

Длины связей, валентные и невалентные углы в комплексах M(II) типа I.

M	Mn	Fe	Co	Ni	Cu	Zn
Длины связей в хелатном узле MN_4 , pm						
(M1N1)	213.5	190.9	188.8	189.2	198.7	199.8
(M1N2)	203.2	190.9	186.6	190.6	196.1	196.7
(M1N3)	216.3	190.0	187.6	187.7	198.9	203.4
(M1N4)	218.9	190.3	188.3	188.5	200.9	211.9
Отдельные длины связей вне хелатного узла, pm						
(N1C1)	136.9	137.7	137.4	136.7	136.0	137.4
(C1C11)	143.7	143.2	143.1	143.2	144.2	144.2
(C11C2)	143.2	142.1	141.8	141.8	142.6	142.6
(C2N3)	130.6	131.8	131.4	131.5	130.7	130.1
(N3C3)	139.2	140.2	140.6	138.7	138.1	139.1
(C3C4)	143.5	142.2	141.9	142.6	144.1	144.4
(C4N2)	135.8	136.9	137.2	135.3	135.1	135.7
(N2C27)	143.2	145.2	145.4	145.0	144.3	143.5
(C27C28)	152.2	152.6	152.6	153.3	153.4	153.2
(C28N5)	147.6	145.6	145.9	146.2	145.6	144.7
(N5C23)	141.7	138.4	138.8	138.9	138.9	137.8
(C23C21)	141.3	141.3	141.1	141.1	141.5	142.0
(C21N4)	139.4	143.0	143.1	143.0	142.1	141.8
(N4C5)	131.4	131.1	130.8	130.3	129.7	129.7
(C5C12)	142.5	143.1	142.8	143.0	143.9	144.4
(C12C6)	144.1	142.8	142.6	142.6	143.1	143.2
(C6N1)	136.3	139.4	138.8	138.1	137.7	138.3
(C1C14)	141.9	141.6	141.8	141.9	142.4	142.0
(C14C19)	138.2	138.4	138.2	138.1	137.9	138.3
(C19C20)	140.4	140.3	140.4	140.5	140.5	140.0
(C20C13)	138.0	138.0	137.9	137.9	137.8	138.1
(C13C11)	141.5	141.6	141.6	141.6	141.7	141.5
(C3C8)	139.9	139.7	139.6	140.0	140.2	140.0
(C8C9)	139.2	139.1	139.3	138.8	138.7	138.8
(C9C10)	139.8	139.7	139.6	140.3	140.3	140.0
(C10C7)	139.0	138.9	139.0	138.5	138.4	138.6
(C7C4)	141.5	141.5	141.3	142.2	142.4	142.2
(C23C25)	139.4	140.9	140.8	140.8	141.0	141.3
(C25C26)	139.5	138.8	138.8	138.8	138.8	138.5
(C26C24)	139.4	139.4	139.4	139.5	139.4	139.5
(C24C22)	139.2	139.1	139.1	139.1	139.0	138.9
(C22C21)	140.4	139.8	139.6	139.6	139.8	140.1

(C6C15)	142.1	141.2	141.3	141.4	141.5	141.4
(C15C18)	137.9	138.6	138.4	138.4	138.4	138.4
(C18C17)	140.8	140.2	140.3	140.3	140.3	140.2
(C17C16)	137.7	138.4	138.2	138.3	138.2	138.2
(C16C12)	141.8	141.0	141.0	140.9	141.1	141.2

Валентные углы в хелатном узле MN₄, град

(N1M1N3)	80.4	91.8	92.5	92.0	90.7	93.8
(N3M1N2)	77.3	84.1	85.5	84.8	83.4	83.7
(N2M1N4)	123.8	101.9	98.9	99.6	106.6	107.1
(N4M1N1)	79.1	89.6	90.7	89.8	88.6	88.6
Сумма углов (VAS)	360.5	361.4	367.6	366.2	369.3	373.2

Невалентные углы в группировке N₄, град

(N1N3N2)	95.0	89.8	88.9	90.8	90.2	87.1
(N3N2N4)	82.8	85.4	86.4	85.5	83.5	82.9
(N2N4N1)	74.1	82.6	83.4	84.6	80.5	77.6
(N4N1N3)	101.4	87.6	86.4	87.1	87.6	86.0
Сумма углов (NVAS)	353.3	345.4	345.1	348.0	341.8	333.6

Валентные углы в 5-членном хелатном цикле, град

(M1N3C3)	113.4	114.1	113.4	113.9	112.3	110.6
(N3C3C4)	114.4	112.6	112.3	112.6	114.2	114.4
(C3C4N2)	116.7	115.6	115.3	115.5	117.3	118.5
(C4N2M1)	117.9	113.5	113.4	112.7	112.6	112.1
(N2M1N3)	77.3	84.1	85.5	84.8	83.4	83.7
Сумма углов (VAS ⁵)	539.7	539.9	539.9	539.5	539.8	539.3

Валентные углы в 6-членном хелатном цикле 1, град

(M1N1C1)	122.0	125.6	125.4	125.1	123.5	123.9
(N1C1C11)	121.7	120.5	120.9	120.4	121.5	122.5
(C1C11C2)	123.4	123.3	122.8	122.6	124.9	126.4
(C11C2N3)	124.7	125.7	125.5	126.1	126.1	126.2
(C2N3M1)	121.2	123.6	125.3	122.8	121.8	123.6
(N3M1N1)	80.4	91.8	92.5	92.0	90.7	93.8
Сумма углов (VAS ⁶¹)	693.4	710.5	712.4	709.0	708.6	716.4

