Electronic Supplementary Information

for

Models for Aerobic Carbon Monoxide Dehydrogenase: Synthesis, Structures and Properties of Paramagnetic $Mo^{V}O(\mu\text{-}S)Cu^{I}$ Complexes

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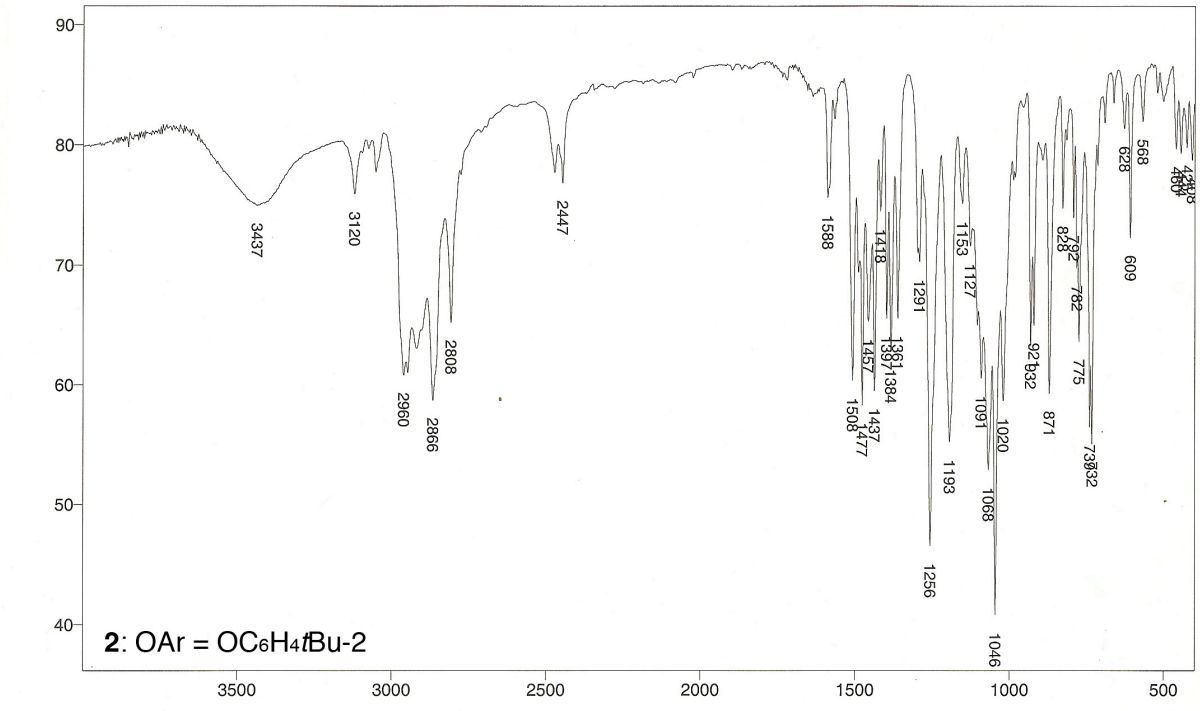
Supplementary Information

