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Table S1.

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6, 2.

atom	x	y	z	B(eq)
Ru(1)	0.11168(4)	0.01253(3)	0.71287(3)	3.50(3)
Ru(2)	0.22381(4)	0.01100(3)	0.82643(3)	3.26(3)
Ru(3)	0.35733(4)	-0.01690(3)	0.74870(3)	3.80(3)
Ru(4)	0.25184(4)	-0.01575(3)	0.63379(3)	3.31(3)
Ru(5)	0.25154(4)	0.08949(3)	0.71848(3)	3.56(3)
Ru(6)	0.20969(4)	-0.09192(3)	0.74124(3)	3.32(3)
Cu(1)	0.02530(6)	0.20452(4)	0.99616(5)	3.89(5)
Cu(2)	0.48893(6)	0.22897(5)	0.52603(5)	4.38(5)
S(1)	0.0950(1)	0.2774(1)	0.9457(1)	5.8(1)
S(2)	-0.0657(2)	0.2506(1)	1.0574(1)	5.6(1)
S(3)	-0.0445(1)	0.1478(1)	0.9190(1)	5.1(1)
S(4)	0.1137(1)	0.14071(9)	1.0582(1)	3.5(1)
S(5)	0.3078(2)	-0.0207(1)	1.0997(1)	6.3(1)
S(6)	0.2338(2)	0.1412(1)	1.2501(1)	7.5(2)
S(7)	0.5947(2)	0.2730(1)	0.4825(2)	7.2(2)
S(8)	0.4297(2)	0.1609(1)	0.4552(1)	6.2(1)
S(9)	0.3970(2)	0.3024(1)	0.5453(1)	7.2(2)
S(10)	0.5187(2)	0.1817(1)	0.6250(1)	5.7(1)
S(11)	0.8054(2)	0.1539(2)	0.6937(2)	9.1(2)
S(12)	0.6718(2)	-0.0084(1)	0.6303(1)	6.7(2)
O(10)	0.0092(4)	0.0092(3)	0.5849(3)	7.9(4)
O(11)	-0.0270(4)	0.0279(3)	0.7987(3)	6.4(4)
O(12)	0.0899(4)	0.1544(3)	0.7049(4)	7.9(4)
O(20)	0.1140(4)	-0.0587(3)	0.9113(3)	6.1(4)
O(21)	0.1828(4)	0.1278(3)	0.8941(3)	6.8(4)

Table S1. (contd)

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	x	y	z	B(eq)
O(22)	0.3795(4)	-0.0092(3)	0.9115(3)	7.5(4)
O(30)	0.5030(4)	0.0649(4)	0.7795(4)	8.6(5)
O(31)	0.4469(4)	-0.1327(3)	0.7868(4)	7.8(4)
O(40)	0.2365(4)	-0.1162(3)	0.5348(3)	7.2(4)
O(41)	0.2316(5)	0.0700(3)	0.5209(3)	8.1(4)
O(42)	0.4311(4)	-0.0320(3)	0.6181(3)	5.9(4)
O(50)	0.3036(6)	0.1678(4)	0.6102(4)	10.3(5)
O(51)	0.3380(7)	0.1839(4)	0.8028(4)	15.2(7)
O(60)	0.2394(6)	-0.1716(3)	0.8594(4)	9.7(5)
O(61)	0.0285(4)	-0.1158(3)	0.7282(4)	7.0(4)
O(62)	0.2297(4)	-0.1992(3)	0.6520(3)	6.7(4)
C(1)	0.2352(4)	-0.0019(3)	0.7286(3)	2.8(3)
C(10)	0.0487(5)	0.0106(4)	0.6332(4)	4.8(5)
C(11)	0.0239(5)	0.0238(4)	0.7652(4)	4.2(4)
C(12)	0.1333(6)	0.1128(4)	0.7089(4)	5.2(5)
C(20)	0.1568(5)	-0.0336(4)	0.8793(4)	4.1(4)
C(21)	0.2006(5)	0.0843(4)	0.8685(4)	4.2(4)
C(22)	0.3313(6)	-0.0045(4)	0.8683(5)	5.3(5)
C(30)	0.4495(6)	0.0345(4)	0.7663(4)	4.9(5)
C(31)	0.4140(6)	-0.0888(4)	0.7715(4)	5.1(5)
C(40)	0.2400(6)	-0.0783(4)	0.5738(4)	4.8(5)
C(41)	0.2409(6)	0.0372(4)	0.5647(4)	5.3(5)
C(42)	0.3757(5)	-0.0250(4)	0.6483(4)	4.1(4)
C(50)	0.2834(6)	0.1365(4)	0.6503(5)	6.1(6)
C(51)	0.3025(8)	0.1485(5)	0.7718(5)	7.8(7)

Table S1. (contd)

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	x	y	z	B(eq)
C(60)	0.2264(7)	-0.1418(4)	0.8147(5)	6.3(6)
C(61)	0.0892(5)	-0.0892(4)	0.7287(4)	4.5(4)
C(62)	0.2227(5)	-0.1571(4)	0.6844(4)	4.1(4)
C(80)	0.0534(7)	0.3499(5)	0.9684(8)	11(1)
C(81)	-0.030(1)	0.3556(5)	0.9847(9)	12(1)
C(82)	-0.0518(7)	0.3315(5)	1.0513(5)	7.8(7)
C(83)	-0.1651(5)	0.2412(5)	1.0129(5)	6.3(6)
C(84)	-0.1781(5)	0.1794(5)	0.9848(6)	7.1(7)
C(85)	-0.1514(6)	0.1670(4)	0.9191(5)	6.0(6)
C(86)	-0.0220(6)	0.1772(5)	0.8410(5)	6.6(6)
C(87)	-0.0121(6)	0.2437(5)	0.8355(4)	6.3(6)
C(88)	0.0709(6)	0.2698(5)	0.8588(5)	6.3(6)
C(89)	0.0891(5)	0.0627(4)	1.0357(4)	4.1(4)
C(90)	0.1472(5)	0.0163(4)	1.0689(4)	4.8(5)
C(91)	0.2329(5)	0.0204(4)	1.0490(4)	4.5(4)
C(92)	0.3101(5)	0.0233(4)	1.1733(4)	5.6(5)
C(93)	0.3422(6)	0.0865(5)	1.1687(5)	6.9(6)
C(94)	0.3356(7)	0.1250(5)	1.2301(5)	7.9(7)
C(95)	0.2013(8)	0.1993(4)	1.1914(5)	7.5(6)
C(96)	0.1117(7)	0.1983(4)	1.1748(4)	6.5(6)
C(97)	0.0804(5)	0.1427(4)	1.1394(4)	4.8(5)
C(98)	0.5884(8)	0.2531(8)	0.4006(7)	11(1)
C(99)	0.552(1)	0.201(1)	0.3786(8)	18(2)
C(100)	0.4736(8)	0.1731(6)	0.3791(6)	9.0(8)
C(101)	0.3279(6)	0.1864(6)	0.4365(5)	7.7(7)

Table S1. (contd)

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	x	y	z	B(eq)
C(102)	0.3126(6)	0.2508(7)	0.4344(6)	9.0(8)
C(103)	0.3034(7)	0.2816(6)	0.4948(6)	9.3(8)
C(104)	0.432(1)	0.3688(8)	0.512(1)	15(1)
C(105)	0.500(1)	0.3775(7)	0.486(1)	21(2)
C(106)	0.5762(9)	0.3537(6)	0.4791(7)	11(1)
C(107)	0.6177(7)	0.2064(4)	0.6551(5)	7.4(6)
C(108)	0.6463(8)	0.1808(6)	0.7206(5)	8.7(7)
C(109)	0.732(1)	0.1923(5)	0.7413(6)	10.8(9)
C(110)	0.7941(6)	0.0785(5)	0.7224(5)	6.6(6)
C(111)	0.8246(6)	0.0305(6)	0.6757(6)	8.4(7)
C(112)	0.7734(6)	0.0217(6)	0.6167(5)	9.2(8)
C(113)	0.6130(5)	0.0196(4)	0.5602(4)	5.2(5)
C(114)	0.5922(5)	0.0861(4)	0.5607(4)	5.4(5)
C(115)	0.5334(5)	0.1018(4)	0.6105(4)	5.1(5)
H(1)	0.0875	0.3643	1.0033	6.0
H(2)	0.0581	0.3757	0.9313	6.0
H(3)	-0.0416	0.3981	0.9847	6.0
H(4)	-0.0633	0.3355	0.9532	6.0
H(5)	-0.1019	0.3502	1.0609	6.0
H(6)	-0.0101	0.3428	1.0829	6.0
H(7)	-0.2061	0.2487	1.0421	6.0
H(8)	-0.1695	0.2702	0.9789	6.0
H(9)	-0.1506	0.1514	1.0137	6.0
H(10)	-0.2352	0.1717	0.9830	6.0
H(11)	-0.1610	0.2022	0.8930	6.0

Table S1. (contd)

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	x	y	z	B(eq)
H(12)	-0.1821	0.1338	0.9007	6.0
H(13)	0.0269	0.1583	0.8299	6.0
H(14)	-0.0657	0.1651	0.8109	6.0
H(15)	-0.0215	0.2542	0.7908	6.0
H(16)	-0.0518	0.2628	0.8595	6.0
H(17)	0.0740	0.3097	0.8407	6.0
H(18)	0.1112	0.2447	0.8425	6.0
H(19)	0.0354	0.0543	1.0471	6.0
H(20)	0.0912	0.0589	0.9901	6.0
H(21)	0.1483	0.0223	1.1145	6.0
H(22)	0.1269	-0.0234	1.0586	6.0
H(23)	0.2482	0.0622	1.0494	6.0
H(24)	0.2335	0.0049	1.0062	6.0
H(25)	0.2560	0.0257	1.1861	6.0
H(26)	0.3435	0.0021	1.2054	6.0
H(27)	0.3983	0.0840	1.1608	6.0
H(28)	0.3128	0.1063	1.1337	6.0
H(29)	0.3618	0.1631	1.2243	6.0
H(30)	0.3622	0.1043	1.2659	6.0
H(31)	0.2154	0.2382	1.2091	6.0
H(32)	0.2279	0.1930	1.1530	6.0
H(33)	0.0854	0.2012	1.2139	6.0
H(34)	0.0982	0.2328	1.1484	6.0
H(35)	0.0225	0.1430	1.1370	6.0
H(36)	0.1001	0.1075	1.1621	6.0

Table S1. (contd)

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	x	y	z	B(eq)
H(37)	0.5612	0.2854	0.3779	6.0
H(38)	0.6434	0.2508	0.3887	6.0
H(39)	0.5575	0.2035	0.3322	6.0
H(40)	0.5872	0.1699	0.3956	6.0
H(41)	0.4774	0.1339	0.3597	6.0
H(42)	0.4363	0.1975	0.3538	6.0
H(43)	0.3104	0.1706	0.3950	6.0
H(44)	0.2953	0.1696	0.4681	6.0
H(45)	0.3563	0.2691	0.4147	6.0
H(46)	0.2632	0.2565	0.4079	6.0
H(47)	0.2719	0.2561	0.5200	6.0
H(48)	0.2745	0.3182	0.4845	6.0
H(49)	0.3918	0.3791	0.4791	6.0
H(50)	0.4321	0.3976	0.5464	6.0
H(51)	0.4808	0.3837	0.4431	6.0
H(52)	0.5152	0.4157	0.5063	6.0
H(53)	0.6123	0.3716	0.5114	6.0
H(54)	0.5901	0.3667	0.4374	6.0
H(55)	0.6550	0.1944	0.6248	6.0
H(56)	0.6164	0.2495	0.6582	6.0
H(57)	0.6145	0.1987	0.7521	6.0
H(58)	0.6383	0.1382	0.7197	6.0
H(59)	0.7411	0.1783	0.7851	6.0
H(60)	0.7415	0.2345	0.7396	6.0
H(61)	0.8247	0.0743	0.7631	6.0