Валентные углы в 6-членном хелатном цикле 2, град

(M1N1C6)	116.4	115.3	115.9	114.8	114.7	115.9
(N1C6C12)	121.2	121.4	121.4	121.3	121.4	120.8
(C6C12C5)	122.8	120.3	120.2	119.8	122.7	124.1
(C12C5N4)	124.8	121.4	122.1	112.6	124.3	125.2
(C5N4M1)	117.6	126.7	126.1	124.4	121.7	119.9
(N4M1N1)	79.1	89.6	90.7	89.8	88.6	88.6
Сумма углов (VAS ⁶²)	681.9	694.7	696.4	682.7	693.4	694.5

Валентные углы в 8-членном хелатном цикле, град						
(M1N2C27)	121.8	131.5	131.9	131.3	129.8	128.4
(N2C27C28)	108.9	116.4	116.6	115.4	113.9	113.7
(C27C28N5)	110.1	116.7	116.6	116.1	117.5	116.3
(C28N5C23)	115.1	125.4	123.0	121.5	126.6	132.1
(N5C23C21)	116.4	123.4	122.4	122.0	124.1	126.2
(C23C21N4)	117.4	120.9	120.2	120.4	121.6	121.6
(C21N4M1)	121.2	114.7	117.3	118.9	119.7	120.7
(N4M1N2)	123.8	101.9	98.9	99.6	106.6	107.1
Сумма углов (VAS ⁸)	934.7	950.9	946.9	945.2	959.8	966.1
Валентные углы вне хелатных циклов, град						
(C1C14C19)	122.1	122.0	122.0	121.8	122.4	122.9
(C14C19C20)	120.7	120.7	120.8	120.8	120.9	120.6
(C19C20C13)	118.7	118.6	118.5	118.7	118.4	118.1
(C20C13C11)	122.3	122.2	122.1	122.0	122.7	123.1
(C13C11C1)	119.1	119.2	119.5	119.5	119.1	118.8
(C11C1C14)	117.2	117.2	116.9	117.2	116.5	116.3
(C13C11C2)	117.3	117.4	117.7	117.9	116.0	114.7
(N3C3C8)	124.9	126.3	126.8	126.1	125.2	124.8
(C3C8C9)	120.8	120.3	120.2	120.0	120.8	121.3
(C8C9C10)	119.2	119.4	119.5	119.4	119.4	118.7
(C9C10C7)	121.1	121.1	120.9	121.4	121.2	121.3
(C10C7C4)	121.1	120.7	120.5	120.5	121.1	121.8
(C7C4C3)	117.1	117.5	117.9	117.0	116.8	115.9
(C4C3C8)	120.6	121.0	120.8	121.3	120.6	120.8
(N2C4C7)	126.1	126.9	126.8	127.4	125.8	125.6
(C22C21C23)	118.7	120.4	120.4	120.5	120.2	120.0
(C21C23C25)	120.1	117.1	117.4	117.4	117.0	116.4
(C23C25C26)	120.5	122.0	121.8	121.7	122.3	122.7
(C25C26C24)	119.7	120.3	120.2	120.2	120.1	120.3
(C26C24C22)	120.3	118.7	118.9	119.0	120.3	118.3
(C24C22C21)	120.6	121.5	121.2	121.1	121.6	122.2
(N4C21C22)	123.6	118.7	119.3	119.0	118.2	118.3
(C6C12C16)	119.3	119.7	119.9	120.2	119.7	119.5
(C12C16C17)	122.0	121.5	121.4	121.3	121.7	121.9
(C16C17C18)	118.8	118.9	118.9	118.8	118.7	118.7
(C17C18C15)	120.9	120.6	120.7	121.0	120.8	120.7
(C18C15C6)	122.0	121.7	121.6	121.5	121.8	122.0
(C15C6C12)	117.0	117.4	117.3	117.1	117.2	117.1
(N1C6C15)	121.8	121.2	121.3	121.6	121.4	119.5

Стандартные энталпии $\Delta H_{f, 298}^0$, энтропии $S_{f, 298}^0$ и энергии Гиббса $\Delta G_{f, 298}^0$ образования для хелатов типа I различных M(II) (в газовой фазе).

M	$\Delta H_{f, 298}^0$, кДж/моль	$S_{f, 298}^0$, Дж/моль·К	$\Delta G_{f, 298}^0$, кДж/моль
Mn	214.3	1025.4	507.0
Fe	370.9	1016.9	664.7
Co	405.3	1009.9	702.0
Ni	433.1	1007.9	730.4
Cu	559.0	1021.6	853.2
Zn	410.9	1027.9	705.8

Стандартные энталпии $\Delta H_{f, 298}^0$, энтропии $S_{f, 298}^0$ и энергии Гиббса $\Delta G_{f, 298}^0$ образования для исходных веществ и конечных продуктов реакции (*) (в газовой фазе).

M	$\Delta H_{f, 298}^0$, кДж/моль	$S_{f, 298}^0$, Дж/моль·К	$\Delta G_{f, 298}^0$, кДж/моль
CoCl ₂	-122.5	315.5	-141.1
CuCl ₂	-19.4	298.9	-32.1
FeCl ₂	-227.5	314.6	-246.7
MnCl ₂	-434.3	309.0	-450.4
NiCl ₂	-70.2	316.8	-89.3
ZnCl ₂	-263.3	289.9	-270.8
HCl	-91.4	192.9	-96.2
H ₂ O	-223.8	197.2	-213.1
C ₁₄ H ₁₈ N ₄	150.9	717.8	400.3
C ₁₄ H ₁₁ NO ₂	-213.9	654.2	-105.7

Примечание:

