Table 3. Hydrogen bonds with water molecules as acceptors (X–H···O_w): Geometry of fairly linear interactions ($\theta > 135°$) with various donors (distances are given in Å). (Database information was retrieved for this article.[10a])

Donor	n	Mean H···O_w distance	Mean X···O_w distance	H···O_w distance (95%)[a]	X···O_w distance (95%)[a]
O–H donors					
H_3O^+	21	1.54(2)	2.49(2)	–	–
N^+–OH	1	1.57(–)	2.55(–)	–	–
S–OH	4	1.58(–)	2.55(–)	–	–
P–OH	73	1.61(1)	2.575(9)	1.44 – 1.77	2.42 – 2.72
Se–OH	4	1.62(–)	2.59(–)	–	–
O=C–OH	244	1.629(4)	2.591(4)	1.51 – 1.78	2.49 – 2.75
N=C–OH	6	1.69(3)	2.60(3)	–	–
N–OH	46	1.68(1)	2.65(1)	–	–
C=C–OH, Ph–OH	162	1.724(8)	2.679(7)	1.55 – 1.96	2.52 – 2.88
As–OH	4	1.75(–)	2.68(–)	–	–
O–OH	2	1.76(–)	2.69(–)	–	–
C_{sp^3}–OH	763	1.804(4)	2.753(3)	1.64 – 2.06	2.61 – 2.97
3(TM)OH[b]	6	1.81(5)	2.76(4)	–	–
2(TM)OH[b]	14	1.85(4)	2.79(4)	–	–
H_2O	2505	1.880(2)	2.825(2)	1.72 – 2.19	2.68 – 3.11
B^-–OH	5	1.91(–)	2.86(–)	–	–
TM–OH[b]	5	1.96(–)	2.89(–)	–	–
$^-$OH	2	2.27(–)	3.22(–)	–	–
N–H donors					
(SO_2,SO_2)NH	7	1.71(1)	2.70(1)	–	–
Im^+N–H	20	1.74(2)	2.73(2)	–	–
Py^+N–H	67	1.78(1)	2.75(1)	1.63 – 2.05	2.63 – 2.96
(C,C,C)N^+–H	40	1.82(2)	2.77(1)	–	–
(C,C)N^+H_2	108	1.87(1)	2.83(1)	1.68 – 2.19	2.68 – 3.06
(C_{sp^2},C_{sp^2})N–H	316	1.860(8)	2.835(7)	1.69 – 2.20	2.69 – 3.13
C–NH_3^+	370	1.878(6)	2.840(5)	1.71 – 2.17	2.71 – 3.08
NH_4^+	86	1.95(1)	2.91(1)	1.74 – 2.24	2.73 – 3.11
(C_{sp^2},C_{sp^3})N–H	178	1.988(9)	2.937(8)	1.79 – 2.25	2.77 – 3.18
(peptide)N–H	118	1.99(1)	2.94(1)	1.80 – 2.31	2.77 – 3.18
C_{sp^2}–NH_2	508	2.016(6)	2.963(5)	1.81 – 2.31	2.78 – 3.21
(TM,C,C)N–H[b]	128	2.05(1)	2.99(1)	1.82 – 2.35	2.82 – 3.24
(TM,C_{sp^2})N–H[b]	18	2.07(3)	3.03(3)	–	–
(TM,C)NH_2[b]	467	2.084(6)	3.031(5)	1.88 – 2.35	2.86 – 3.27
TM–NH_3[b]	68	2.09(2)	3.03(1)	1.90 – 2.35	2.89 – 3.28
(C_{sp^3},C_{sp^3})N–H	13	2.14(3)	3.08(2)	–	–
C_{sp^3}–NH_2	20	2.12(4)	3.09(4)	–	–
N–NH_2	5	2.16(–)	3.09(–)	–	–
S–H donors					
C–SH	1	2.16(–)	3.48(–)	–	–
C–H donors					
Cl_3C–H	2	2.06(–)	3.07(–)	–	–
C≡C–H	3	2.10(–)	3.16(–)	–	–
Cl_2CH_2	2	2.16(–)	3.22(–)	–	–
(N,N)C_{sp^2}–H	32	2.41(3)	3.38(3)	–	–
(Cl,C)C_{sp^3}–H	6	2.46(9)	3.44(5)	–	–
(N,C)C_{sp^2}–H	276	2.48(1)	3.47(1)	> 2.12	> 3.14
(C,C)C_{sp^2}–H	1369	2.553(4)	3.540(4)	> 2.22	> 3.23
(C,C,C)C_{sp^3}–H	29	2.59(2)	3.59(2)	–	–
O–CH_3	80	2.59(2)	3.59(2)	> 2.32	> 3.32
C_{sp^3}–CH_3	533	2.632(6)	3.613(6)	> 2.37	> 3.35

[a] The "95% ranges" of H···O_w and X···O_w distances include 95% of the hydrogen bonds. They are given only if $n > 50$. For distributions without a pronounced maximum, the 2.5th percentile is given instead of the central 95%. [b] TM = transition metal atom.

[10] Database information retrieved for this article was obtained from the Cambridge Structural Database (CSD: F. H. Allen, O. Kennard, *Chem. Des. Autom. News.* **1993**, *8*, 1), update 5.20 (Oct. 2000) with 224400 entries, ordered and error-free organic and organometallic crystal structures with *R* values < 0.06, X–H bond lengths normalized. Standard uncertainties of mean values were calculated only if $n > 5$. Geometric cutoff criteria were used as specified: a) Tables 3, 5, 6: for X = O, N: $d < 2.4$ Å; for X = S, C: $d < 2.8$ Å, $\theta > 135°$. b) For