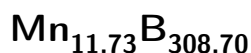


A Borreiche Boride

A.1 Ausgewählte Bindungswinkel und -längen in



Winkel (Angles) in Grad, Abstände (Distance) in Å.

B1 -	Distance	Angles
B7_\$19	1.8341 (0.0023)	
B2	1.8466 (0.0022)	58.71 (0.08)
B9_\$19	1.8654 (0.0024)	104.49 (0.11) 106.01 (0.11)
B2_\$7	1.8655 (0.0022)	105.10 (0.11) 59.72 (0.10) 58.76 (0.09)
B1_\$8	1.9041 (0.0031)	58.73 (0.06) 106.60 (0.07) 59.31 (0.06) 106.43 (0.07)
B1_\$6	1.9283 (0.0032)	117.02 (0.08) 119.94 (0.07) 129.08 (0.08) 128.46 (0.07) 120.00
Mn1	2.1603 (0.0019)	64.12 (0.09) 114.58 (0.10) 116.85 (0.10) 167.91 (0.10) 63.85 (0.04) 63.49 (0.04)
Mn3	2.3628 (0.0016)	115.57 (0.09) 172.83 (0.10) 70.41 (0.08) 120.86 (0.09) 66.24 (0.04) 65.92 (0.04) 63.31 (0.07)
Mn2	2.4028 (0.0017)	118.89 (0.08) 68.19 (0.07) 117.80 (0.08) 67.99 (0.07) 173.63 (0.04) 66.34 (0.04) 121.24 (0.07)
	B1 -	B7_\$19 B2 B9_\$19 B2_\$7 B1_\$8 B1_\$6 Mn1

B2 -	Distance	Angles
B3_\$14	1.7434 (0.0022)	
B7_\$19	1.8045 (0.0020)	115.74 (0.12)
B9_\$24	1.8303 (0.0020)	119.61 (0.11) 59.92 (0.10)
B1	1.8466 (0.0022)	117.65 (0.11) 60.30 (0.09) 109.46 (0.10)
B2_\$7	1.8481 (0.0030)	127.44 (0.07) 107.05 (0.10) 107.41 (0.10) 60.65 (0.09)
B1_\$7	1.8655 (0.0022)	126.17 (0.11) 108.49 (0.11) 60.62 (0.10) 110.04 (0.10) 59.63 (0.09)
Mn2	2.4260 (0.0016)	65.61 (0.07) 119.07 (0.10) 174.76 (0.10) 66.85 (0.07) 67.67 (0.06) 116.51 (0.09)
Mn2_\$30	2.4277 (0.0016)	70.34 (0.08) 173.90 (0.11) 118.13 (0.10) 117.23 (0.09) 67.57 (0.06) 66.58 (0.07) 62.27 (0.05)
	B2 -	B3_\$14 B7_\$19 B9_\$24 B1 B2_\$7 B1_\$7 Mn2

B3 -	Distance	Angles
B2_\$9	1.7436 (0.0022)	
B12	1.7899 (0.0017)	123.83 (0.12)
B8_\$9	1.7970 (0.0024)	121.57 (0.12) 105.38 (0.12)
B4	1.8124 (0.0021)	119.04 (0.11) 62.05 (0.10) 57.54 (0.09)
B13_\$19	1.8142 (0.0032)	124.04 (0.14) 62.24 (0.12) 104.85 (0.12) 111.30 (0.14)
B3_\$8	1.9022 (0.0031)	122.42 (0.07) 107.38 (0.08) 58.04 (0.06) 106.49 (0.07) 58.38 (0.08)
Mn2_\$9	2.3307 (0.0016)	71.44 (0.07) 112.14 (0.10) 119.23 (0.09) 169.47 (0.10) 58.81 (0.11) 65.92 (0.04)
Mn2_\$13	2.4667 (0.0017)	67.93 (0.07) 66.09 (0.08) 170.45 (0.11) 118.38 (0.09) 67.80 (0.09) 119.07 (0.04) 63.01 (0.04)
	B3 -	B2_\$9 B12 B8_\$9 B4 B13_\$19 B3_\$8 Mn2_\$9

B4 -	Distance	Angles
B4_\$16	1.6758 (0.0030)	
B8_\$9	1.7372 (0.0020)	121.22 (0.08)
B3	1.8124 (0.0021)	122.77 (0.14) 60.78 (0.10)
B10_\$19	1.8493 (0.0020)	118.66 (0.14) 62.05 (0.10) 110.69 (0.11)
B11	1.8503 (0.0022)	123.38 (0.11) 106.02 (0.11) 106.11 (0.11) 58.10 (0.09)
B12	1.8569 (0.0022)	126.59 (0.10) 105.03 (0.11) 58.38 (0.08) 105.27 (0.12) 57.94 (0.10)
	B4 -	B4_\$16 B8_\$9 B3 B10_\$19 B11

B5 -	Distance	Angles
B7	1.7072 (0.0031)	
B6_\$19	1.7522 (0.0022)	122.57 (0.10)
B6_\$3	1.7523 (0.0022)	122.57 (0.10) 106.40 (0.18)
B6_\$20	1.7623 (0.0031)	122.40 (0.17) 59.31 (0.08) 59.32 (0.08)
B5_\$2	1.7778 (0.0038)	122.15 (0.08) 59.52 (0.08) 107.07 (0.09) 106.96 (0.09)
B5_\$1	1.7778 (0.0039)	122.15 (0.09) 107.06 (0.09) 59.52 (0.08) 106.96 (0.09) 60.00 (0.00)
Mn1_\$18	2.1260 (0.0031)	66.78 (0.11) 116.99 (0.09) 116.98 (0.09) 170.82 (0.15) 65.28 (0.06) 65.28 (0.06)

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	B5 -	B7	B6_\$19	B6_\$3	B6_\$20	B5_\$2	B5_\$1
B6 -	Distance	Angles					
B8	1.6282 (0.0031)						
B6_\$21	1.7390 (0.0026)	122.23 (0.03)					
B6_\$22	1.7391 (0.0026)	122.23 (0.03)	107.57 (0.14)				
B5_\$3	1.7523 (0.0022)	119.34 (0.14)	109.16 (0.11)	60.63 (0.10)			
B5_\$19	1.7522 (0.0022)	119.34 (0.14)	60.63 (0.10)	109.16 (0.11)	60.97 (0.16)		
B5_\$17	1.7624 (0.0031)	122.17 (0.17)	60.05 (0.12)	60.05 (0.12)	109.83 (0.14)	109.83 (0.14)	
	B6 -	B8	B6_\$21	B6_\$22	B5_\$3	B5_\$19	
B7 -	Distance	Angles					
B5	1.7072 (0.0031)						
B2_\$3	1.8045 (0.0020)	119.77 (0.09)					
B2_\$4	1.8046 (0.0021)	119.77 (0.09)	110.15 (0.15)				
B9_\$23	1.8153 (0.0032)	118.76 (0.16)	60.75 (0.08)	60.74 (0.08)			
B1_\$3	1.8342 (0.0023)	120.82 (0.14)	60.98 (0.08)	111.47 (0.13)	110.69 (0.13)		
B1_\$4	1.8342 (0.0023)	120.82 (0.13)	111.47 (0.13)	60.98 (0.08)	110.68 (0.13)	62.54 (0.12)	
Mn1_\$18	2.1384 (0.0023)	66.02 (0.13)	117.52 (0.09)	117.52 (0.09)	175.22 (0.16)	65.36 (0.10)	65.36 (0.10)
	B7 -	B5	B2_\$3	B2_\$4	B9_\$23	B1_\$3	B1_\$4
B8 -	Distance	Angles					
B6	1.6282 (0.0031)						
B4_\$15	1.7372 (0.0020)	116.52 (0.09)					
B4_\$14	1.7373 (0.0020)	116.52 (0.09)	115.03 (0.16)				
B3_\$15	1.7969 (0.0024)	120.93 (0.13)	61.68 (0.08)	114.74 (0.13)			
B3_\$14	1.7970 (0.0024)	120.93 (0.13)	114.74 (0.13)	61.68 (0.08)	63.91 (0.12)		
B10_\$13	1.8511 (0.0031)	117.35 (0.16)	61.95 (0.08)	61.94 (0.08)	111.31 (0.13)	111.31 (0.13)	
	B8 -	B6	B4_\$15	B4_\$14	B3_\$15	B3_\$14	
B9 -	Distance	Angles					
B10	1.7302 (0.0030)						
B7_\$23	1.8154 (0.0032)	116.91 (0.16)					
B2_\$12	1.8303 (0.0020)	119.54 (0.09)	59.33 (0.08)				
B2_\$11	1.8304 (0.0020)	119.54 (0.09)	59.34 (0.08)	107.87 (0.14)			
B1_\$4	1.8654 (0.0024)	125.12 (0.13)	108.03 (0.12)	109.55 (0.12)	60.62 (0.08)		
B1_\$3	1.8654 (0.0024)	125.12 (0.13)	108.03 (0.12)	60.62 (0.08)	109.55 (0.12)	61.38 (0.12)	
Mn3_\$18	2.4713 (0.0022)	72.31 (0.11)	170.77 (0.14)	117.15 (0.09)	117.15 (0.09)	64.26 (0.08)	64.26 (0.08)
	B9 -	B10	B7_\$23	B2_\$12	B2_\$11	B1_\$4	B1_\$3
B10 -	Distance	Angles					
B9	1.7302 (0.0030)						
B11_\$19	1.7964 (0.0020)	124.32 (0.13)					
B11_\$3	1.7965 (0.0020)	124.32 (0.14)	63.57 (0.16)				
B4_\$3	1.8492 (0.0020)	120.36 (0.09)	110.46 (0.13)	60.97 (0.09)			
B4_\$4	1.8492 (0.0020)	120.36 (0.09)	60.98 (0.09)	110.46 (0.13)	104.83 (0.14)		
B8_\$13	1.8510 (0.0031)	122.41 (0.16)	103.58 (0.13)	103.58 (0.13)	56.00 (0.08)	56.00 (0.08)	
Mn3_\$18	2.5501 (0.0022)	67.41 (0.10)	68.24 (0.09)	68.24 (0.09)	120.62 (0.08)	120.62 (0.08)	170.17 (0.13)
	B10 -	B9	B11_\$19	B11_\$3	B4_\$3	B4_\$4	B8_\$13
B11 -	Distance	Angles					
B14	1.7647 (0.0036)						
B12	1.7956 (0.0030)	58.56 (0.12)					
B10_\$3	1.7964 (0.0020)	103.16 (0.09)	110.18 (0.09)				
B10_\$19	1.7965 (0.0020)	103.16 (0.09)	110.18 (0.09)	139.09 (0.19)			
B4_\$6	1.8502 (0.0022)	103.83 (0.11)	61.22 (0.09)	60.92 (0.08)	138.93 (0.14)		
B4	1.8503 (0.0022)	103.83 (0.11)	61.21 (0.09)	138.94 (0.14)	60.92 (0.08)	82.86 (0.14)	
B11_\$1	1.8924 (0.0038)	57.57 (0.08)	107.49 (0.09)	58.22 (0.08)	114.22 (0.08)	106.30 (0.07)	160.44 (0.08)
B11_\$2	1.8924 (0.0038)	57.58 (0.08)	107.49 (0.08)	114.22 (0.08)	58.22 (0.08)	160.45 (0.08)	106.30 (0.07)
Mn3	2.5166 (0.0022)	116.02 (0.13)	174.57 (0.14)	70.23 (0.09)	70.24 (0.09)	122.26 (0.09)	122.26 (0.09)
	B11 -	B14	B12	B10_\$3	B10_\$19	B4_\$6	B4
B12 -	Distance	Angles					
B14	1.7413 (0.0022)						
B3_\$6	1.7898 (0.0017)	104.04 (0.09)					
B3	1.7899 (0.0017)	104.04 (0.09)	139.72 (0.16)				
B11	1.7956 (0.0030)	59.84 (0.16)	109.46 (0.08)	109.46 (0.08)			
B4	1.8569 (0.0022)	104.50 (0.14)	137.02 (0.14)	59.57 (0.07)	60.85 (0.09)		
B4_\$6	1.8569 (0.0022)	104.50 (0.14)	59.57 (0.07)	137.02 (0.14)	60.84 (0.09)	82.50 (0.13)	
B13_\$3	1.8629 (0.0027)	58.39 (0.15)	59.52 (0.12)	115.01 (0.15)	109.62 (0.14)	161.61 (0.15)	107.21 (0.12)
B13_\$19	1.8630 (0.0027)	58.39 (0.15)	115.01 (0.15)	59.52 (0.12)	109.61 (0.14)	107.20 (0.11)	161.61 (0.15)
Mn2_\$13	2.3894 (0.0023)	118.57 (0.16)	70.69 (0.08)	70.69 (0.08)	178.41 (0.14)	120.19 (0.09)	120.19 (0.09)

A.1 Ausgewählte Bindungswinkel und -längen in Mn_{11.73}B_{308.70}

	B12 -	B14	B3_§6	B3	B11	B4	B4_§6	B13_§3
B13 -	Distance	Angles						
B15	1.7148 (0.0034)							
B14_§18	1.7614 (0.0045)	104.37 (0.19)						
B3_§4	1.8142 (0.0032)	138.28 (0.14)	102.23 (0.17)					
B3_§3	1.8142 (0.0032)	138.28 (0.14)	102.23 (0.17)	63.24 (0.15)				
B13_§2	1.8454 (0.0058)	57.45 (0.09)	58.41 (0.11)	114.69 (0.08)	160.37 (0.11)			
B13_§1	1.8454 (0.0059)	57.45 (0.09)	58.41 (0.11)	160.38 (0.11)	114.68 (0.08)	60.00 (0.00)		
B12_§19	1.8629 (0.0027)	113.29 (0.13)	57.35 (0.11)	58.24 (0.09)	108.05 (0.17)	60.31 (0.11)	107.59 (0.11)	
B12_§3	1.8630 (0.0027)	113.28 (0.13)	57.35 (0.11)	108.05 (0.17)	58.24 (0.09)	107.59 (0.11)	60.31 (0.11)	105.79 (0.20)
Mn2_§13	2.0843 (0.0034)	81.24 (0.13)	174.40 (0.22)	73.06 (0.12)	73.06 (0.12)	126.06 (0.07)	126.06 (0.07)	120.70 (0.12)
Mn2_§9	2.4484 (0.0017)	70.96 (0.08)	114.85 (0.08)	68.88 (0.07)	124.07 (0.16)	67.86 (0.08)	120.08 (0.08)	65.69 (0.07)
Mn2_§29	2.4484 (0.0017)	70.96 (0.08)	114.85 (0.08)	124.07 (0.16)	68.88 (0.07)	120.07 (0.08)	67.86 (0.08)	171.42 (0.16)
	B13 -	B15	B14_§18	B3_§4	B3_§3	B13_§2	B13_§1	B12_§19
B14 -	Distance	Angles						
B12_§1	1.7413 (0.0022)							
B12	1.7413 (0.0022)	117.13 (0.08)						
B12_§2	1.7414 (0.0022)	117.13 (0.08)	117.13 (0.08)					
B13_§3	1.7614 (0.0045)	64.26 (0.10)	64.26 (0.10)	117.36 (0.24)				
B13_§19	1.7614 (0.0045)	117.36 (0.24)	64.26 (0.10)	64.26 (0.10)	63.18 (0.22)			
B13_§18	1.7614 (0.0045)	64.26 (0.10)	117.36 (0.24)	64.26 (0.10)	63.18 (0.22)	63.18 (0.22)		
B11_§1	1.7647 (0.0036)	61.61 (0.11)	116.07 (0.14)	116.07 (0.14)	115.98 (0.10)	178.97 (0.21)	115.98 (0.11)	
B11	1.7647 (0.0036)	116.07 (0.14)	61.61 (0.11)	116.07 (0.14)	115.98 (0.10)	115.98 (0.11)	178.97 (0.21)	64.85 (0.17)
B11_§2	1.7647 (0.0036)	116.07 (0.14)	116.07 (0.14)	61.60 (0.11)	178.96 (0.20)	115.98 (0.10)	115.98 (0.10)	64.85 (0.17)
	B14 -	B12_§1	B12	B12_§2	B13_§3	B13_§19	B13_§18	B11_§1
B15 -	Distance	Angles						
B13_§3	1.7148 (0.0033)							
B13_§2	1.7148 (0.0033)	180.00 (0.14)						
B13_§18	1.7148 (0.0034)	65.11 (0.18)	114.89 (0.18)					
B13_§1	1.7148 (0.0034)	114.89 (0.18)	65.11 (0.18)	114.89 (0.18)				