Table S1. (contd)

Positional parameters and B(eq) for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	x	y	z	B(eq)
H(62)	0.7382	0.0710	0.7277	6.0
H(63)	0.8769	0.0436	0.6635	6.0
H(64)	0.8301	-0.0070	0.6979	6.0
H(65)	0.7994	-0.0072	0.5905	6.0
H(66)	0.7667	0.0589	0.5946	6.0
H(67)	0.6434	0.0121	0.5236	6.0
H(68)	0.5636	-0.0028	0.5559	6.0
H(69)	0.6409	0.1087	0.5696	6.0
H(70)	0.5681	0.0969	0.5191	6.0
H(71)	0.5531	0.0837	0.6504	6.0
H(72)	0.4819	0.0849	0.5968	6.0

Table S2.

Intramolecular Distances Involving the Nonhydrogen Atoms for 2.

atom	atom	distance	atom	atom	distance
Ru(1)	Ru(2)	2.8755(8)	Ru(4)	C(40)	1.852(9)
Ru(1)	Ru(4)	2.9891(8)	Ru(4)	C(41)	1.841(9)
Ru(1)	Ru(5)	2.8480(8)	Ru(4)	C(42)	2.045(9)
Ru(1)	Ru(6)	2.8377(8)	Ru(5)	C(1)	2.037(7)
Ru(1)	C(1)	2.057(7)	Ru(5)	C(12)	2.01(1)
Ru(1)	C(10)	1.880(9)	Ru(5)	C(50)	1.85(1)
Ru(1)	C(11)	1.883(9)	Ru(5)	C(51)	1.86(1)
Ru(1)	C(12)	2.233(9)	Ru(6)	C(1)	2.040(7)
Ru(1)	C(61)	2.290(9)	Ru(6)	C(60)	1.88(1)
Ru(2)	Ru(3)	2.882(1)	Ru(6)	C(61)	1.979(9)
Ru(2)	Ru(5)	2.8836(9)	Ru(6)	C(62)	1.875(9)
Ru(2)	Ru(6)	2.8638(9)	Cu(1)	S(1)	2.267(3)
Ru(2)	C(1)	2.066(7)	Cu(1)	S(2)	2.269(3)
Ru(2)	C(20)	1.883(9)	Cu(1)	S(3)	2.266(3)
Ru(2)	C(21)	1.881(9)	Cu(1)	S(4)	2.333(2)
Ru(2)	C(22)	1.939(9)	Cu(2)	S(7)	2.236(3)
Ru(3)	Ru(4)	2.8359(9)	Cu(2)	S(8)	2.262(3)
Ru(3)	Ru(5)	2.9502(9)	Cu(2)	S(9)	2.265(3)
Ru(3)	Ru(6)	2.927(1)	Cu(2)	S(10)	2.315(3)
Ru(3)	C(1)	2.046(7)	S(1)	C(80)	1.81(1)
Ru(3)	C(30)	1.902(9)	S(1)	C(88)	1.82(1)
Ru(3)	C(31)	1.87(1)	S(2)	C(82)	1.80(1)
Ru(3)	C(42)	2.129(9)	S(2)	C(83)	1.825(9)
Ru(4)	Ru(5)	2.8994(9)	S(3)	C(85)	1.81(1)
Ru(4)	Ru(6)	2.9064(9)	S(3)	C(86)	1.80(1)
Ru(4)	C(1)	2.024(7)	S(4)	C(89)	1.812(8)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S2.
Intramolecular Distances Involving the Nonhydrogen Atoms cont

atom	atom	distance	atom	atom	distance
S(4)	C(97)	1.806(9)	O(41)	C(41)	1.16(1)
S(5)	C(91)	1.801(8)	O(42)	C(42)	1.15(1)
S(5)	C(92)	1.80(1)	O(50)	C(50)	1.15(1)
S(6)	C(94)	1.79(1)	O(51)	C(51)	1.14(1)
S(6)	C(95)	1.81(1)	O(60)	C(60)	1.14(1)
S(7)	C(98)	1.75(2)	O(61)	C(61)	1.16(1)
S(7)	C(106)	1.80(1)	O(62)	C(62)	1.15(1)
S(8)	C(100)	1.80(1)	C(80)	C(81)	1.43(2)
S(8)	C(101)	1.78(1)	C(81)	C(82)	1.54(2)
S(9)	C(103)	1.85(1)	C(83)	C(84)	1.49(2)
S(9)	C(104)	1.72(2)	C(84)	C(85)	1.48(2)
S(10)	C(107)	1.78(1)	C(86)	C(87)	1.47(1)
S(10)	C(115)	1.799(9)	C(87)	C(88)	1.52(1)
S(11)	C(109)	1.82(2)	C(89)	C(90)	1.52(1)
S(11)	C(110)	1.77(1)	C(90)	C(91)	1.50(1)
S(12)	C(112)	1.84(1)	C(92)	C(93)	1.49(1)
S(12)	C(113)	1.791(9)	C(93)	C(94)	1.54(1)
O(10)	C(10)	1.15(1)	C(95)	C(96)	1.49(2)
O(11)	C(11)	1.13(1)	C(96)	C(97)	1.49(1)
O(12)	C(12)	1.16(1)	C(98)	C(99)	1.36(3)
O(20)	C(20)	1.14(1)	C(99)	C(100)	1.42(3)
O(21)	C(21)	1.14(1)	C(101)	C(102)	1.43(2)
O(22)	C(22)	1.15(1)	C(102)	C(103)	1.44(2)
O(30)	C(30)	1.12(1)	C(104)	C(105)	1.30(3)
O(31)	C(31)	1.14(1)	C(105)	C(106)	1.37(2)
O(40)	C(40)	1.16(1)	C(107)	C(108)	1.51(1)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S2.
Intramolecular Distances Involving the Nonhydrogen Atoms cont

atom	atom	distance	atom	atom	distance
C(108)	C(109)	1.47(2)			
C(110)	C(111)	1.54(2)			
C(111)	C(112)	1.44(2)			
C(113)	C(114)	1.50(1)			
C(114)	C(115)	1.50(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S3.
Intramolecular Bond Angles Involving the Nonhydrogen Atoms for 2.

atom	atom	atom	angle	atom	atom	atom	angle
Ru(2)	Ru(1)	Ru(4)	88.38(2)	C(1)	Ru(1)	C(10)	127.4(3)
Ru(2)	Ru(1)	Ru(5)	60.50(2)	C(1)	Ru(1)	C(11)	136.0(3)
Ru(2)	Ru(1)	Ru(6)	60.16(2)	C(1)	Ru(1)	C(12)	90.0(3)
Ru(2)	Ru(1)	C(1)	45.9(2)	C(1)	Ru(1)	C(61)	89.7(3)
Ru(2)	Ru(1)	C(10)	173.3(3)	C(10)	Ru(1)	C(11)	96.4(4)
Ru(2)	Ru(1)	C(11)	90.2(2)	C(10)	Ru(1)	C(12)	94.0(4)
Ru(2)	Ru(1)	C(12)	87.0(2)	C(10)	Ru(1)	C(61)	91.1(3)
Ru(2)	Ru(1)	C(61)	88.4(2)	C(11)	Ru(1)	C(12)	91.2(4)
Ru(4)	Ru(1)	Ru(5)	59.51(2)	C(11)	Ru(1)	C(61)	84.7(3)
Ru(4)	Ru(1)	Ru(6)	59.77(2)	C(12)	Ru(1)	C(61)	173.9(3)
Ru(4)	Ru(1)	C(1)	42.5(2)	Ru(1)	Ru(2)	Ru(3)	90.85(2)
Ru(4)	Ru(1)	C(10)	85.0(3)	Ru(1)	Ru(2)	Ru(5)	59.28(2)
Ru(4)	Ru(1)	C(11)	175.4(3)	Ru(1)	Ru(2)	Ru(6)	59.26(2)
Ru(4)	Ru(1)	C(12)	93.1(2)	Ru(1)	Ru(2)	C(1)	45.6(2)
Ru(4)	Ru(1)	C(61)	90.8(2)	Ru(1)	Ru(2)	C(20)	96.5(2)
Ru(5)	Ru(1)	Ru(6)	91.53(2)	Ru(1)	Ru(2)	C(21)	103.2(2)
Ru(5)	Ru(1)	C(1)	45.6(2)	Ru(1)	Ru(2)	C(22)	150.9(3)
Ru(5)	Ru(1)	C(10)	116.1(3)	Ru(3)	Ru(2)	Ru(5)	61.55(2)
Ru(5)	Ru(1)	C(11)	123.3(3)	Ru(3)	Ru(2)	Ru(6)	61.25(2)
Ru(5)	Ru(1)	C(12)	44.5(2)	Ru(3)	Ru(2)	C(1)	45.2(2)
Ru(5)	Ru(1)	C(61)	135.3(2)	Ru(3)	Ru(2)	C(20)	135.7(3)
Ru(6)	Ru(1)	C(1)	45.9(2)	Ru(3)	Ru(2)	C(21)	129.0(3)
Ru(6)	Ru(1)	C(10)	115.4(3)	Ru(3)	Ru(2)	C(22)	60.4(3)
Ru(6)	Ru(1)	C(11)	115.8(3)	Ru(5)	Ru(2)	Ru(6)	90.27(2)
Ru(6)	Ru(1)	C(12)	135.6(2)	Ru(5)	Ru(2)	C(1)	44.9(2)
Ru(6)	Ru(1)	C(61)	43.8(2)	Ru(5)	Ru(2)	C(20)	153.3(3)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S3.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
Ru(5)	Ru(2)	C(21)	84.1(3)	Ru(5)	Ru(3)	C(1)	43.6(2)
Ru(5)	Ru(2)	C(22)	105.0(3)	Ru(5)	Ru(3)	C(30)	91.1(3)
Ru(6)	Ru(2)	C(1)	45.4(2)	Ru(5)	Ru(3)	C(31)	173.4(3)
Ru(6)	Ru(2)	C(20)	85.6(2)	Ru(5)	Ru(3)	C(42)	89.1(2)
Ru(6)	Ru(2)	C(21)	161.6(2)	Ru(6)	Ru(3)	C(1)	44.2(2)
Ru(6)	Ru(2)	C(22)	99.6(3)	Ru(6)	Ru(3)	C(30)	171.6(3)
C(1)	Ru(2)	C(20)	126.7(3)	Ru(6)	Ru(3)	C(31)	86.2(3)
C(1)	Ru(2)	C(21)	127.4(3)	Ru(6)	Ru(3)	C(42)	94.5(2)
C(1)	Ru(2)	C(22)	105.5(4)	C(1)	Ru(3)	C(30)	134.4(3)
C(20)	Ru(2)	C(21)	91.6(4)	C(1)	Ru(3)	C(31)	130.4(3)
C(20)	Ru(2)	C(22)	101.7(4)	C(1)	Ru(3)	C(42)	91.4(3)
C(21)	Ru(2)	C(22)	98.8(4)	C(30)	Ru(3)	C(31)	94.5(4)
Ru(2)	Ru(3)	Ru(4)	91.29(3)	C(30)	Ru(3)	C(42)	93.8(4)
Ru(2)	Ru(3)	Ru(5)	59.25(2)	C(31)	Ru(3)	C(42)	94.1(4)
Ru(2)	Ru(3)	Ru(6)	59.07(2)	Ru(1)	Ru(4)	Ru(3)	89.47(3)
Ru(2)	Ru(3)	C(1)	45.8(2)	Ru(1)	Ru(4)	Ru(5)	57.82(2)
Ru(2)	Ru(3)	C(30)	113.4(3)	Ru(1)	Ru(4)	Ru(6)	57.52(2)
Ru(2)	Ru(3)	C(31)	115.1(3)	Ru(1)	Ru(4)	C(1)	43.3(2)
Ru(2)	Ru(3)	C(42)	137.0(2)	Ru(1)	Ru(4)	C(40)	118.3(3)
Ru(4)	Ru(3)	Ru(5)	60.11(2)	Ru(1)	Ru(4)	C(41)	105.0(3)
Ru(4)	Ru(3)	Ru(6)	60.55(2)	Ru(1)	Ru(4)	C(42)	137.7(2)
Ru(4)	Ru(3)	C(1)	45.5(2)	Ru(3)	Ru(4)	Ru(5)	61.90(2)
Ru(4)	Ru(3)	C(30)	125.7(3)	Ru(3)	Ru(4)	Ru(6)	61.28(2)
Ru(4)	Ru(3)	C(31)	118.6(3)	Ru(3)	Ru(4)	C(1)	46.1(2)
Ru(4)	Ru(3)	C(42)	46.0(2)	Ru(3)	Ru(4)	C(40)	125.6(3)
Ru(5)	Ru(3)	Ru(6)	87.75(3)	Ru(3)	Ru(4)	C(41)	132.4(3)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S3.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
Ru(2)	Ru(6)	Ru(4)	90.24(2)	S(7)	Cu(2)	S(8)	109.5(1)
Ru(2)	Ru(6)	C(1)	46.1(2)	S(7)	Cu(2)	S(9)	108.2(1)
Ru(2)	Ru(6)	C(60)	87.8(3)	S(7)	Cu(2)	S(10)	115.5(1)
Ru(2)	Ru(6)	C(61)	95.2(2)	S(8)	Cu(2)	S(9)	108.9(1)
Ru(2)	Ru(6)	C(62)	168.7(3)	S(8)	Cu(2)	S(10)	109.3(1)
Ru(3)	Ru(6)	Ru(4)	58.17(2)	S(9)	Cu(2)	S(10)	105.2(1)
Ru(3)	Ru(6)	C(1)	44.3(2)	Cu(1)	S(1)	C(80)	106.7(5)
Ru(3)	Ru(6)	C(60)	102.4(3)	Cu(1)	S(1)	C(88)	108.1(3)
Ru(3)	Ru(6)	C(61)	143.8(3)	C(80)	S(1)	C(88)	106.1(6)
Ru(3)	Ru(6)	C(62)	109.2(3)	Cu(1)	S(2)	C(82)	108.0(4)
Ru(4)	Ru(6)	C(1)	44.1(2)	Cu(1)	S(2)	C(83)	105.7(3)
Ru(4)	Ru(6)	C(60)	157.9(3)	C(82)	S(2)	C(83)	100.9(5)
Ru(4)	Ru(6)	C(61)	100.1(2)	Cu(1)	S(3)	C(85)	108.2(3)
Ru(4)	Ru(6)	C(62)	85.1(3)	Cu(1)	S(3)	C(86)	107.9(3)
C(1)	Ru(6)	C(60)	130.5(4)	C(85)	S(3)	C(86)	100.5(5)
C(1)	Ru(6)	C(61)	99.6(3)	Cu(1)	S(4)	C(89)	108.0(3)
C(1)	Ru(6)	C(62)	128.6(3)	Cu(1)	S(4)	C(97)	106.1(3)
C(60)	Ru(6)	C(61)	102.0(4)	C(89)	S(4)	C(97)	100.6(4)
C(60)	Ru(6)	C(62)	92.7(4)	C(91)	S(5)	C(92)	101.2(4)
C(61)	Ru(6)	C(62)	95.8(4)	C(94)	S(6)	C(95)	102.5(5)
S(1)	Cu(1)	S(2)	108.7(1)	Cu(2)	S(7)	C(98)	106.9(5)
S(1)	Cu(1)	S(3)	108.0(1)	Cu(2)	S(7)	C(106)	107.9(5)
S(1)	Cu(1)	S(4)	111.17(9)	C(98)	S(7)	C(106)	102.2(7)
S(2)	Cu(1)	S(3)	108.6(1)	Cu(2)	S(8)	C(100)	106.7(4)
S(2)	Cu(1)	S(4)	111.69(9)	Cu(2)	S(8)	C(101)	106.5(4)
S(3)	Cu(1)	S(4)	108.63(8)	C(100)	S(8)	C(101)	101.2(5)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S3.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
Ru(3)	Ru(4)	C(42)	48.5(2)	Ru(2)	Ru(5)	C(12)	91.2(3)
Ru(5)	Ru(4)	Ru(6)	89.12(3)	Ru(2)	Ru(5)	C(50)	172.5(3)
Ru(5)	Ru(4)	C(1)	44.6(2)	Ru(2)	Ru(5)	C(51)	92.7(3)
Ru(5)	Ru(4)	C(40)	172.4(3)	Ru(3)	Ru(5)	Ru(4)	57.99(2)
Ru(5)	Ru(4)	C(41)	87.8(3)	Ru(3)	Ru(5)	C(1)	43.8(2)
Ru(5)	Ru(4)	C(42)	92.1(2)	Ru(3)	Ru(5)	C(12)	140.8(3)
Ru(6)	Ru(4)	C(1)	44.6(2)	Ru(3)	Ru(5)	C(50)	113.9(3)
Ru(6)	Ru(4)	C(40)	93.8(3)	Ru(3)	Ru(5)	C(51)	101.1(3)
Ru(6)	Ru(4)	C(41)	160.4(3)	Ru(4)	Ru(5)	C(1)	44.3(2)
Ru(6)	Ru(4)	C(42)	97.0(2)	Ru(4)	Ru(5)	C(12)	100.9(3)
C(1)	Ru(4)	C(40)	138.2(3)	Ru(4)	Ru(5)	C(50)	88.3(3)
C(1)	Ru(4)	C(41)	130.2(3)	Ru(4)	Ru(5)	C(51)	153.1(4)
C(1)	Ru(4)	C(42)	94.5(3)	C(1)	Ru(5)	C(12)	97.3(3)
C(40)	Ru(4)	C(41)	87.1(4)	C(1)	Ru(5)	C(50)	132.3(4)
C(40)	Ru(4)	C(42)	94.5(4)	C(1)	Ru(5)	C(51)	133.0(4)
C(41)	Ru(4)	C(42)	102.4(4)	C(12)	Ru(5)	C(50)	96.3(4)
Ru(1)	Ru(5)	Ru(2)	60.22(2)	C(12)	Ru(5)	C(51)	105.7(5)
Ru(1)	Ru(5)	Ru(3)	90.02(3)	C(50)	Ru(5)	C(51)	85.6(4)
Ru(1)	Ru(5)	Ru(4)	62.67(2)	Ru(1)	Ru(6)	Ru(2)	60.57(2)
Ru(1)	Ru(5)	C(1)	46.2(2)	Ru(1)	Ru(6)	Ru(3)	90.69(2)
Ru(1)	Ru(5)	C(12)	51.3(3)	Ru(1)	Ru(6)	Ru(4)	62.70(2)
Ru(1)	Ru(5)	C(50)	124.9(3)	Ru(1)	Ru(6)	C(1)	46.4(2)
Ru(1)	Ru(5)	C(51)	139.8(4)	Ru(1)	Ru(6)	C(60)	133.2(3)
Ru(2)	Ru(5)	Ru(3)	59.20(2)	Ru(1)	Ru(6)	C(61)	53.2(2)
Ru(2)	Ru(5)	Ru(4)	89.99(3)	Ru(1)	Ru(6)	C(62)	125.2(3)
Ru(2)	Ru(5)	C(1)	45.8(2)	Ru(2)	Ru(6)	Ru(3)	59.69(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S3.
Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
Cu(2)	S(9)	C(103)	105.2(4)	Ru(1)	C(12)	O(12)	132.9(7)
Cu(2)	S(9)	C(104)	106.6(7)	Ru(5)	C(12)	O(12)	142.8(8)
C(103)	S(9)	C(104)	105.9(8)	Ru(2)	C(20)	O(20)	177.2(7)
Cu(2)	S(10)	C(107)	107.5(3)	Ru(2)	C(21)	O(21)	176.8(8)
Cu(2)	S(10)	C(115)	108.1(3)	Ru(2)	C(22)	O(22)	155.8(9)
C(107)	S(10)	C(115)	103.0(4)	Ru(3)	C(30)	O(30)	176.8(8)
C(109)	S(11)	C(110)	99.2(5)	Ru(3)	C(31)	O(31)	177.9(9)
C(112)	S(12)	C(113)	101.2(5)	Ru(4)	C(40)	O(40)	176.1(8)
Ru(1)	C(1)	Ru(2)	88.5(3)	Ru(4)	C(41)	O(41)	177.9(9)
Ru(1)	C(1)	Ru(3)	177.4(4)	Ru(3)	C(42)	Ru(4)	85.6(3)
Ru(1)	C(1)	Ru(4)	94.2(3)	Ru(3)	C(42)	O(42)	135.6(7)
Ru(1)	C(1)	Ru(5)	88.2(3)	Ru(4)	C(42)	O(42)	138.8(7)
Ru(1)	C(1)	Ru(6)	87.7(3)	Ru(5)	C(50)	O(50)	176.7(9)
Ru(2)	C(1)	Ru(3)	89.0(3)	Ru(5)	C(51)	O(51)	176(1)
Ru(2)	C(1)	Ru(4)	177.3(4)	Ru(6)	C(60)	O(60)	177(1)
Ru(2)	C(1)	Ru(5)	89.3(3)	Ru(1)	C(61)	Ru(6)	83.0(3)
Ru(2)	C(1)	Ru(6)	88.5(3)	Ru(1)	C(61)	O(61)	129.8(7)
Ru(3)	C(1)	Ru(4)	88.3(3)	Ru(6)	C(61)	O(61)	147.2(7)
Ru(3)	C(1)	Ru(5)	92.5(3)	Ru(6)	C(62)	O(62)	176.4(8)
Ru(3)	C(1)	Ru(6)	91.5(3)	S(1)	C(80)	C(81)	121.5(9)
Ru(4)	C(1)	Ru(5)	91.1(3)	C(80)	C(81)	C(82)	118(1)
Ru(4)	C(1)	Ru(6)	91.3(3)	S(2)	C(82)	C(81)	116.2(8)
Ru(5)	C(1)	Ru(6)	175.3(4)	S(2)	C(83)	C(84)	113.4(7)
Ru(1)	C(10)	O(10)	179.1(8)	C(83)	C(84)	C(85)	118.8(9)
Ru(1)	C(11)	O(11)	176.0(8)	S(3)	C(85)	C(84)	113.5(7)
Ru(1)	C(12)	Ru(5)	84.3(3)	S(3)	C(86)	C(87)	117.1(7)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S3.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C(86)	C(87)	C(88)	116.7(8)	S(12)	C(113)	C(114)	116.0(6)
S(1)	C(88)	C(87)	118.0(7)	C(113)	C(114)	C(115)	112.8(8)
S(4)	C(89)	C(90)	113.3(5)	S(10)	C(115)	C(114)	116.1(6)
C(89)	C(90)	C(91)	113.9(7)				
S(5)	C(91)	C(90)	115.1(6)				
S(5)	C(92)	C(93)	115.5(7)				
C(92)	C(93)	C(94)	114.3(8)				
S(6)	C(94)	C(93)	115.1(7)				
S(6)	C(95)	C(96)	112.3(8)				
C(95)	C(96)	C(97)	115.0(8)				
S(4)	C(97)	C(96)	111.0(6)				
S(7)	C(98)	C(99)	122(1)				
C(98)	C(99)	C(100)	137(2)				
S(8)	C(100)	C(99)	119(1)				
S(8)	C(101)	C(102)	118.5(8)				
C(101)	C(102)	C(103)	118(1)				
S(9)	C(103)	C(102)	117.9(8)				
S(9)	C(104)	C(105)	128(1)				
C(104)	C(105)	C(106)	144(2)				
S(7)	C(106)	C(105)	122(1)				
S(10)	C(107)	C(108)	114.5(8)				
C(107)	C(108)	C(109)	115(1)				
S(11)	C(109)	C(108)	115.1(9)				
S(11)	C(110)	C(111)	112.4(8)				
C(110)	C(111)	C(112)	115.2(9)				
S(12)	C(112)	C(111)	113.5(8)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S4. Anisotropic Thermal Parameters.

