Übergangsmetall-Cluster

2. Konzepte

Isolobale Fragmente

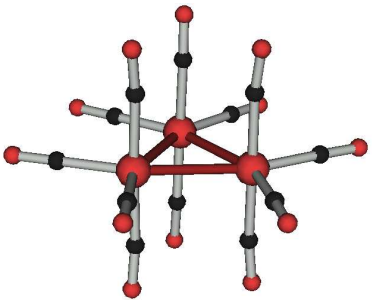
isolobales Fragment	Koordinationszahl des TM, auf die sich die Herleitung isolobaler Fragmente gründet				
	9	8	7	6	5
CH_3, H	$d^1 - ML_8$	$d^3 - ML_7$	$d^5 - ML_6$	$d^7 - ML_5$	$d^9 - ML_4$
CH_2, O, S	$d^2 - ML_7$	$d^4 - ML_6$	$d^6 - ML_5$	$d^8 - ML_4$	$d^{10} - ML_3$
CH, N, P	$d^3 - ML_6$	$d^5 - ML_5$	$d^7 - ML_4$	$d^9 - ML_3$	-
C, BH, B^-	$d^4 - ML_5$	$d^6 - ML_4$	$d^8 - ML_3$	$d^{10} - ML_2$	-

Erweiterte Wade-Regeln

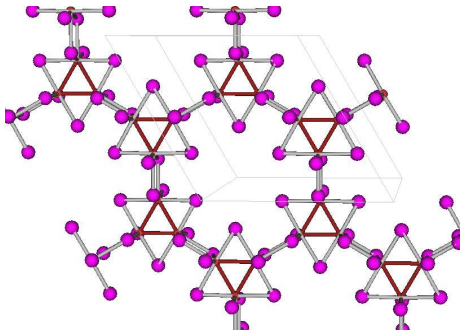
Gerüstbindungs-Elektronenpaare	Struktur	Geometrie
n-1	-	(n-2)-Polyeder, 2 Flächen überdacht
n	-	(n-1)-Polyeder, 1 Fläche überdacht
n+1	closo	n-Polyeder, keine freien Ecken
n+2	nido	(n+1)-Polyeder, eine freie Ecke
n+3	arachno	(n+2)-Polyeder, zwei freie Ecken
n+4	hypho	(n+3)-Polyeder, drei freie Ecken

3. Beispiele nach Zahl der M-Atome

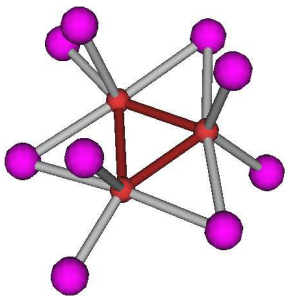
M_3-Cluster



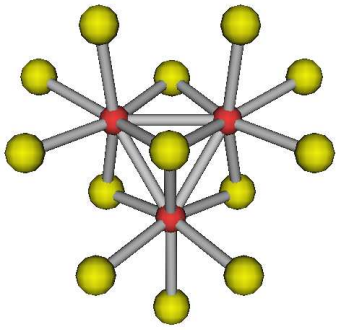
$Ru_3(CO)_{12}$



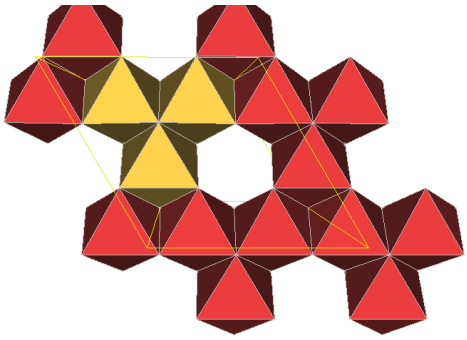
Re_3Cl_9



Re_3I_9

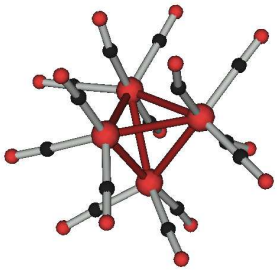


Nb_3Br_8

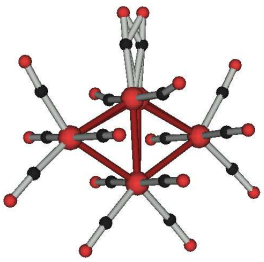


Nb_3Br_8

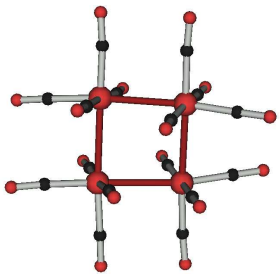
$M_{4/5}$-Cluster



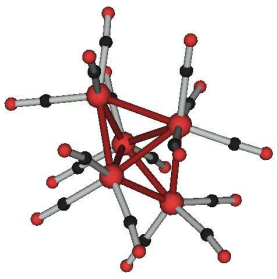
$Os_4(CO)_{14}$



$Os_4(CO)_{15}$



$Os_4(CO)_{16}$



$Os_5(CO)_{16}$