an acetonitrile solution containing 0.03 mL (0.36 mmol) of concentrated hydrochloric acid and 20.4 mg (0.18 mmol) of 30% hydrogen peroxide. The mixture was stirred for 10 min at room temperature and filtered. The resulting black solid was washed with acetonitrile and dried under a nitrogen stream. Soxhlet extraction of the solid overnight with carbon disulfide afford a deeply colored solution that deposited black crystals upon slow evaporation. IR (KBr, cm^{-1}): 2320 (m), 1435 (s), 1365 (s), 912 (s). UV-vis (CH_2Cl_2, λ_{max}, nm (ϵ)): 830 (1374), 710 (3531), 485 (2045).

Anal. Calcd for $C_8H_{12}NiSe_4$: C, 19.89; H, 2.49; Ni, 17.16; Se, 65.47. Found: C, 19.75; H, 2.53; Ni, 16.84; Se, 61.38.

Registry No. III, 17107-91-4; IV, 66251-92-1; VIa·Bu_4N, 97316-36-4; VIb·Bu_4N, 97316-38-6; $[NiSe_4C_4(CF_3)_4]AsPh_4$, 20413-89-2; $NiSe_4C_4(CH_3)_4$, 97316-39-7; $Ni(OAc)_2$, 373-02-4; hexafluoro-2-butyne, 692-50-2.

Contribution from the AFRC Unit of Nitrogen Fixation,
University of Sussex, Brighton BN1 9RQ,
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A Convenient One-Step Synthesis of Thiolato Complexes with Molybdenum–Molybdenum Triple Bonds. X-ray Crystal Structure of $[Mo_2(SC_6H_2\text{-}i\text{-}Pr_3)_6]$

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There is considerable current interest in the chemistry of dinuclear complexes with metal–metal multiple bonds,[2a,b] particularly involving alkoxide ligands. The recent reports of the multistage synthesis of $[Mo_2(SC_6H_2Me_3)_6]$[2c] and related species in low yield prompts us to report a very convenient one-step route into the same series of complexes.

The sodium salt of the bulky thiolate 2,4,6-triisopropylthiophenolate (TIPTNa) reacts with $[MoCl_4(thf)_2]$ (thf = tetrahydrofuran) in the presence of CO to give $[Mo(CO)_2(TIPT)_3]^-$,[3] and in the absence of CO no characterizable species were obtained. However, in 1,2-dimethoxyethane as solvent $MoCl_4$ gives a mixture of $[Mo_2(TIPT)_6]$ (I) and $[MoO(TIPT)_4]^-$ (II) in yields of 20–25% and 45–50%, respectively.

Experimental Section

All reactions were carried out under an atmosphere of dinitrogen with use of conventional Schlenk-tube techniques. The solvents were dried over appropriate drying agents and freshly distilled under dinitrogen prior to use. ^1H NMR spectra were recorded on a JEOL FX90Q instrument in deuteriodichloromethane with tetramethylsilane as internal standard. Infrared spectra were recorded on a Unicam SP 2000 spectrophotometer. Microanalyses were performed by Mrs. A. Olney at the University of Sussex or C. J. Macdonald at the Unit of Nitrogen Fixation. 2,4,6-Triisopropylthiophenol and 2,4,6-trimethylthiophenol were prepared by $LiAlH_4$ reduction of the commercially available sulfonyl chlorides. $MoCl_4$[4] was prepared by literature methods.

Preparation of $[Mo_2(SC_6H_2Me_3)_6]$. 2,4,6-Trimethylthiophenol (TMTH) (0.72 mL, 4.7 mmol) in 1,2-dimethoxyethane (40 mL) was treated with sodium metal (0.5 g in small pieces) and stirred at 50 °C for 1 h. It was then cooled to room temperature and filtered to remove excess sodium. $MoCl_4$ (0.28 g, 0.12 mmol) was then added to the solution of the sodium salt. The solution became dark purple and after stirring for 0.5 h was orange-brown. It was then filtered through Celite filter aid and evaporated to dryness. Extraction with hexane gave orange-red $[Mo_2(SC_6H_2Me_3)_6]$, which was recrystallized from thf–hexane; yield 28%. Anal. Calcd for $Mo_2C_{54}H_{66}S_6$: C, 59.0; H, 6.0. Found: C, 58.7; H, 6.4.