U values for Ru6C(CO)16Cu2(SCH2CH2CH2)6, 2.

atom	U11	U22	U33	U12	U13	U23
Ru(1)	0.0417(4)	0.0468(4)	0.0449(4)	0.0027(4)	0.0041(3)	-0.0027(4)
Ru(2)	0.0527(4)	0.0383(4)	0.0328(4)	-0.0028(3)	0.0044(3)	-0.0012(3)
Ru(3)	0.0407(4)	0.0507(5)	0.0526(5)	-0.0010(4)	-0.0010(3)	0.0025(4)
Ru(4)	0.0489(4)	0.0426(4)	0.0347(4)	-0.0022(4)	0.0074(3)	-0.0011(3)
Ru(5)	0.0602(5)	0.0331(4)	0.0419(4)	-0.0062(3)	0.0043(3)	0.0020(3)
Ru(6)	0.0518(4)	0.0306(4)	0.0448(4)	-0.0025(3)	0.0099(3)	0.0005(3)
Cu(1)	0.0467(6)	0.0509(6)	0.0498(6)	0.0070(5)	0.0015(5)	0.0052(5)
Cu(2)	0.0556(7)	0.0539(7)	0.0557(7)	0.0062(6)	-0.0052(6)	-0.0022(6)
S(1)	0.052(2)	0.072(2)	0.097(2)	-0.003(1)	0.006(1)	0.023(2)
S(2)	0.071(2)	0.082(2)	0.060(2)	0.026(1)	0.011(1)	0.008(1)
S(3)	0.072(2)	0.053(1)	0.066(2)	0.005(1)	-0.018(1)	0.004(1)
S(4)	0.044(1)	0.046(1)	0.041(1)	0.005(1)	0.001(1)	0.002(1)
S(5)	0.073(2)	0.076(2)	0.088(2)	0.033(2)	-0.004(1)	-0.005(2)
S(6)	0.133(3)	0.098(2)	0.050(2)	0.001(2)	-0.013(2)	0.006(2)
S(7)	0.059(2)	0.107(2)	0.109(2)	-0.015(2)	0.007(2)	0.009(2)
S(8)	0.085(2)	0.067(2)	0.079(2)	-0.004(1)	-0.023(2)	-0.002(1)
S(9)	0.115(2)	0.081(2)	0.082(2)	0.038(2)	0.034(2)	0.003(2)
S(10)	0.092(2)	0.067(2)	0.058(2)	0.018(2)	0.000(1)	-0.002(1)

