluster and is on the opposite side of the Os_3 plane from the benzyne ligand. The bond distances Os(3)-C(27) = 2.082(14)Å, Os(2)-N = 2.186(9)Å and C(27)-N = 1.274(14)Å are very similar to the distances Os-C = 2.075(9)Å, Os-N = 2.150(6)Å,

(continued on p. 246)

* The table of final observed and calculated structure factor amplitudes has been deposited as NAPS Document No. 03427 (29 pages). Order form ASIS/NAPS, c/o Microfiche Publications, P.O. Box 3513, Grand Central Station, New York, N.Y. 10017. A copy may be secured by citing the document number, remitting $7.25 for photocopies or $3.00 for microfiche. Advance payment is required. Make checks payable to Microfiche Publications.

Table 3. Final Anisotropic Thermal Parameters with Esds for $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC=NC_6H_5)Os_3(CO)_8$

Atom	β(1,1)	β(2,2)	β(3,3)	β(1,2)	β(1,3)	β(2,3)
OS1	0.00948(6)	0.00871(6)	0.00539(3)	-0.0059(1)	-0.00542(7)	-0.00155(7)
OS2	0.01300(7)	0.00906(6)	0.00492(3)	-0.0032(1)	-0.00826(6)	-0.00229(7)
OS3	0.01061(7)	0.01056(6)	0.00524(3)	-0.0088(1)	-0.00485(7)	-0.00317(7)
O1	0.019(2)	0.020(2)	0.0040(7)	-0.005(4)	-0.001(2)	0.001(2)
O2	0.021(2)	0.009(2)	0.0118(12)	-0.005(3)	-0.008(3)	-0.003(2)
O3	0.019(2)	0.022(2)	0.0177(12)	-0.013(3)	-0.020(2)	-0.012(2)
O4	0.033(2)	0.017(2)	0.0110(9)	-0.022(3)	-0.019(2)	-0.005(2)
O5	0.032(3)	0.013(2)	0.0053(7)	-0.008(4)	-0.009(2)	0.001(2)
O6	0.021(2)	0.016(2)	0.0131(9)	0.009(3)	-0.022(2)	-0.010(2)
O7	0.020(2)	0.042(3)	0.0080(7)	-0.020(3)	-0.010(2)	-0.016(2)
O8	0.025(3)	0.019(2)	0.0163(18)	-0.025(4)	-0.007(4)	0.002(3)
N	0.012(2)	0.008(1)	0.0041(6)	-0.003(2)	-0.004(2)	-0.002(1)
C1	0.009(2)	0.010(2)	0.0091(12)	0.004(4)	-0.006(2)	-0.004(3)
C2	0.013(2)	0.013(2)	0.0075(10)	-0.007(3)	-0.006(2)	-0.006(2)
C3	0.017(3)	0.007(2)	0.0062(10)	-0.007(3)	-0.003(3)	-0.002(2)
C4	0.018(2)	0.016(3)	0.0073(9)	0.000(4)	-0.014(2)	-0.007(2)
C5	0.022(3)	0.007(2)	0.0064(9)	-0.007(3)	-0.011(2)	-0.000(2)
C6	0.018(2)	0.008(2)	0.0081(9)	-0.002(3)	-0.013(2)	-0.004(2)
C7	0.014(3)	0.017(3)	0.0056(10)	-0.012(4)	-0.001(3)	-0.002(3)
C8	0.019(3)	0.022(3)	0.0065(11)	-0.026(4)	-0.001(3)	-0.005(3)
C11	0.009(2)	0.006(1)	0.0047(7)	-0.004(2)	-0.003(2)	-0.003(1)
C12	0.011(2)	0.008(2)	0.0054(8)	-0.004(3)	-0.006(2)	-0.002(2)
C13	0.012(2)	0.017(2)	0.0052(8)	-0.008(4)	-0.004(2)	-0.005(2)
C14	0.014(3)	0.018(3)	0.0073(11)	-0.000(5)	-0.007(3)	-0.007(3)
C15	0.021(3)	0.012(2)	0.0076(11)	-0.000(5)	-0.008(3)	-0.005(3)
C16	0.018(3)	0.012(2)	0.0072(9)	-0.002(4)	-0.009(2)	-0.007(2)

Table 3. (cont.)

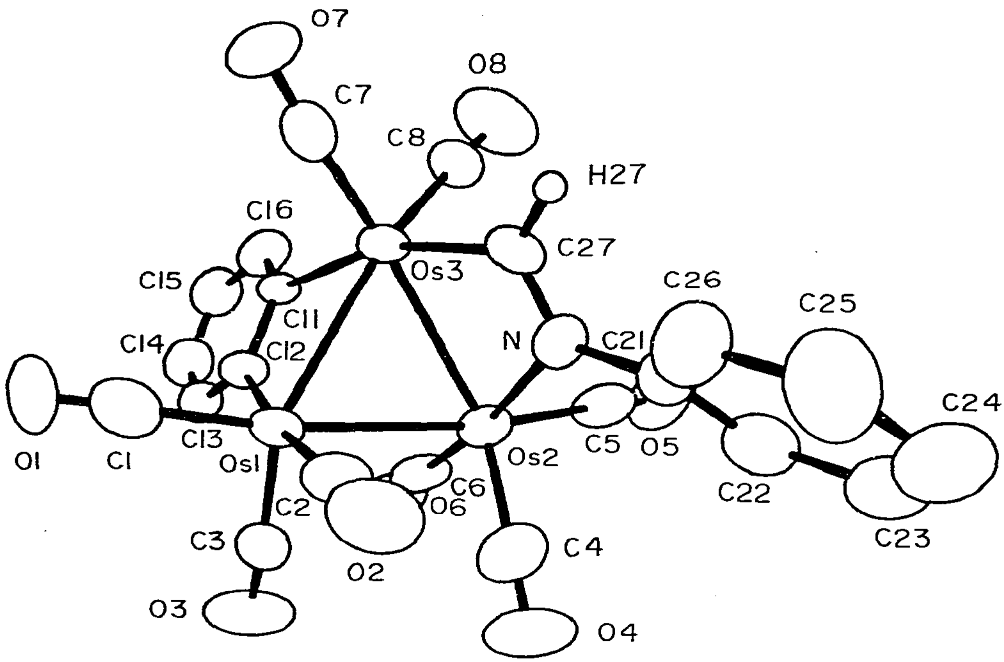
Atom	β(1,1)	β(2,2)	β(3,3)	β(1,2)	β(1,3)	β(2,3)
C21	0.012(2)	0.012(2)	0.0041(7)	-0.007(3)	-0.002(2)	-0.003(2)
C22	0.013(2)	0.014(2)	0.0076(11)	-0.005(4)	-0.007(2)	-0.004(3)
C23	0.018(3)	0.015(2)	0.0059(10)	-0.012(4)	-0.005(2)	-0.004(2)
C24	0.019(3)	0.008(2)	0.0133(17)	-0.003(4)	-0.004(4)	-0.010(3)
C25	0.017(3)	0.022(4)	0.0063(12)	0.003(6)	-0.005(3)	-0.003(4)
C26	0.018(3)	0.013(2)	0.0044(9)	-0.004(5)	-0.005(2)	-0.001(2)
C27	0.010(2)	0.023(3)	0.0040(7)	-0.017(3)	-0.004(2)	-0.001(2)

The form of the anisotropic thermal parameter is:

$$\mathrm{Exp}[-(\beta(1,1)h^2 + \beta(2,2)k^2 + \beta(3,3)\ \ell^2 + \beta(1,2)hk + \beta(1,3)h\ell + \beta(2,3)k\ell\ )]$$

Table 4. Bond Distances with Esds for $H_3(\mu\text{-}\eta^2\text{-}HC{=}NC_6H_5)Os_3(CO)_8$.

Atoms	Distance (Å)	Atoms	Distance (Å)
Os(1)-Os(2)	2.866(1)	C(27)-N	1.274(14)
Os(1)-Os(3)	2.942(1)	N-C(21)	1.444(13)
Os(2)-Os(3)	2.944(1)	C(21)-C(22)	1.415(17)
Os(1)-C(1)	1.940(15)	C(22)-C(23)	1.371(18)
Os(1)-C(2)	1.963(12)	C(23)-C(24)	1.386(21)
Os(1)-C(3)	1.895(13)	C(24)-C(25)	1.414(22)
Os(1)-C(12)	2.107(10)	C(25)-C(26)	1.373(19)
Os(2)-C(4)	1.925(15)	C(26)-C(21)	1.352(16)
Os(2)-C(5)	1.992(13)	C(1)-O(1)	1.124(20)
Os(2)-C(6)	1.923(12)	C(2)-O(2)	1.138(14)
Os(2)-N	2.186(9)	C(3)-O(3)	1.166(15)
Os(3)-C(7)	1.904(14)	C(4)-O(4)	1.107(16)
Os(3)-C(8)	1.940(15)	C(5)-O(5)	1.082(18)
Os(3)-C(11)	2.165(9)	C(6)-O(6)	1.119(15)
Os(3)-C(27)	2.082(14)	C(7)-O(7)	1.146(15)
C(11)-C(12)	1.381(13)	C(8)-O(8)	1.070(17)
C(12)-C(13)	1.405(16)		
C(13)-C(14)	1.343(19)		
C(14)-C(15)	1.332(21)		
C(15)-C(16)	1.404(19)		
C(16)-C(11)	1.364(14)		