Table I. Summary of Crystal Data and Experimental Details for the Structural Study of $[Mo_2(SC_6H_2\text{-}i\text{-}Pr_3)_6]$

(A) Crystal Parameters[a] at 23 °C

a = 17.679 (3) Å	V = 8998.3 (14) Å^3
b = 21.019 (4) Å	space group: *Pban*
c = 24.215 (5) Å	Z = 4
	D_{calcd} = 1.18 g/cm^3

(B) Measurement of Intensity Data

cryst dimens: 0.20 × 0.24 × 0.17 mm
instrument: Nicolet R3m
radiation: Mo Kα (λ = 0.71069 Å)
scan mode: coupled θ(cryst)–2θ(counter)
scan rate: variable, 3–30°/min
scan range: $2 \leq 2\theta \leq 45°$
scan length: from $[2\theta(K\alpha_1) - 1.0]°$ to $[2\theta(K\alpha_2) + 1.0]°$
bkgd measmt: stationary counter, stationary cryst at beginning and end of each 2θ scan, each taken for 0.5 the time of the scan
stds: 3 collected every 197 reflcns; no signif dev over the 70 h of data collecn
no. of reflcns collected: 6631
no. of indep reflcns used in soln: 2525 with $I_o \geq 3\sigma(I_o)$

(C) Reduction of Intensity Data and Summary of Structure and Refinement[b]

data redn: data corrected for bkgd, attenuation, Lorentz, and polarization effects in the usual fashion
abs coeff: 8.5 cm^{-1}
abs cor: none (T_{max}/T_{min} = 1.05)
structure soln: Mo atom position located from a sharpened Patterson map all non-H atoms located on subsequent difference Fourier maps; H atoms included as fixed contributors in the final refinement cycles
atomic scattering factors: neutral atomic scattering factors used throughout anal.
anamalous dispersion: applied to all non-H atoms
final discrepancy factor:[c] R = 0.070; R_w = 0.073
goodness of fit:[d] 1.69

[a] From a least-squares fitting of the setting angle of 25 reflections. [b] All calculations were performed on a Data General Nova 3 computer with 32K of 16-bit words using local versions of the Nicolet SHELXTL interactive crystallographic software package as described in: Sheldrick, G. M. "Nicolet SHELXTL Operations Manual"; Nicolet XRD Corp.: Cupertino, CA, 1979. [c] $R = \sum[|F_o| - |F_c|/\sum|F_o|]$; $R_w = [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2}$; $w = 1/\delta^2(F_o) + g^*(F_o)^2$; g = 0.001. [d] GOF $= [\sum w(|F_o| - |F_c|)^2/(NO - NV)]^{1/2}$, where NO is the number of observations and NV is the number of variables.

Preparation of $[Mo_2(SC_6H_2\text{-}i\text{-}Pr_3)_6]$ (I). A 1,2-dimethoxyethane (40 mL) solution of the sodium salt of 2,4,6-triisopropylthiophenol (2.1 mL, 9.8 mmol) was prepared as above and a solution of $MoCl_4$ (0.38 g, 2.0 mmol) in 1,2-dimethoxyethane (20 mL) added. The resulting mixture was stirred at room temperature for 16 h and filtered through Celite filter aid. Washing of the resulting filtered solid with methanol and addition of $[Ph_4P]Br$ gave $[Ph_4P][MoO(SC_6H_2\text{-}i\text{-}Pr_3)_4]$ as a blue crystalline solid (30% yield). The filtrate was evaporated to dryness and the residue triturated with pentane (30 mL). The resulting pink-brown solid was filtered off, washed with methanol until the washings were no longer blue, and recrystallized as red prisms from dichloromethane–acetonitrile; yield 25%. Anal. Calcd for $Mo_2C_{90}H_{138}S_6$: C, 67.4; H, 8.6. Found: C, 67.2; H, 8.9.

X-ray Data Collection and Structure Solution. Red prisms of I suitable for a structure determination were obtained by slow diffusion of acetonitrile into a dichloromethane solution. The details of data collection and structure solution are summarized in Table I. Atomic positional and isotropic thermal parameters are listed in Table II.

Results and Discussion

The orange-red derivatives $[Mo_2(SAr)_6]$ (Ar = TIPT, TMT) are isolated as dark-red crystals that are indefinitely stable in air as solids and can be recrystallized in reagent grade solvents in air. The other products, the blue complexes $[MoO(SAr)_4]^-$, are

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(2) (a) Chisholm, M. H.; Rothwell, I. P. *Prog. Inorg. Chem.* **1982**, *29*, 1. (b) Cotton, F. A.; Walton, R. A. "Multiple Bonds Between Metal Atoms"; Wiley: New York, 1981. (c) Chisholm, M. H.; Corning, J. F.; Huffmann, J. C. *J. Am. Chem. Soc.* **1983**, *105*, 5924.
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0020-1669/85/1324-2866$01.50/0

Table II. Atom Coordinates (×10^4) and Temperature Factors (Å^2 × 10^3)

atom	*x*	*y*	*z*	*U*
Mo	9535 (1)	−361 (1)	22 (1)	35 (1)[a]
S(1)	8639 (2)	313 (2)	398 (2)	43 (1)[a]
S(2)	9447 (2)	−542 (2)	−933 (2)	45 (1)[a]
S(3)	10172 (2)	−1030 (2)	617 (2)	49 (1)[a]
C(11)	7980 (7)	−59 (6)	854 (5)	40 (4)
C(12)	7989 (8)	138 (6)	1406 (6)	50 (4)
C(13)	7414 (8)	−78 (7)	1777 (6)	55 (4)
C(14)	6863 (8)	−481 (7)	1581 (6)	57 (4)
C(15)	6875 (8)	−709 (7)	1036 (6)	54 (4)
C(16)	7430 (7)	−492 (6)	671 (5)	41 (4)
C(121)	8578 (10)	608 (8)	1633 (7)	67 (5)
C(122)	9008 (14)	337 (11)	2082 (9)	144 (9)
C(123)	8219 (14)	1223 (10)	1750 (10)	148 (9)
C(161)	7417 (8)	−754 (7)	93 (6)	48 (4)
C(162)	7828 (8)	−1387 (7)	78 (7)	68 (5)
C(163)	6641 (9)	−801 (8)	−152 (7)	79 (6)
C(141)	6235 (12)	−674 (11)	2009 (9)	96 (7)
C(142)	6326 (17)	−1336 (12)	2153 (12)	198 (13)
C(143)	5520 (15)	−605 (15)	1734 (13)	211 (14)
C(21)	8532 (8)	−808 (6)	−1177 (5)	44 (4)
C(22)	8441 (8)	−1454 (6)	−1324 (6)	46 (4)
C(23)	7756 (9)	−1637 (7)	−1575 (6)	58 (5)
C(24)	7220 (8)	−1228 (7)	−1675 (6)	57 (5)
C(25)	7294 (8)	−576 (7)	−1555 (6)	53 (4)
C(26)	7971 (8)	−366 (7)	−1297 (5)	49 (4)
C(221)	9065 (9)	−1946 (7)	−1264 (7)	57 (4)
C(222)	8778 (10)	−2592 (8)	−1079 (7)	87 (6)
C(223)	9515 (10)	−2003 (8)	−1778 (7)	83 (5)
C(241)	3066 (8)	4655 (7)	1184 (6)	56 (4)
C(242)	3443 (10)	4337 (8)	1680 (7)	83 (6)
C(243)	7321 (9)	675 (8)	−1049 (7)	85 (6)
C(261)	6469 (16)	−1443 (14)	−1938 (12)	140 (9)
C(262)	6092 (16)	−1941 (15)	−1602 (14)	212 (14)
C(263)	6321 (21)	−1294 (18)	−2420 (17)	292 (22)
C(31)	9825 (8)	−1834 (6)	567 (5)	44 (4)
C(32)	10165 (8)	−2243 (6)	196 (5)	46 (4)
C(33)	9929 (8)	−2895 (6)	178 (6)	53 (4)
C(34)	9358 (9)	−3072 (8)	537 (7)	67 (5)
C(35)	9047 (9)	−2686 (7)	927 (7)	67 (5)
C(36)	9269 (8)	−2052 (6)	946 (6)	48 (4)
C(321)	10859 (9)	−2053 (7)	−142 (6)	60 (5)
C(322)	10972 (10)	−2455 (8)	−653 (7)	92 (6)
C(323)	11545 (9)	−2054 (8)	212 (7)	84 (6)
C(341)	8966 (10)	−1622 (8)	1391 (7)	71 (5)
C(342)	8191 (10)	−1833 (9)	1608 (8)	96 (6)
C(343)	9519 (10)	−1569 (8)	1867 (7)	91 (6)
C(361)	9088 (17)	−3760 (14)	560 (11)	135 (9)
C(362)	8353 (19)	−3835 (14)	354 (14)	193 (15)
C(363)	9531 (20)	−4187 (16)	704 (14)	272 (17)

[a] Equivalent isotropic *U* defined as one-third of the trace of the orthogonalized U_{ij} tensor.

direct analogues of the previously reported $[MoO(SPh)_4]^-$.[7] The two products are readily separable by virtue of the insolubility of the sodium salt of the ionic oxo complex in dimethoxyethane. The source of the oxo group is unclear as the yield of oxo complex is only slightly diminished on carrying out the reaction in very carefully dried solvent in a glovebox at less 1 ppm of dioxygen. It is possible that it originates from the solvent or that there are oxo impurities present in the $MoCl_4$, although this contains no IR bands assignable to $Mo{=}O$.

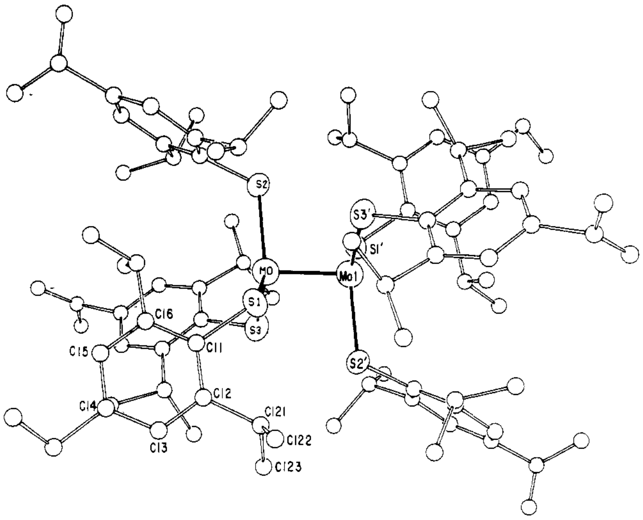

Figure 1. ORTEP diagram of the structure of $[Mo_2(SC_6H_2\text{-}i\text{-}Pr_3)_6]$ showing atom-labeling scheme.

Table III. Comparative Bond Lengths (Å) and Angles (deg) for $[Mo_2(SC_6H_2\text{-}i\text{-}Pr_3)_6]$ and $[Mo_2(SC_6H_2Me_3)_6]$

	$[Mo_2(SC_6H_2\text{-}i\text{-}Pr_3)_6]$	$[Mo_2(SC_6H_2Me_3)_6]$[a]
Mo–Mo′	2.239 (2)	2.228 (1)
Mo–S1	2.313 (4)	2.325 (2)
Mo–S2	2.348 (4)	
Mo–S3	2.306 (4)	
S1–C11	1.786 (13)	1.792 (5)
S2–C21	1.815 (14)	
S3–C31	1.798 (14)	
∠Mo′–Mo–S1	96.1 (4)	96.6 (2)
∠Mo′–Mo–S2	96.4 (1)	
∠Mo′–Mo–S3	94.9 (1)	
∠Mo–S1–C11	114.9 (4)	110.1 (2)
∠Mo–S2–C21	115.7 (2)	
∠Mo–S3–C31	111.3 (2)	
∠S1–Mo–S2	116.2 (1)	118.7 (1)
∠S1–Mo–S3	117.5 (1)	
∠S2–Mo–S3	123.3 (1)	

[a] $[Mo_2(SC_6H_2Me_3)_6]$ has crystallographically imposed S_6 symmetry.

The ^1H NMR spectrum of I is much more complex than that of $[Mo_2(TMT)_6]$, which Chisholm et al. reported to display a simple pattern distinguishing only *o*- and *p*-methyl groups, with *o*-methyls all equivalent. By contrast I shows three distinct multiplets of equal intensity for the *i*-Pr methyne protons. A well-defined heptet at 2.85 ppm is assigned to the equivalent *p*-*i*-Pr methyne protons, while a low-field unresolved multiplet ($\delta = 4.6$) is assigned to the *o*-*i*-Pr methyne protons proximal to the Mo–Mo bond axis and the higher field unresolved multiplet ($\delta = 2.4$) is ascribed to the distal methyne protons.[2b] Whereas concerted rotation of the $-SC_4H_2Me_3$ groups about the Mo–S bonds in $[Mo_2(TMT)_6]$ results in exchange of proximal and distal methyl groups at room temperature, the considerably more significant steric requirements of the TIPT group inhibit rotation and the proximal and distal methyne groups are frozen out.[8] The infrared spectra of the dinuclear complexes show only bands assignable to the coordinated thiolate ligands. The oxo complexes showed $\nu(Mo{=}O)$ as a medium-intensity band at 940 cm^{-1} and were shown to be identical with samples prepared in high yield by other routes. Full details of the chemistry, spectroscopy, and redox properties of the complexes $[MoO(SAr)_4]^-$ (M = Mo, W, Re; Ar = bulky thiol) will be presented elsewhere.

Confirmation of the presence of a $Mo{\equiv}Mo$ bond in I was obtained from an X-ray structure determination. An ORTEP drawing of the complex indicating the atom-labeling scheme is shown in Figure 1. Table III summarizes selected bond lengths and angles and compares these values with those reported for $[Mo_2(SC_6H_2Me_3)_6]$.[2c] The most striking feature of the two structures is their similarity, although the change from methyl to isopropyl substituents does cause a reduction in overall symmetry. The greater steric interactions within complex I are manifested in a slight increase in the Mo–Mo distance (from 2.228 (1) to 2.239 (2) Å) and wider ∠Mo–S–C angles (113.8 (2)° (av) compared to 110.1 (2)°).

