

Accessory publication**Trace metals in the open oceans: speciation modelling based on humic type ligands**Anthony Stockdale,^{A,C,D} Edward Tipping,^A John Hamilton-Taylor^B and Stephen Lofts^A^ACentre for Ecology and Hydrology, Lancaster Environment Centre, Bailrigg, Lancaster LA1 4AP, UK.^BLancaster Environment Centre (LEC), Lancaster University, Bailrigg, Lancaster LA1 4YQ, UK.^CPresent address: School of Chemistry, University of Manchester, Oxford Road, Manchester, M13 9PL, UK.^DCorresponding author. Email address: tony@biogeochemistry.org.uk**DOC estimates for all locations and depths***Tables of DOC estimates*

Estimates are derived from literature sources for the nearest available station to where a metal measurement was taken (see methods section in the main manuscript for details). Full station and depth information (in parentheses) is included to allow easy identification of all metal measurement sites obtained from the published literature.

Table A1. DOC estimates for Fe data

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)	Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
[21]	Station 163 (20 m)	0.60	[21]	Station 167 (150 m)	0.60
	Station 163 (40 m)	0.60	Cont...	Station 167 (250 m)	0.60
	Station 163 (80 m)	0.60		Station 167 (500 m)	0.60
	Station 163 (100 m)	0.60		Station 167 (750 m)	0.50
	Station 163 (150 m)	0.60		Station 167 (1000 m)	0.50
	Station 163 (250 m)	0.60		Station 169 (20 m)	0.60
	Station 163 (298 m)	0.60		Station 169 (60 m)	0.60
	Station 163 (478 m)	0.60		Station 169 (100 m)	0.60
	Station 163 (701 m)	0.50		Station 169 (250 m)	0.60
	Station 165 (40 m)	0.60		Station 169 (300 m)	0.60
	Station 165 (60 m)	0.60		Station 169 (400 m)	0.60
	Station 165 (80 m)	0.60		Station 169 (2000 m)	0.50
	Station 165 (100 m)	0.60		Station 169 (3000 m)	0.50
	Station 165 (129 m)	0.60		Station 169 (4000 m)	0.50
	Station 165 (150 m)	0.60		Station 169 (4500 m)	0.50
	Station 165 (250 m)	0.60		Station 182 (40 m)	0.60
	Station 165 (293 m)	0.60		Station 182 (60 m)	0.60
	Station 165 (528 m)	0.60		Station 182 (100 m)	0.60
	Station 167 (40 m)	0.60		Station 182 (150 m)	0.60
	Station 167 (80 m)	0.60		Station 182 (200 m)	0.60
	Station 167 (100 m)	0.60		Station 182 (271 m)	0.60

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)	Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
[21]	Station 182 (610 m)	0.60	[22]	Surface (3)	0.90
Cont...	Station 182 (986 m)	0.50	Cont...	Surface (4)	0.90
	Station 185 (50 m)	0.60		Surface (5)	0.90
	Station 185 (100 m)	0.60		Surface (6)	0.90
	Station 185 (250 m)	0.60		Surface (7)	0.90
	Station 185 (500 m)	0.60		Surface (8)	0.90
	Station 185 (1000 m)	0.50		Surface (9)	0.90
	Station 185 (1500 m)	0.50		Surface (10)	0.90
	Station 185 (2500 m)	0.50	[23]	SIE D145 BIO2	0.60
	Station 185 (3500 m)	0.50		SIE D166 BIO2	0.60
	Station 185 (4500 m)	0.50		SIE D174 (50 m)	0.60
	Station 190 (20 m)	0.60		SIE D174 (100 m)	0.60
	Station 190 (40 m)	0.60		SIE D201 BIO3	0.60
	Station 190 (60 m)	0.60		D203/D208 (10 m)	0.60
	Station 190 (80 m)	0.60		D203/D208 (30 m)	0.60
	Station 190 (100 m)	0.60		D203/D208 (50 m)	0.60
	Station 190 (130 m)	0.60		D203/D208 (100 m)	0.60
	Station 190 (250 m)	0.60		D203/D208 (150 m)	0.60
	Station 190 (400 m)	0.60		D203/D208 (200 m)	0.60
	Station 190 (700 m)	0.60		D203/D208 (300 m)	0.60
	Station 190 (1000 m)	0.50		D203/D208 (400 m)	0.60
[22]	Romanche F. (15 m)	0.91		APF D318 BIO5 r1	0.60
	RF (60 m)	0.77		APF D318 BIO5 r2	0.60
	RF (110 m)	0.67		APF D318 BIO5 r3	0.60
	RF (180 m)	0.66		APF D324 BIO5	0.60
	RF (500 m)	0.62		APF D345 BIO5	0.50
	RF (850 m)	0.60		APF D353 BIO6 r1	0.60
	RF (1500 m)	0.60		APF D353 BIO6 r2	0.60
	RF (2000 m)	0.60	[24]	Station 2 (10 m)	0.80
	RF (3000 m)	0.60		Station 2 (25 m)	0.79
	RF (5300 m)	0.60		Station 2 (75 m)	0.77
	Station 6 (40 m)	0.80		Station 2 (150 m)	0.73
	Station 6 (83 m)	0.73		Station 2 (200 m)	0.72
	Station 6 (110 m)	0.67		Station 4 (10 m)	0.80
	Station 6 (170 m)	0.66		Station 4 (25 m)	0.79
	Station 6 (850 m)	0.66		Station 4 (50 m)	0.78
	Station 6 (1150 m)	0.60		Station 4 (75 m)	0.77
	Station 6 (2000 m)	0.60		Station 4 (125 m)	0.74
	Station 6 (3400 m)	0.60		Station 4 (150 m)	0.73
	Station 6 (4700 m)	0.60		Station 4 (200 m)	0.72
	Station 6 (5050 m)	0.60		Station 6 (10 m)	0.80
	Station 6 (50 m)	0.60		Station 6 (30 m)	0.79
	Station 8 (60 m)	0.77		Station 6 (50 m)	0.78
	Station 8 (110 m)	0.67		Station 6 (75 m)	0.77
	Station 8 (170 m)	0.66		Station 6 (100 m)	0.73
	Station 8 (850 m)	0.60		Station 6 (250 m)	0.70
	Station 8 (1150 m)	0.60		Station 6 (1000 m)	0.60
	Station 8 (2000 m)	0.60		Station 6 (1500 m)	0.60
	Station 8 (3400 m)	0.60		Station 6 (2000 m)	0.60
	Station 8 (4700 m)	0.60		Station 8 (10 m)	0.80
	Station 8 (5050 m)	0.60		Station 8 (20 m)	0.79
	Surface (1)	0.90		Station 8 (30 m)	0.79
	Surface (2)	0.90		Station 8 (40 m)	0.78

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)	Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
[24]	Station 8 (50 m)	0.78	[25]	22-Mar (0800 hours)	0.80
Cont...	Station 8 (75 m)	0.77	Cont...	22-Mar (1200 hours)	0.80
	Station 8 (100 m)	0.76		22-Mar (2000 hours)	0.80
	Station 8 (150 m)	0.73		23-Mar (0400 hours)	0.80
	Station 8 (200 m)	0.72		23-Mar (1200 hours)	0.80
	Station 8 (250 m)	0.70		23-Mar (1600 hours)	0.80
	Station 8 (500 m)	0.64		23-Mar (2000 hours)	0.80
	Station 8 (750 m)	0.60	[26]	A1 (20 m)	0.60
	Station 8 (900 m)	0.60		A1 (60 m)	0.60
	Station 8 (1000 m)	0.60		A1 (100 m)	0.60
	Station 8 (1500 m)	0.60		A1 (200 m)	0.60
	Station 8 (1750 m)	0.60		A1 (300 m)	0.60
	Station 8 (2000 m)	0.60		A1 (400 m)	0.60
	Station 9 (15 m)	0.80		A1 (500 m)	0.60
	Station 9 (20 m)	0.79		A1 (600 m)	0.60
	Station 9 (30 m)	0.79		A1 (620 m)	0.60
	Station 9 (40 m)	0.79		A3(I) (20 m)	0.60
	Station 9 (50 m)	0.78		A3(I) (40 m)	0.60
	Station 9 (65 m)	0.78		A3(I) (60 m)	0.60
	Station 9 (115 m)	0.76		A3(I) (80 m)	0.60
	Station 9 (165 m)	0.73		A3(I) (100 m)	0.60
	Station 9 (200 m)	0.72		A3(I) (150 m)	0.60
	Station 9 (250 m)	0.70		A3(I) (200 m)	0.60
	Station 9 (500 m)	0.64		A3(I) (500 m)	0.60
	Station 9 (890 m)	0.60		A3(II) (20 m)	0.60
	Station 9 (1000 m)	0.60		A3(II) (60 m)	0.60
	Station 9 (1065 m)	0.60		A3(II) (80 m)	0.60
	Station 9 (1500 m)	0.60		A3(II) (100 m)	0.60
	Station 9 (2000 m)	0.60		A3(II) (150 m)	0.60
	Station 10 (10 m)	0.80		A3(II) (200 m)	0.60
	Station 10 (20 m)	0.79		A3(II) (300 m)	0.60
	Station 10 (30 m)	0.79		A3(II) (400 m)	0.60
	Station 10 (40 m)	0.78		A3(II) (450 m)	0.60
	Station 10 (50 m)	0.78		A3(II) (500 m)	0.60
	Station 10 (75 m)	0.77		A34(III) (120 m)	0.60
	Station 10 (100 m)	0.76		A34(III) (150 m)	0.60
	Station 10 (150 m)	0.73		A34(III) (200 m)	0.60
	Station 10 (200 m)	0.72		A34(III) (350 m)	0.60
	Station 10 (250 m)	0.70		A34(III) (400 m)	0.60
	Station 10 (500 m)	0.64		A5 (40 m)	0.60
	Station 10 (650 m)	0.60		A5 (80 m)	0.60
	Station 10 (770 m)	0.60		A5 (110 m)	0.60
	Station 10 (840 m)	0.60		A5 (130 m)	0.60
	Station 10 (960 m)	0.60		A5 (150 m)	0.60
	Station 10 (1250 m)	0.60		A5 (200 m)	0.60
	Station 10 (1500 m)	0.60		A5 (300 m)	0.60
	Station 10 (1750 m)	0.60		A5 (350 m)	0.60
	Station 10 (2000 m)	0.60		A5 (400 m)	0.60
[25]	21-Mar (0400 hours)	0.80		A5 (450 m)	0.60
	21-Mar (1200 hours)	0.80		A7 (20 m)	0.60
	21-Mar (1600 hours)	0.80		A7 (40 m)	0.60
	21-Mar (2200 hours)	0.80		A7 (60 m)	0.60
	22-Mar (0000 hours)	0.80			

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)	Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
[26]	A7 (80 m)	0.60	[26]	N A3(I) (60 m)	0.60
Cont...	A7 (100 m)	0.60	Cont...	N A3(I) (80 m)	0.60
	A7 (150 m)	0.60		N A3(I) (100 m)	0.60
	A7 (200 m)	0.60		N A3(I) (150 m)	0.60
	A7 (300 m)	0.60		N A3(I) (200 m)	0.60
	A7 (400 m)	0.60		N A3(I) (400 m)	0.60
	A7 (550 m)	0.60		N A3(I) (450 m)	0.60
	A8 (40 m)	0.60		N A3(I) (500 m)	0.60
	A8 (60 m)	0.60		N A3(III) (40 m)	0.60
	A8 (80 m)	0.60		N A3(III) (80 m)	0.60
	A8 (125 m)	0.60		N A3(III) (120 m)	0.60
	A8 (200 m)	0.60		N A3(III) (150 m)	0.60
	A8 (400 m)	0.60		N A3(III) (200 m)	0.60
	A8 (600 m)	0.60		N A3(III) (300 m)	0.60
	A8 (800 m)	0.50		N A3(III) (350 m)	0.60
	A8 (1150 m)	0.50		N A3(III) (400 m)	0.60
	A11 (125 m)	0.60		N A3(III) (450 m)	0.60
	A11 (150 m)	0.60		N C11(I) (80 m)	0.60
	A11 (200 m)	0.60		N C11(I) (100 m)	0.60
	A11 (400 m)	0.60		N C11(I) (150 m)	0.60
	A11 (600 m)	0.60		N C11(I) (200 m)	0.60
	C11 (80 m)	0.60		N C11(I) (800 m)	0.50
	C11 (100 m)	0.60		N C11(I) (1000 m)	0.50
	C11 (150 m)	0.60		N C11(I) (1500 m)	0.50
	C11 (200 m)	0.60		N C11(I) (2000 m)	0.50
	C11 (500 m)	0.60		N C11(I) (2500 m)	0.50
	C11 (1500 m)	0.50	[27]	Station 199 (25 m)	0.60
	C11 (2000 m)	0.50		Station 199 (50 m)	0.60
	C11 (2500 m)	0.50		Station 199 (75 m)	0.60
	B5 (40 m)	0.60		Station 199 (100 m)	0.60
	B5 (43 m)	0.60		Station 199 (150 m)	0.60
	B5 (80 m)	0.60		Station 199 (200 m)	0.60
	B5 (93 m)	0.60		Station 199 (300 m)	0.60
	B5 (120 m)	0.60		Station 199 (400 m)	0.60
	B5 (150 m)	0.60		Station 199 (600 m)	0.60
	B5 (200 m)	0.60		Station 199 (800 m)	0.50
	B5 (300 m)	0.60			
	C11(II) (120 m)	0.60			
	C11(II) (200 m)	0.60			
	N A3(I) (20 m)	0.60			

Table A2. DOC estimates for Co, Ni, Cu, Zn, Cd and Pb data

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)	Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
Co: [28]	St204 (20 m)	0.6	[31]	Longitude (86.4°W)	0.84
	St204 (40 m)	0.6	Cont...	Longitude (80.9°W)	0.84
	St204 (6 m)	0.6		Longitude (80.3°W)	0.84
	St204 (80 m)	0.6	Cu:	St4 (500 m)	0.48
	St204 (120 m)	0.6	[32]	St4 (1500 m)	0.48
	St204 (200 m)	0.6		St4 (3000 m)	0.48
	St204 (400 m)	0.6		St6 (500 m)	0.48
	St204 (600 m)	0.6		St6 (1000 m)	0.48
	St204 (800 m)	0.5		St6 (1500 m)	0.48
	St204 (1000 m)	0.5	[33]	Sargasso (60 m)	0.78
	St200 (20 m)	0.6		Sargasso (105 m)	0.76
	St200 (40 m)	0.6	[34]	VERT. T4,4 (20 m)	0.88
	St200 (60 m)	0.6		VERT. T4,4 (40 m)	0.83
	St200 (80 m)	0.6		VERT. T4,4 (60 m)	0.79
	St200 (200 m)	0.6		VERT. T4,4 (80 m)	0.76
[29]	St200 (400 m)	0.6		VERT. T4,4 (100 m)	0.73
	St200 (600 m)	0.6		VERT. T4,4 (150 m)	0.66
	St200 (800 m)	0.5		VERT. T4,4 (200 m)	0.60
	St200 (1000 m)	0.5		VERT. T4,4 (300 m)	0.53
	MER. st9 (15 m)	0.79		VERT. T4,4 (500 m)	0.50
	MER. st9 (30 m)	0.79		VERT. T5 (20 m)	0.88
	MER. st9 (40 m)	0.78		VERT. T5 (40 m)	0.83
	MER. st9 (65 m)	0.78		VERT. T5 (60 m)	0.79
	MER. st9 (115 m)	0.76		VERT. T5 (80 m)	0.76
	MER. st9 (165 m)	0.73		VERT. T5 (100 m)	0.73
	MER. st9 (200 m)	0.72		VERT. T5 (150 m)	0.66
	MER. st9 (250 m)	0.7		VERT. T5 (200 m)	0.60
	MER. st9 (500 m)	0.64		VERT. T5 (300 m)	0.53
	MER. st9 (1000 m)	0.6		VERT. T5 (500 m)	0.50
	MER. st9 (1250 m)	0.6		VERT. T6 (8 m)	0.89
[30]	7-Mar-98 (2400 hours)	0.8		VERT. T6 (20 m)	0.88
	9-Mar-98 (1700 hours)	0.8		VERT. T6 (40 m)	0.83
	10-Mar-98 (0400 hours)	0.8		VERT. T6 (60 m)	0.79
	11-Mar-98 (2400 hours)	0.8		VERT. T6 (80 m)	0.76
	12-Mar-98 (0400 hours)	0.8		VERT. T6 (100 m)	0.73
	20-Mar-98 (0800 hours)	0.8		VERT. T6 (150 m)	0.66
	20-Mar-98 (1600 hours)	0.8		VERT. T6 (200 m)	0.60
	20-Mar-98 (2400 hours)	0.8		VERT. T6 (300 m)	0.53
	22-Mar-98 (0000 hours)	0.8		VERT. T6 (500 m)	0.50
	22-Mar-98 (1600 hours)	0.8		VERT. T7 (8 m)	0.89
	23-Mar-98 (2000 hours)	0.8		VERT. T7 (20 m)	0.88
	BATS (15 m)	0.83		VERT. T7 (40 m)	0.83
	BATS (25 m)	0.83		VERT. T7 (60 m)	0.79
	BATS (40 m)	0.83		VERT. T7 (80 m)	0.76
Ni: [31]	BATS (85 m)	0.76		VERT. T7 (100 m)	0.73
	BATS (100 m)	0.73		VERT. T7 (150 m)	0.66
	BATS (125 m)	0.7		VERT. T7 (300 m)	0.53
	Longitude (91.4°W)	0.84		VERT. T7 (500 m)	0.50
	Longitude (90.0°W)	0.84		VERT. T8 (8 m)	0.89
	Longitude (89.2°W)	0.84		VERT. T8 (20 m)	0.88
	Longitude (88.1°W)	0.84		VERT. T8 (40 m)	0.83
	Longitude (87.9°W)	0.84		VERT. T8 (60 m)	0.79

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)	Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
[34]	VERT. T8 (80 m)	0.76	Cd:	VERTEX IV (22 m)	0.86
Cont...	VERT. T8 (100 m)	0.73	[2]	VERTEX IV (25 m)	0.86
	VERT. T8 (150 m)	0.66		VERTEX IV (40 m)	0.84
	VERT. T8 (200 m)	0.60		VERTEX IV (50 m)	0.83
Zn:	Challenger St. 13 (18 m)	0.80		VERTEX IV (50 m)	0.83
[35]	CS 13 (58 m)	0.79		VERTEX IV (60 m)	0.80
	CS 13 (107 m)	0.76		VERTEX IV (75 m)	0.77
	CS 13 (258 m)	0.70		VERTEX IV (100 m)	0.73
	CS 13 (754 m)	0.60		VERTEX IV (125 m)	0.71
	CS 13 (1003 m)	0.60		VERTEX IV (150 m)	0.68
	CS 13 (1299 m)	0.60		VERTEX IV (175 m)	0.65
	CS 13 (1991 m)	0.60		VERTEX IV (200 m)	0.62
	9-Mar-98 (2400 hours)	0.80		VERTEX IV (300 m)	0.54
	19-Mar-98 (2100 hours)	0.80		VERTEX IV (400 m)	0.48
	20-Mar-98 (2000 hours)	0.80		VERTEX IV (500 m)	0.48
	22-Mar-98 (0400 hours)	0.80		VERTEX IV (600 m)	0.48
	23-Mar-98 (0800 hours)	0.80	[37]	Mar 2002 (20 m)	0.61
[36]	VERT. (IV) (22 m)	0.86		Mar-2002 (30 m)	0.61
	VERT. (IV) (50 m)	0.83		Mar-2002 (40 m)	0.61
	VERT. (IV) (50 m)	0.83		Mar-2002 (60 m)	0.61
	VERT. (IV) (90 m)	0.74		Mar-2002 (80 m)	0.61
	VERT. (IV) (100 m)	0.73		Jul-2002 (20 m)	0.61
	VERT. (IV) (125 m)	0.71		Jul-2002 (30 m)	0.61
	VERT. (IV) (150 m)	0.68		Jul-2002 (40 m)	0.61
	VERT. (IV) (175 m)	0.65		Jul-2002 (60 m)	0.61
	VERT. (IV) (200 m)	0.62		Jul-2002 (80 m)	0.61
	VERT. (IV) (300 m)	0.54		Dec-2002 (14 m)	0.61
	VERT. (IV) (400 m)	0.52		Dec-2002 (32 m)	0.61
	VERT. (IV) (500 m)	0.48		Dec-2002 (42 m)	0.61
	VERT. (IV) (600 m)	0.48		Jan-2003 (3 m)	0.61
[37]	Mar-2002 (20 m)	0.61		Jan-2003 (15 m)	0.61
	Mar-2002 (30 m)	0.61		Jan-2003 (44 m)	0.61
	Mar-2002 (40 m)	0.61		Jan-2003 (60 m)	0.61
	Mar-2002 (60 m)	0.61	[39]	Station 8	0.54
	Mar-2002 (80 m)	0.61		Station 9	0.54
	Jul-2002 (20 m)	0.61		Station 10	0.54
	Jul-2002 (30 m)	0.61		Station 12	0.54
	Jul-2002 (40 m)	0.61		Station 13	0.54
	Jul-2002 (60 m)	0.61		Station 16	0.54
	Jul-2002 (80 m)	0.61		Station 17	0.54
	Dec-2002 (14 m)	0.61		Station 22	0.54
	Dec-2002 (32 m)	0.61		Station 28	0.54
	Dec-2002 (42 m)	0.61		Station 31	0.54
	Jan-2003 (3 m)	0.61		Station 37	0.54
	Jan-2003 (15 m)	0.61		Station 46	0.54
	Jan-2003 (26 m)	0.61	Pb:	Station T8	0.88
	Jan-2003 (32 m)	0.61	[40]	Station T7.5	0.88
	Jan-2003 (44 m)	0.61		Station T7	0.88
	Jan-2003 (60 m)	0.61		Station TA	0.88
[38]	(20 m)	0.85		Station TC	0.88
	(60 m)	0.9		Station TD	0.88
	(80 m)	0.88		Station TE	0.88
	(150 m)	0.7		Station TF	0.88