An ORTEP diagram of $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC{=}NC_6H_5)Os_3(CO)_8$ showing 50% probability ellipsoids. The hydrogen atom H27 is shown in an idealized position with an artificial temperature factor of 1.0.

and C-N = 1.320(10)Å which were found for an edge-bridging phenylfomimidoyl ligand in the complex $(\mu-H)(\mu-\eta^2-HC{=}NC_6H_5)Os_3(CO)_9(P(OCH_3)_3)$, [2]. The short carbon-nitrogen, C(27)-N, distance emphasizes the double bond character of this bond. The hydrogen atom H(27) was not observed crystallographically and is shown in the figure in an idealized position. The most convincing evidence for its location on the carbon atom C(27) is provided by the ^1H NMR spectrum which shows a resonance at δ = 10.58 ppm. These shifts are well-known to be characteristic of hydrogen atoms on formimidoyl ligands [2,8-12].

The metal-hydride ligands were not observed crystallographically either. On the basis of the ^1H NMR spectrum which showed resonances at δ = -10.64, -10.83, and -12.51 ppm, the number of hydride ligands appears to be three. This is also consistent with bonding considerations assuming the benzyne ligand serves as a two electron donor and an overall charge on the complex as zero.

Table 5. Bond Angles with Esds for $H_3(\mu-\eta^2-C_6H_4)(\mu-\eta^2-HC=NC_6H_5)Os_3(CO)_8$

Atoms	Angle(deg)	Atoms	Angle(deg)
Os(1)-Os(2)-Os(3)	60.84(1)	C(7)-Os(3)-C(8)	92.6(6)
Os(2)-Os(1)-Os(3)	60.88(1)	C(7)-Os(3)-c(27)	95.3(5)
Os(1)-Os(3)-Os(2)	58.28(1)	C(7)-Os(3)-C(11)	100.0(5)
Os(2)-Os(1)-C(1)	172.0(4)	C(8)-Os(3)-C(27)	95.4(6)
Os(2)-Os(1)-C(2)	84.7(4)	C(8)-Os(3)-C(11)	97.3(5)
Os(2)-Os(1)-C(3)	90.4(4)	C(27)-Os(3)-C(11)	159.7(4)
Os(2)-Os(1)-C(12)	89.4(3)	Os(1)-C(12)-C(11)	115.0(7)
Os(3)-Os(1)-C(1)	111.2(4)	Os(1)-C(12)-C(13)	131.1(9)
Os(3)-Os(1)-C(2)	103.2(4)	Os(3)-C(11)-C(12)	107.5(6)
Os(3)-Os(1)-C(3)	143.7(3)	Os(3)-C(11)-C(16)	128.4(9)
Os(3)-Os(1)-C(12)	67.7(3)	C(11)-C(12)-C(13)	113.1(9)
C(1)-Os(1)-C(2)	97.4(5)	C(12)-C(13)-C(14)	124.9(12)
C(1)-Os(3)-C(3)	97.1(5)	C(13)-C(14)-C(15)	119.8(13)
C(1)-Os(1)-C(12)	87.5(4)	C(14)-C(15)-C(16)	119.6(13)
C(2)-Os(1)-C(3)	95.0(5)	C(15)-C(16)-C(11)	118.9(13)
C(2)-Os(1)-C(12)	70.8(5)	C(16)-C(11)-C(12)	123.6(10)
C(3)-Os(1)-C(12)	92.1(4)	Os(2)-N-C(27)	112.4(7)
Os(1)-Os(2)-C(4)	89.6(4)	Os(2)-N-C(21)	125.7(7)
Os(1)-Os(2)-C(5)	168.1(3)	Os(3)-C(27)-N	113.3(8)
Os(1)-Os(2)-C(6)	84.4(4)	C(27)-N-C(21)	122.0(10)
Os(1)-Os(2)-N	90.5(2)	N-C(21)-C(26)	122.1(10)
Os(3)-Os(2)-C(4)	142.2(4)	N-C(21)-C(22)	120.5(10)
Os(3)-Os(2)-C(5)	110.1(13)	C(21)-C(22)-C(23)	122.3(12)
Os(3)-Os(2)-C(6)	107.6(3)	C(22)-C(23)-C(24)	118.8(13)
Os(3)-Os(2)-N	65.3(2)	C(23)-C(24)-C(25)	119.7(13)
C(4)-Os(2)-C(5)	101.7(5)	C(24)-C(25)-C(26)	119.0(13)
C(4)-Os(2)-C(6)	90.9(5)	C(25)-C(26)-C(21)	122.9(12)
C(4)-Os(2)-N	94.3(4)	C(26)-C(21)-C(22)	117.3(10)
C(5)-Os(2)-C(6)	91.8(5)	Os(1)-C(1)-O(1)	179.0(10)
C(5)-Os(2)-N	92.2(4)	Os(1)-C(2)-O(2)	177.3(12)
C(6)-Os(2)-N	170.7(4)	Os(1)-C(3)-O(3)	176.8(12)
Os(1)-Os(3)-C(7)	106.8(4)	Os(2)-C(4)-O(4)	178.7(12)
Os(1)-Os(3)-C(8)	157.8(5)	Os(2)-C(5)-O(5)	174.5(12)
Os(1)-Os(3)-C(27)	93.6(3)	Os(2)-C(6)-C(6)	178.6(12)
Os(1)-Os(3)-C(11)	69.1(2)	Os(3)-C(7)-O(7)	175.3(12)
Os(2)-Os(3)-C(7)	155.5(4)	Os(3)-C(8)-O(8)	176.2(16)
Os(2)-Os(3)-C(8)	106.7(4)		
Os(2)-Os(3)-C(27)	68.6(3)		
Os(2)-Os(3)-C(11)	92.5(2)		