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Although there is an extensive range of metal–metal-bonded alkoxides, there are none reported with ortho-substituted aryl oxides. This prevents a precise comparison of the effect of changing oxygen to sulfur on the observed chemistry. However, complex I does not react with CO at room temperature in contrast to species such as $[Mo_2(O\text{-}i\text{-}Pr)_6]$, which forms a series of carbonyl complexes.[2a,b]

The electrochemistry of complex I was studied by cyclic voltammetry in thf solution with $[n\text{-}Bu_4N][BF_4]$ as supporting electrolyte and a platinum working electrode. The complex undergoes a one-electron reversible reduction at $E_{1/2} = -0.88$ V (vs. SCE calibrated vs. the ferrocene/ferrocenium couple at +0.54 V) followed by a further irreversible one-electron reduction at $E_p = -1.72$ V. The second irreversible reduction was accompanied by thiolate anion loss. Although CO does not react with the unreduced dimer, under CO the second reduction process becomes a two-electron process due to interaction with CO. However, there was no indication of interaction with N_2 at any redox level. No oxidation waves were observed at potentials up to +1.2 V.

Acknowledgment. We thank Dr. C. J. Pickett for performing the cyclic voltammetric measurements and the NIH for the award of a grant to J.Z.

Registry No. I, 97352-51-7; I (salt entry), 97352-52-8; $[Mo_2(SC_6H_2Me_3)_6]$, 86350-27-8; $[Mo_2(SC_6H_2Me_3)_6]$ (salt entry), 97069-07-3; $MoCl_4$, 13320-71-3; $[Ph_4P][MoO(SC_6H_2\text{-}i\text{-}Pr_3)_4]$, 97352-54-0; Mo, 7439-98-7.

Supplementary Material Available: Tables of observed and calculated structure factors, bond lengths and angles, anisotropic thermal parameters, and hydrogen atom positions (36 pages). Ordering information is given on any current masthead page.

Contribution from the Department of Chemistry,
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Convenient Synthesis of *trans*-Diacidotetraammineruthenium(III) Complexes

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The chemistry of trans ruthenium(II) and ruthenium(III) tetraammine complexes has been the subject of extensive research over the past decade.[1] However, the reported synthesis[2] of *trans*-$[Ru(NH_3)_4Cl_2]Cl$, a key starting material in ruthenium ammine chemistry, was rather inefficient and inconvenient, involving several steps. We have recently found that high-valent ruthenium(VI) amine oxo complexes could easily be converted into the corresponding ruthenium(IV) and ruthenium(III) species.[3] Here an efficient synthetic procedure for *trans*-$[Ru(NH_3)_4X_2]^+$ (X = Cl, I, NCS) utilizing *trans*-$[Ru(NH_3)_4O_2]^{2+}$ as the starting material is described.

Experiment Section

Materials. Ruthenium(III) chloride trihydrate (Aldrich) was used as supplied. *trans*-$[Ru(NH_3)_4O_2]Cl_2$ was prepared according to the literature method.[4] All chemicals used were of reagent grade, and deionized water was used throughout the experiment.

***trans*-$[Ru(NH_3)_4Cl_2]Cl$.** A mixture of *trans*-$[Ru(NH_3)_4O_2]Cl_2$ (0.2 g) and ascorbic acid (2 g) in HCl (2 M, 15 cm^3) was stirred for 1 day. An orange microcrystalline solid gradually deposited upon standing (yield >60%). The purity of the complex was checked by comparing its molar extinction coefficient at 331 nm with the known value. Alternatively, $SnCl_2$ or 2-propanol could be used instead of ascorbic acid.

Table I. UV–Vis Absorption Spectra of Some *trans*-Diacidotetraammineruthenium(III) Complexes

complex	solvent	λ_{max}/nm (ϵ_{max}/cm^{-1} dm^3 mol^{-1})[a]
trans-$[Ru(NH_3)_4Cl_2]Cl$	HCl (1 M)	331 (5270)[b]
trans-$[Ru(NH_3)_4Br_2]Br$	HBr (0.1 M)	399 (5133)[b]
trans-$[Ru(NH_3)_4(NCS)_2]NCS$	H_2O	524 (12 600), 430 sh (1410), 330 br (770)
trans-$[Ru(NH_3)_4I_2]I$	H_2O	552 (5800), 425 sh (1190), 304 (12 100)

[a] Abbreviations: br, broad; sh, shoulder. [b] Isabirye, D. A. Ph.D. Thesis, University of Hong Kong, 1977.

***trans*-$[Ru(NH_3)_4I_2]I$.** An aqueous solution (20 cm^3) of *trans*-$[Ru(NH_3)_4O_2]Cl_2$ (0.1 g), ascorbic acid (2 g), and NaI (2 g) was stirred for 2 h. A dark violet-blue microcrystalline solid gradually deposited. This was filtered and purified from a hot (~70 °C) NaI solution (1 M) (overall yield >70%). Anal. Calcd for $[Ru(NH_3)_4I_2]I$: N, 10.17; I, 69.20. Found: N, 10.27; I, 68.90. IR: ν(NH) 3240, 3200, 3130 cm^{-1}; δ(NH) 1620 cm^{-1}.

***trans*-$[Ru(NH_3)_4(NCS)_2]NCS$.** An aqueous solution (20 cm^3) of *trans*-$[Ru(NH_3)_4O_2]Cl_2$ (0.1 g), ascorbic acid (2 g), and NaNCS (2 g) was stirred for 2–3 h. A dark violet-red solid gradually precipitated out. This was filtered off, washed with an ethanol–diethyl ether mixture (1:10), and dried under vacuum. Anal. Calcd for $[Ru(NH_3)_4(NCS)_2]NCS$: C, 10.50; H, 3.49; N, 28.56; S, 28.0. Found: C, 10.37; H, 3.33; N, 28.14; S, 28.4. IR: ν(NH) 3240, 3200, 3130 cm^{-1}; ν(C≡N) 2060 cm^{-1}; δ(NH) 1620 cm^{-1}, δ(NCS) 790 cm^{-1}.

Physical Measurements. Elemental analyses of the newly prepared compounds were performed by the Australian Microanalytical Service Unit. Infrared spectra were measured in Nujol mulls on a Perkin-Elmer 577 spectrophotometer (4000–200 cm^{-1}). Electronic absorption spectra of freshly prepared solutions were measured with a Beckman Acta CIII spectrophotometer and the results were tabulated in Table I.

Results and Discussion

Previous work of Taube and his co-workers[5] has shown that reduction of *trans*-$[Os(NH_3)_4O_2]Cl_2$ by $SnCl_2$ in HCl (6 M) produced *trans*-$[Os(NH_3)_4Cl_2]^+$. This synthetic method has been found to be more efficient for the general synthesis of *trans*-$[Ru(NH_3)_4X_2]^+$ (X = Cl, I, NCS). Other mild reductants, such as ascorbic acid and 2-propanol, can also very efficiently reduce *trans*-$[Ru(NH_3)_4O_2]^{2+}$, as it is a better oxidant than *trans*-$[Os(NH_3)_4O_2]^{2+}$.

The complex *trans*-$[Ru(NH_3)_4Cl_2$ prepared here is identical with that reported in the literature. The newly prepared *trans*-$[Ru(NH_3)_4I_2]I$ and *trans*-$[Ru(NH_3)_4(NCS)_2]NCS$ complexes are stable in the solid state and in acidic solutions. The similarities of their UV–vis absorption spectra with those of the reported *trans*-$[Ru(en)_2X_2]^+$[6] (X = I, NCS) support the assignment of a trans configuration. As expected, the ligand-to-metal charge-transfer energy of *trans*-$[Ru(NH_3)_4X_2]^+$ decreases in the order of X = Cl > Br > NCS > I (see Table I). *trans*-$[Ru(NH_3)_4(NCS)_2]NCS$ has also been characterized by its IR absorption bands at 2060 and 790 cm^{-1} assignable to ν(CN) and ν(CS), respectively.[7] It is difficult to ascertain whether it is an N- or S-bonded thiocyanate species. Preliminary redox kinetic work showed that this species is a good mediator for electron-transfer reactions,[8] a full account of which will be reported.

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