Study	Station/sample identifier (depth)	DOC (mg L ⁻¹)
[39]	Station TG	0.88
	Station TH	0.88
	Station RB	0.54
	Station 8	0.54
	Station 9	0.54
	Station 10	0.54
	Station 12	0.54
	Station 13	0.54
	Station 16	0.54
	Station 22	0.54
	Station 28	0.54
	Station 31	0.54
	Station 37	0.54
	Station 46	0.54

Comparison of side reaction coefficients between WHAM modelling and literature

The side reaction coefficient is calculated by dividing the total concentration of all the inorganic species by the free ion concentration.

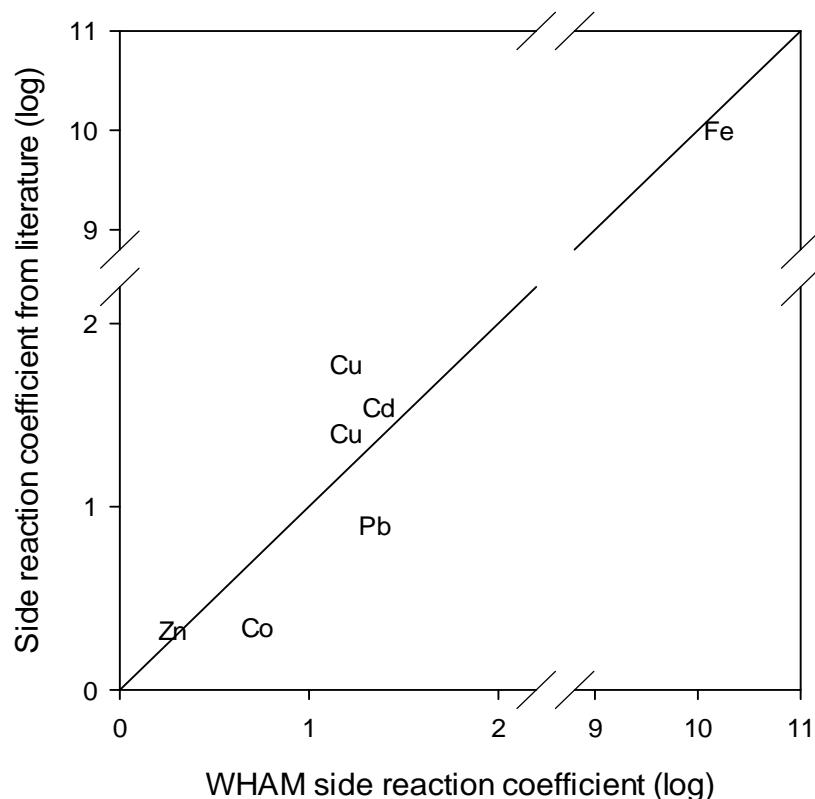


Fig. A1. Comparison of side reaction coefficients (SRC) used in the literature to those calculated using data in the WHAM data base. From the literature cited in the compilation of data, only the SRC values for Cu vary between studies. Hence only one point is shown for all other metals.