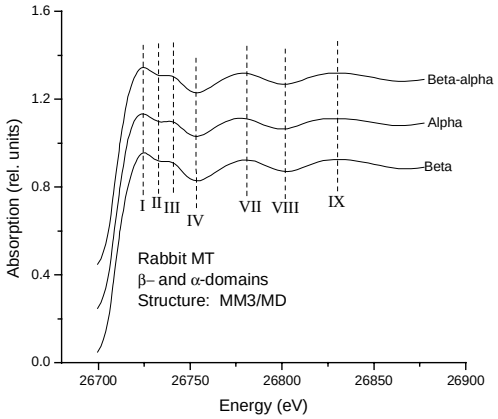
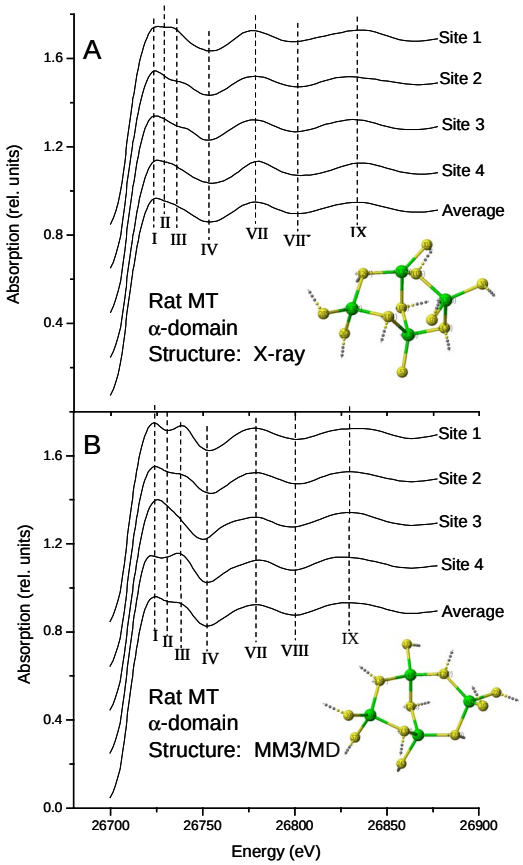
XAFS spectral analysis of the cadmium coordination geometry in cadmium-thiolate clusters in metallothionein[**]

by Jayna Chan[*], Maureen E. Merrifield[*], Alexander V. Soldatov[†] and Martin J. Stillman[,*]*

Supplementary Figures



Supplementary Figure 1. Contributions of the XAFS spectra of the individual domains to the XAFS spectrum of the complete molecule in rabbit liver metallothionein.



Supplementary Figure 2. Site-specific and averaged XAFS spectra for the α domain of rat MT prior to and following energy minimization.

Supplementary Table

Table 1. Connectivities and Cd-S bond lengths and angles in the β and α domains of rabbit and rat metallothioneins.

