

Supplementary Information for:

Conversions Between Metal-Ligand Multiple Bond (MLMB) Types and Their Applications

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Summary of CSD search

The CSD was searched for each of the metals of interest with bonds to N, C, and O atoms that are classified as having either 2 or 3 bonds. Initial data Table 1 is with the raw files from the CSD up to the May 5, 2020 update. This did not eliminate duplicate entries. Table 2 give the data from the November, 2009 data base where duplicates are removed based on the R values of duplicated entries.¹

1. J. van de Streek, *Acta Cryst.* (2006) B62, 567-579.
<http://dx.doi.org/10.1107/S0108768106019677>

Table1. CSD hits for Multiply Bonded M-N, -C, or -O atom structures. Duplicates remain. All updates up to May, 2010 included.

Metal	C	N	O	Total
Ti	42	323	53	418
V	28	200	2982	3210
Cr	366	98	264	728
Mn	148	53	25	226
Fe	213	42	13	268
Co	30	12	3	45
Zr	12	48	7	67
Nb	28	145	170	343
Mo	316	783	4229	5328
Tc	3	128	213	344
Ru	726	49	33	808
Rh	73	1	1	75
Hf	3	13	1	17
Ta	92	201	20	313
W	779	583	1772	3134
Re	171	462	1740	2373
Os	208	188	175	571
Ir	99	10	2	111

Table 2. CSD hits for Multiply Bonded M-N, -C, or -O atom structures. Duplicates removed. Only November 2090 database used.

Metal	C	N	O	Total
Ti	20	209	30	259
V	12	140	1593	1745
Cr	293	67	152	512
Mn	103	34	11	148
Fe	144	22	1	167
Co	22	9	0	31
Zr	8	26	3	37
Nb	14	105	79	198
Mo	192	452	2289	2933
Tc	2	76	151	229
Ru	402	33	16	451
Rh	45	0	0	45
Hf	2	8	1	11
Ta	58	132	13	203
W	560	373	752	1685
Re	111	350	1151	1612
Os	115	119	117	351
Ir	64	6	1	71

In these lists, a structure was counted for each unique MLMB in the compound. In other words, a compound with multiple oxo ligands was counted once. If one compound has both an oxo and an imido it would be counted once in each category.