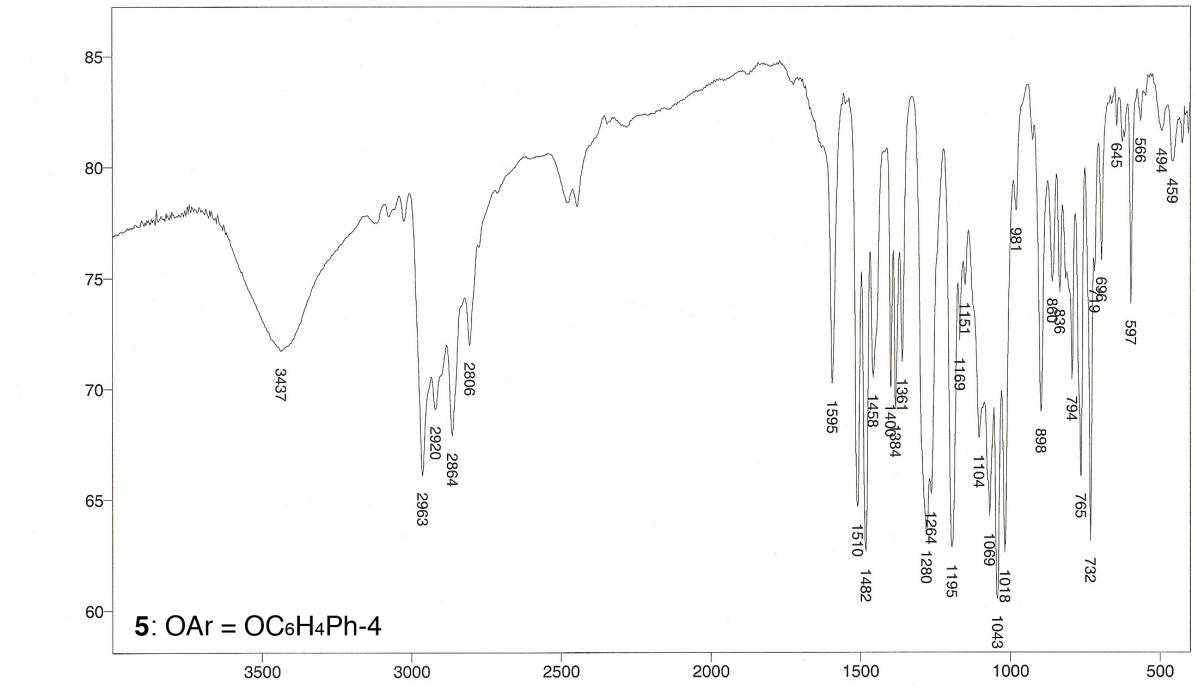
Table S1. Microanalytical, mass spectrometric and selected IR data.

Cmpd (Yield)	Elemental Analysis, %, found (calcd)				*m/z*	Major Infrared Bands (cm^{-1})		
OAr	C	H	N	S	$[M+H]^+$	ν(BH)	ν(CN)	ν(Mo=O)
1	49.07	6.92	14.98	3.74	812.2	2445	1508	896
OPh	(48.86)	(6.71)	(15.54)	(3.95)		2482		
2	50.80	7.29	13.97	3.49	866.9[a]	2444	1508	922[b]
$OC_6H_4{}^tBu$-2	(51.24)	(7.21)	(14.54)	(3.70)		2476		932[b]
3	51.18	7.12	14.21	3.45	868.5	2445	1508	904
$OC_6H_4{}^sBu$-2	(51.24)	(7.21)	(14.54)	(3.70)		2478		
4	50.59	7.21	13.85	3.45	868.3	2445	1503	904
$OC_6H_4{}^sBu$-4	(51.24)	(7.21)	(14.54)	(3.70)		2474		
5	52.54	6.61	14.04	3.45	888.6	2448	1510	895
OC_6H_4Ph-4	(52.79)	(6.59)	(14.21)	(3.61)		2481		
6	51.37	7.19	13.87	3.38	868.3	2441	1507	898
$OC_6H_4{}^tBu$-3	(51.24)	(7.21)	(14.54)	(3.70)		2485		
7	53.31	7.50	13.61	3.47	925.6	2446	1508	907
$OC_6H_3{}^tBu_2$-3,5	(53.33)	(7.64)	(13.65)	(3.47)		2474		

[a] For $[M]^+$. [b] Single band at 918 cm^{-1} observed in solution (MeCN).

Section S1. Representative Infrared Spectra, Synthetic Yields and Full IR Band Listings.





1 (OPh): Yield 30%. IR (cm^{-1}) KBr: 2965 s, 2927 s, 2866 s, 2808 m, ν(BH) 2482 w and 2445 w, 1585 m, ν(CN) 1508 s, 1488 s, 1481 s, 1459 m, 1400 m, 1384 m, 1362 m, 1296 s, 1282 m, 1266 s, 1247 m, ν(CC) 1194 s, 1163 m, 1106 w, 1081 w, 1070 s, ν(CC) 1047 s, 1020 s, 985 w, 957 w, 929 w, ν(Mo=O) 902 s, 855 m, 842 m, 817 w, 794 m, 772 m, 755 m, 733 s, 691 w, 628 w, 595 m, 504w, 459 w, 426 w.

2 ($OC_6H_4{}^tBu$-2): Yield 34%. IR (cm^{-1}) KBr: 2960 s, 2918 s, 2866 s, 2808 m, ν(BH) 2476 w and 2447 w, 1588 m, ν(CN) 1508 s, 1477 s, 1457 m, 1437 m, 1418 w, 1397 m, 1384 m, 1361 m, 1291 w, 1256 s, ν(CC) 1193 s, 1153 w, 1153 w, 1127 m, 1104 m, 1091 m, 1068 s, ν(CC) 1046 s, 1020 s, 981 w, ν(Mo=O) 932 s and 922 s (918 s in MeCN), 871 m, 828 w, 792 m, 782 m, 775 m, 739 s, 732 s, 628 w, 609 m, 568 w, 460 w, 444 w, 425 w.

3 ($OC_6H_4{}^sBu$-2): Yield 53%. IR (cm^{-1}) KBr: 2962 s, 2925 s, 2867 s, 2807 m, ν(BH) 2477 w and 2447 w, 1588 m, ν(CN) 1508 s, 1478 s, 1459 m, 1444 m, 1399 m, 1384 m, 1362 m, 1296 m, 1264 sh, 1249 s, ν(CC) 1194, 1151 w, 1105 w, 1069 s, ν(CC) 1045 s, 1019 s, 983 w, 929 w, ν(Mo=O) 9032 s, 875 w, 844 m, 817 w, 794 m, 794 m, 773 m, 733 s, 631 m, 610 w, 489 w, 425 w.

4 ($OC_6H_4{}^sBu$-4): Yield 41%. IR (cm^{-1}) KBr: 2962 s, 2924 s, 2867 s, 2807 m, ν(BH) 2474 w and 2445 w, 1601 m, ν(CN) 1503 s, 1458 m, 1399 m, 1382 m, 1361 m, 1297 m, 1277 s, 1267 s, ν(CC) 1194, 1170 w, 1152 w, 1128 m, 1105 m, 1098 m, 1068 s, ν(CC) 1045 s, 1019 s, 982 w, ν(Mo=O) 904 s, 865 w, 830 w, 817 w, 794 m, 773 m, 766 m, 733 s, 717 w, 628 w, 590 w, 566 w, 551 w, 492 w, 427 w.

5 (OC_6H_4Ph-4): Yield 47%. IR (cm^{-1}) KBr: 2963 s, 2920 s, 2864 s, 2806 m, ν(BH) 2481 w and 2448 w, 1595 m, ν(CN) 1510 s, 1482 s, 1458 m, 1400 m, 1384 m, 1361 m, 1280 s, 1264 s, ν(CC) 1195 s, 1169 m, 1151 w, 1116 m, 1104 m, 1069 s, ν(CC) 1043 s, 1018 s, 981 w, ν(Mo=O) 898 s, 860 w, 836 m, 794 m, 765 m, 732 s, 710 w, 696 w, 645 w, 597 m, 494 w, 459 w.

6 ($OC_6H_4{}^tBu$-3): Yield 33%. IR (cm^{-1}) KBr: 2960 s, 2924 s, 2864 s, 2805 m, ν(BH) 2468 w and 2441 w, 1587 m, 1563 m, ν(CN) 1506 s, 1481 s, 1460 m, 1418 m, 1398 m, 1380 m,

1359 m, 1286 s, 1262 s,1239 m, ν(CC) 1191 s, 1151 w, 1104 w, 1095 w, 1068 m, ν(CC) 1045 s, 1018 m, 995 m, 983 w, 938 m, ν(Mo=O) 897 s, 874 w, 823 m, 815 w, 793 m, 775 m, 733 s, 700 w, 664 w, 639 w, 620 m, 566 w, 520 w, 492 w, 446 w, 424 w.

7 ($OC_6H_3{}^tBu_2$-3,5): Yield 42%. IR (cm^{-1}) KBr: 2964 s, 2925 s, 2865 s, 2806 m, ν(BH) 2474 w and 2446 w, 1579 m, ν(CN) 1509 s, 1491 s, 1459 m, 1423 m, 1400 m, 1384 m, 1361 m, 1300 m, 1245 w, 1224 w, ν(CC) 1199, 1151 w, 1104 w, 1092 w, 1069 m, ν(CC) 1045 s, 1022 m, 978 w, 927 w, ν(Mo=O) 907 s, 865 w, 818 w, 794 m, 772 m, 732 s, 647 m, 627 m, 566 w, 521 w, 494 w, 460 m, 425 w.