Table 6 lists least squares planes of important atomic groupings. The benzyne and formimidoyl ligands are nearly perpendicular to the plane of the Os_3 triangle. The dihedral angles are 79.0° and 72.9°, respectively.

There are no unusually short intermolecular contacts. The shortest contacts are between oxygen atoms of the carbonyl ligands, e.g. O(1)---O(3) = 3.12Å, O(4)---O(5) = 3.09Å.

Table 6. Unit Weighted Least Squares Atomic Planes for $H_3(\mu\text{-}\eta^2\text{-}C_6H_4)(\mu\text{-}\eta^2\text{-}HC{=}NC_6H_5)Os_3(CO)_8$.

A)

Plane No.	Atoms	Distance from Plane (Å)
1	Os(1)	0.00
	Os(2)	0.00
	Os(3)	0.00
	C(11)*	1.94(2)
	C(12)*	1.90(2)
	C(27)*	-1.83(2)
	N *	-1.91(1)
2	C(11)	0.01(2)
	C(12)	-0.02(2)
	C(13)	0.01(2)
	C(14)	0.01(2)
	C(15)	-0.02(2)
	C(16)	0.01(2)
	Os(1)*	-0.080(1)
	Os(2)*	2.540(1)
	Os(3)*	0.311(1)
3	Os(2)	0.019(1)
	Os(3)	-0.021(1)
	C(27)	0.05(2)
	N	-0.05(2)
	Os(1)*	-2.391(1)
4	C(21)	0.01(2)
	C(22)	-0.01(2)
	C(23)	0.00(2)
	C(24)	0.02(3)
	C(25)	-0.01(3)
	C(26)	0.00(2)
	N *	0.05(2)
	C(27)*	0.71(2)

B) Dihedral Angles between Planes

Planes	Angles(deg)
1-2	79.0
1-3	72.9
1-4	-86.2
2-3	48.5
2-4	79.2
3-4	35.0

C) Equations of the Planes are of the Form

$$Ax + By + Cz - D = 0$$

Plane	A	B	C	D
1	-0.5776	0.8153	-0.0418	-1.5775
2	-0.2723	-0.0075	-0.9622	-6.1474
3	0.3108	0.5412	-0.7814	1.3690
4	0.7852	0.4538	-0.4212	5.6593

*These atoms were not used in defining the plane.

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