U values for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	U11	U22	U33	U12	U13	U23
S(11)	0.089(2)	0.128(3)	0.125(3)	-0.048(2)	-0.034(2)	0.056(2)
S(12)	0.093(2)	0.084(2)	0.075(2)	0.010(2)	-0.016(2)	0.012(2)
O(10)	0.098(6)	0.131(7)	0.065(5)	0.024(5)	-0.028(4)	-0.013(5)
O(11)	0.064(5)	0.107(6)	0.075(5)	0.016(4)	0.026(4)	-0.016(4)
O(12)	0.086(5)	0.052(4)	0.165(8)	0.022(4)	0.023(5)	0.027(5)
O(20)	0.088(5)	0.078(5)	0.070(5)	-0.026(4)	0.029(4)	0.013(4)

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Table S4. (contd)

O(21)	0.110(6)	0.056(4)	0.092(5)	0.003(4)	0.016(4)	-0.025(4)
O(22)	0.074(5)	0.145(7)	0.065(5)	0.018(5)	-0.010(4)	-0.003(5)
O(30)	0.079(5)	0.127(7)	0.118(7)	-0.060(5)	-0.008(5)	-0.003(5)
O(31)	0.092(6)	0.076(5)	0.127(7)	0.037(4)	0.003(5)	0.018(5)
O(40)	0.129(6)	0.072(5)	0.073(5)	-0.029(4)	0.019(4)	-0.022(4)
O(41)	0.176(8)	0.077(5)	0.057(5)	0.032(5)	0.014(5)	0.018(4)
O(42)	0.058(4)	0.094(5)	0.077(5)	-0.000(4)	0.023(4)	-0.003(4)
O(50)	0.21(1)	0.111(7)	0.074(6)	-0.061(6)	0.039(6)	0.026(5)
O(51)	0.34(1)	0.141(8)	0.087(6)	-0.14(1)	-0.014(8)	-0.037(6)
O(60)	0.21(1)	0.087(6)	0.075(6)	0.032(6)	0.024(6)	0.036(5)
O(61)	0.064(5)	0.064(4)	0.141(7)	-0.023(4)	0.021(4)	-0.017(4)
O(62)	0.128(6)	0.044(4)	0.085(5)	-0.005(4)	0.028(4)	-0.021(4)