	Cd-S Connectivity	Bridging/ Terminal	Bond Lengths (pm)	S-Cd-S Connectivity	Bridging/ Terminal	Bond Angles (°)		Cd-S Connectivity	Bridging/ Terminal	Bond Lengths (pm)	S-Cd-S Connectivity	Bridging/ Terminal	Bond Angles (°)
2MRB rabbit	Cd1-S9	T	253.4	S5-Cd1-S9	TT	110.7	2MRB rabbit	Cd1-S9	T	246.8	S5-Cd1-S9	TT	105.5
beta NMR	Cd1-S5	T	252.7	S5-Cd1-S7	TB	104.2	beta	Cd1-S5	T	246.2	S9-Cd1-S4	TB	118.8
	Cd1-S7	B	253.6	S5-Cd1-S4	TB	113.9	Energy	Cd1-S4	B	256.7	S9-Cd1-S7	TB	109.7
	Cd1-S4	B	259.8	S9-Cd1-S7	TB	119.4	Minimized	Cd1-S7	B	256.5	S5-Cd1-S4	BB	113.8
				S9-Cd1-S4	TB	108.2					S5-Cd1-S7	TB	108.4
				S4-Cd1-S7	BB	100.3					S4-Cd1-S7	TB	100.2
	Cd3-S6	T	253.0	S6-Cd3-S1	TT	115.2		Cd2-S3	T	246.5	S3-Cd2-S8	TB	109.7
	Cd3-S1	T	253.0	S6-Cd3-S7	TB	111.9		Cd2-S8	T	246.4	S3-Cd2-S4	TT	111.2
	Cd3-S7	B	261.0	S6-Cd3-S2	TB	100.1		Cd2-S4	B	256.3	S3-Cd2-S2	TB	110.6
	Cd3-S2	B	254.0	S1-Cd3-S7	TB	107.3		Cd2-S2	B	256.4	S4-Cd2-S8	TB	103.4
				S1Cd3-S2	TB	111.2					S8-Cd2-S2	TB	113.5
				S2-Cd3-S7	BB	110.6					S2-Cd2-S4	BB	108.3
	Cd2-S3	T	253.1	S3-Cd2-S8	TT	109.8		Cd3-S6	T	245.6	S1-Cd3-S6	TB	105.8
	Cd2-S8	T	253.5	S3-Cd2-S4	TB	113.5		Cd3-S1	B	247.0	S1-Cd3-S7	TB	123.3
	Cd2-S4	B	253.0	S3-Cd2-S2	TB	108.5		Cd3-S7	B	255.8	S1-Cd3-S2	TB	107.2
	Cd2-S2	B	270.4	S8-Cd2-S4	TB	131.6		Cd3-S2	B	256.4	S6-Cd3-S7	BB	103.5
				S2-Cd2-S8	TB	96.4					S2-Cd3-S6	BB	96.2
				S2-Cd2-S4	BB	89.4					S2-Cd3-S7	BB	96.2
		Avg.	255.9		Avg.	109.0			Avg.	251.4		Avg.	108.1
		S. D.	5.3		S. D.	9.2			S. D.	5.2		S. D.	7.0
1MRB rabbit	Cd1-S9	T	250.4	S9-Cd1-S10	TT	106.6	1MRB rabbit	Cd1-S9	T	246.3	S10-Cd1-S9	TT	104.4
alpha NMR	Cd1-S10	T	246.7	S10-Cd1-S8	TB	111.4	alpha	Cd1-S10	T	248.3	S9-Cd1-S11	TB	102.4
	Cd1-S8	B	252.7	S10-Cd1-S11	TB	126.8	Energy	Cd1-S11	B	259.1	S9-Cd1-S8	TB	107.4
	Cd1-S11	B	263.8	S8-Cd1-S11	BB	95.0	Minimized	Cd1-S8	B	257.1	S10-Cd1-S11	BB	124.2
				S9-Cd1-S8	TB	108.6					S10-Cd1-S8	TB	107.9
				S9-Cd1-S11	TB	107.2					S8-Cd1-S11	TB	109.2
	Cd2-S1	T	252.2	S7-Cd2-S2	TB	104.3		Cd2-S1	T	246.4	S1-Cd2-S6	TB	107.7
	Cd2-S7	T	250.3	S1-Cd2-S7	TT	123.8		Cd2-S7	T	247.9	S1-Cd2-S7	TT	115.0
	Cd2-S2	B	262.6	S1-Cd2-S6	TB	112.8		Cd2-S6	B	258.7	S1-Cd2-S2	TB	107.8
	Cd2-S6	B	253.3	S7-Cd2-S6	TB	104.3		Cd2-S2	B	258.0	S7-Cd2-S6	TB	114.6
				S1-Cd2-S2	TB	103.1					S7-Cd2-S2	TB	103.7
				S6-Cd2-S2	BB	107.3					S2-Cd2-S6	BB	107.5
	Cd3-S5	T	248.1	S5-Cd3-S6	TB	92.2		Cd3-S5	T	247.0	S5-Cd3-S11	TB	102.9
	Cd3-S6	B	264.0	S5-Cd3-S4	TB	120.2		Cd3-S11	B	256.0	S5-Cd3-S4	TB	105.9
	Cd3-S4	B	272.4	S5-Cd3-S11	TB	135.2		Cd3-S4	B	255.8	S5-Cd3-S6	TB	118.7
	Cd3-S11	B	249.0	S4-Cd3-S6	BB	115.1		Cd3-S6	B	258.2	S11-Cd3-S4	BB	106.1
				S4-Cd3-S11	BB	90.5					S4-Cd3-S6	BB	105.4
				S6-Cd3-S11	BB	103.8					S11-Cd3-S6	BB	116.8
	Cd4-S3	T	244.4	S3-Cd4-S8	TB	110.4		Cd4-S3	T	248.3	S3-Cd4-S2	TB	109.5
	Cd4-S8	B	269.5	S3-Cd4-S4	TB	133.6		Cd4-S2	B	258.0	S3-Cd4-S4	TB	111.6
	Cd4-S4	B	243.7	S3-Cd4-S2	TB	109.3		Cd4-S8	B	258.0	S3-Cd4-S8	TB	107.8
	Cd4-S2	B	247.2	S4-Cd4-S8	BB	96.1		Cd4-S4	B	257.5	S2-Cd4-S4	BB	104.6
				S4-Cd4-S2	BB	104.6					S8-Cd4-S4	BB	106.1
				S2-Cd4-S8	BB	96.3					S8-Cd4-S2	BB	117.2
		Avg.	254.4		Avg.	109.1			Avg.	253.8		Avg.	109.4
		S. D.	9.1		S. D.	12.0			S. D.	5.2		S. D.	5.6
4MT2 rat	Cd1-S10	T	250.5	S10-Cd1-S9	TT	111.7	4MT2 rat	Cd1-S9	T	245.6	S10-Cd1-S9	TT	105.5
alpha X-ray	Cd1-S9	T	250.4	S10-Cd1-S11	TB	122.5	alpha	Cd1-S10	T	248.3	S9-Cd1-S11	TB	116.0
	Cd1-S8	B	257.2	S10-Cd1-S8	TB	100.2	Energy	Cd1-S11	B	258.1	S9-Cd1-S8	TB	101.4
	Cd1-S11	B	249.5	S8-Cd1-S11	BB	104.4	Minimized	Cd1-S8	B	257.0	S10-Cd1-S11	TB	116.2
				S9-Cd1-S11	TB	102.3					S10-Cd1-S8	TB	115.0
				S9-Cd1-S8	TB	116.5					S8-Cd1-S11	BB	102.1
	Cd2-S1	T	254.9	S1-Cd2-S6	TB	102.5		Cd2-S1	T	247.6	S1-Cd2-S6	TB	107.8
	Cd2-S7	T	247.3	S1-Cd2-S7	TT	101.4		Cd2-S7	T	247.7	S1-Cd2-S7	TT	107.4
	Cd2-S2	B	244.8	S1-Cd2-S2	TB	115.0		Cd2-S6	B	258.3	S1-Cd2-S2	TB	112.6
	Cd2-S6	B	262.1	S7-Cd2-S2	TB	111.8		Cd2-S2	B	258.6	S7-Cd2-S6	TB	112.1
				S7-Cd2-S6	TB	110.2					S7-Cd2-S2	TB	104.3
				S2-Cd2-S6	BB	114.9					S2-Cd2-S6	BB	112.6
	Cd3-S5	T	248.3	S5-Cd3-S11	TB	101.0		Cd3-S5	T	248.3	S5-Cd3-S11	TB	108.8
	Cd3-S11	B	259.8	S5-Cd3-S4	TB	99.9		Cd3-S11	B	258.3	S5-Cd3-S4	TB	120.7
	Cd3-S4	B	251.7	S5-Cd3-S6	TB	118.9		Cd3-S4	B	255.7	S5-Cd3-S6	TB	106.5
	Cd3-S6	B	250.7	S4-Cd3-S11	BB	96.1		Cd3-S6	B	255.9	S11-Cd3-S4	BB	97.2
				S6-Cd3-S11	BB	114.6					S4-Cd3-S6	BB	103.6
				S6-Cd3-S4	BB	122.1					S11-Cd3-S6	BB	120.8
	Cd4-S3	T	248.6	S3-Cd4-S2	TB	97.9		Cd4-S3	T	247.8	S3-Cd4-S2	TB	121.9
	Cd4-S8	B	250.2	S3-Cd4-S4	TB	132.2		Cd4-S2	B	257.3	S3-Cd4-S4	TB	108.3
	Cd4-S4	B	244.0	S3-Cd4-S8	TB	113.2		Cd4-S8	B	257.5	S3-Cd4-S8	TB	103.6
	Cd4-S2	B	250.6	S4-Cd4-S2	BB	97.8		Cd4-S4	B	256.6	S2-Cd4-S4	BB	107.3
				S8-Cd4-S2	BB	100.2					S8-Cd4-S4	BB	112.6
				S8-Cd4-S4	BB	107.8					S8-Cd4-S2	BB	103.0
		Avg.	251.3		Avg.	109.0			Avg.	253.7		Avg.	109.5
		S. D.	5.0		S. D.	9.5			S. D.	5.0		S. D.	6.6