U values for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	U11	U22	U33	U12	U13	U23
C(1)	0.038(4)	0.037(4)	0.032(4)	0.006(3)	0.004(3)	0.004(3)
C(10)	0.058(6)	0.068(6)	0.058(6)	0.010(5)	0.014(5)	0.000(5)
C(11)	0.048(6)	0.059(6)	0.051(6)	0.009(5)	0.003(5)	-0.005(5)
C(12)	0.085(7)	0.053(6)	0.062(6)	0.012(6)	0.012(5)	0.015(5)
C(20)	0.066(6)	0.043(5)	0.044(6)	-0.005(5)	-0.004(5)	-0.004(4)
C(21)	0.060(6)	0.044(6)	0.053(6)	-0.001(5)	-0.004(5)	0.002(5)
C(22)	0.060(7)	0.070(7)	0.071(7)	0.007(5)	0.003(5)	0.000(6)
C(30)	0.058(6)	0.068(7)	0.060(6)	-0.006(5)	0.003(5)	0.001(5)
C(31)	0.062(6)	0.069(7)	0.064(6)	0.002(6)	-0.000(5)	0.009(6)
C(40)	0.079(7)	0.050(6)	0.054(6)	-0.014(5)	0.022(5)	-0.000(5)
C(41)	0.108(8)	0.048(6)	0.044(6)	0.016(6)	0.008(6)	0.003(5)
C(42)	0.049(6)	0.052(6)	0.053(6)	-0.006(5)	0.008(5)	0.002(5)
C(50)	0.114(9)	0.055(6)	0.063(7)	-0.022(6)	0.018(6)	0.003(6)
C(51)	0.17(1)	0.064(7)	0.060(7)	-0.044(8)	0.009(7)	-0.005(6)

Table S4. (contd)

C(60)	0.12(1)	0.054(7)	0.066(7)	0.007(6)	0.023(7)	0.008(6)
C(61)	0.057(6)	0.057(6)	0.059(6)	-0.007(5)	0.019(5)	-0.013(5)
C(62)	0.060(6)	0.040(5)	0.058(6)	-0.003(5)	0.015(5)	0.012(5)
C(80)	0.077(9)	0.074(9)	0.26(2)	-0.013(7)	-0.00(1)	0.04(1)

U values for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	U11	U22	U33	U12	U13	U23
C(81)	0.15(1)	0.050(7)	0.23(2)	0.008(9)	-0.03(1)	0.01(1)
C(82)	0.12(1)	0.083(8)	0.087(9)	0.046(7)	-0.006(8)	-0.035(7)
C(83)	0.042(6)	0.080(8)	0.12(1)	0.016(5)	0.017(6)	0.026(7)
C(84)	0.039(6)	0.12(1)	0.11(1)	-0.003(6)	-0.014(6)	0.043(8)
C(85)	0.065(7)	0.063(6)	0.097(8)	-0.011(5)	-0.024(6)	0.018(6)
C(86)	0.097(8)	0.081(8)	0.068(7)	0.007(6)	-0.018(6)	0.007(6)
C(87)	0.093(8)	0.100(9)	0.047(6)	0.005(7)	0.005(6)	0.017(6)
C(88)	0.066(7)	0.096(8)	0.080(8)	-0.002(6)	0.012(6)	0.045(6)
C(89)	0.040(5)	0.049(5)	0.065(6)	-0.002(4)	-0.008(4)	-0.008(5)
C(90)	0.061(6)	0.046(5)	0.076(7)	-0.003(5)	-0.001(5)	-0.005(5)
C(91)	0.062(6)	0.062(6)	0.045(5)	0.015(5)	-0.004(4)	-0.010(5)
C(92)	0.058(6)	0.082(7)	0.070(7)	-0.001(6)	-0.011(5)	0.021(6)
C(93)	0.071(7)	0.12(1)	0.066(7)	-0.032(7)	-0.014(6)	0.014(7)
C(94)	0.12(1)	0.095(8)	0.072(8)	-0.032(7)	-0.046(7)	0.001(7)
C(95)	0.16(1)	0.048(6)	0.074(8)	-0.024(7)	-0.029(8)	-0.007(6)
C(96)	0.14(1)	0.057(7)	0.052(6)	0.019(7)	0.016(7)	-0.000(5)
C(97)	0.072(6)	0.064(6)	0.047(6)	0.017(5)	0.006(5)	-0.001(5)
C(98)	0.11(1)	0.19(2)	0.13(1)	0.00(1)	0.07(1)	-0.02(1)

Table S4. (contd)

U values for Ru6C(CO)16Cu2(SCH2CH2CH2)6

atom	U11	U22	U33	U12	U13	U23
C(99)	0.33(3)	0.27(2)	0.10(1)	-0.13(2)	0.13(2)	-0.10(1)
C(100)	0.10(1)	0.16(1)	0.079(9)	0.031(9)	-0.010(8)	-0.053(9)
C(101)	0.076(8)	0.11(1)	0.098(9)	-0.020(7)	-0.027(7)	0.031(8)
C(102)	0.053(7)	0.16(1)	0.12(1)	0.013(8)	-0.022(7)	0.05(1)
C(103)	0.071(8)	0.18(1)	0.10(1)	0.065(9)	-0.002(7)	-0.01(1)
C(104)	0.25(2)	0.12(1)	0.22(2)	0.07(2)	0.14(2)	0.02(1)
C(105)	0.14(2)	0.052(9)	0.59(5)	0.01(1)	-0.00(2)	0.09(2)
C(106)	0.12(1)	0.10(1)	0.20(2)	-0.04(1)	0.04(1)	0.05(1)
C(107)	0.13(1)	0.062(7)	0.079(8)	0.008(6)	-0.049(7)	0.003(6)
C(108)	0.14(1)	0.13(1)	0.049(7)	0.04(1)	-0.023(7)	-0.013(7)
C(109)	0.22(2)	0.067(8)	0.12(1)	-0.01(1)	-0.06(1)	-0.017(8)
C(110)	0.062(7)	0.103(9)	0.082(8)	-0.002(6)	-0.009(6)	0.021(7)
C(111)	0.071(8)	0.16(1)	0.09(1)	0.013(8)	0.009(7)	-0.011(9)
C(112)	0.070(8)	0.20(1)	0.075(8)	0.030(9)	-0.002(6)	-0.017(9)
C(113)	0.066(6)	0.077(7)	0.051(6)	0.005(6)	-0.006(5)	-0.008(5)
C(114)	0.070(7)	0.060(6)	0.077(7)	0.010(5)	0.002(5)	0.010(6)
C(115)	0.075(7)	0.063(6)	0.058(6)	0.006(5)	0.020(5)	0.003(5)