B13_§19	1.7148 (0.0034)	65.11 (0.18)	114.89 (0.18)	65.11 (0.18)	180.00 (0.00)			
B13	1.7148 (0.0034)	114.90 (0.18)	65.10 (0.18)	180.00 (0.00)	65.11 (0.18)	114.89 (0.18)		
Mn2_§28	2.4891 (0.0008)	68.41 (0.04)	111.59 (0.04)	68.40 (0.04)	55.85 (0.11)	124.15 (0.11)	111.60 (0.04)	
Mn2_§9	2.4891 (0.0008)	111.59 (0.04)	68.41 (0.04)	111.60 (0.04)	124.15 (0.11)	55.85 (0.11)	68.40 (0.04)	180.00
Mn2_§27	2.4891 (0.0008)	111.59 (0.04)	68.41 (0.04)	55.85 (0.11)	68.41 (0.04)	111.59 (0.04)	124.15 (0.11)	60.54 (0.00)
Mn2_§13	2.4891 (0.0008)	68.41 (0.04)	111.59 (0.04)	124.15 (0.11)	111.59 (0.04)	68.41 (0.04)	55.85 (0.11)	119.46 (0.00)
Mn2_§31	2.4892 (0.0008)	124.15 (0.11)	55.85 (0.11)	68.40 (0.04)	111.60 (0.04)	68.40 (0.04)	111.59 (0.04)	119.45 (0.00)
Mn2_§29	2.4892 (0.0008)	55.85 (0.11)	124.15 (0.11)	111.60 (0.04)	68.40 (0.04)	111.60 (0.04)	68.41 (0.04)	60.55 (0.00)
	B15 -	B13_§3	B13_§2	B13_§18	B13_§1	B13_§19	B13	Mn2_§28
Mn1 -	Distance	Angles						
B5_§18	2.1260 (0.0031)							
B5_§3	2.1260 (0.0031)	49.43 (0.11)						
B5_§19	2.1260 (0.0031)	49.43 (0.11)	49.43 (0.11)					
B7_§18	2.1384 (0.0023)	47.20 (0.09)	91.34 (0.10)	91.34 (0.10)				
B7_§19	2.1384 (0.0023)	91.34 (0.10)	91.34 (0.10)	47.20 (0.09)	114.40 (0.07)			
B7_§3	2.1384 (0.0023)	91.34 (0.10)	47.20 (0.09)	91.34 (0.10)	114.39 (0.07)	114.39 (0.07)		
B1	2.1603 (0.0019)	140.76 (0.10)	113.95 (0.06)	91.88 (0.07)	148.78 (0.07)	50.51 (0.06)	96.57 (0.05)	
B1_§6	2.1604 (0.0019)	140.76 (0.10)	91.88 (0.07)	113.95 (0.06)	148.78 (0.07)	96.56 (0.05)	50.51 (0.06)	53.01 (0.09)
B1_§8	2.1604 (0.0019)	113.95 (0.06)	140.76 (0.10)	91.88 (0.07)	96.57 (0.05)	50.51 (0.06)	148.78 (0.07)	52.30 (0.09)
B1_§5	2.1604 (0.0019)	91.88 (0.07)	113.95 (0.06)	140.76 (0.10)	50.51 (0.06)	148.78 (0.07)	96.57 (0.05)	124.99 (0.14)
B1_§2	2.1604 (0.0019)	91.88 (0.07)	140.76 (0.10)	113.95 (0.06)	50.51 (0.06)	96.57 (0.05)	148.78 (0.07)	100.38 (0.09)
B1_§1	2.1604 (0.0019)	113.95 (0.06)	91.88 (0.07)	140.76 (0.10)	96.56 (0.05)	148.78 (0.07)	50.51 (0.06)	100.38 (0.09)
	Mn1 -	B5_§18	B5_§3	B5_§19	B7_§18	B7_§19	B7_§3	B1
Mn2 -	Distance	Angles						
B13_§13	2.0842 (0.0034)							
B3_§15	2.3306 (0.0016)	48.13 (0.09)						
B3_§14	2.3307 (0.0016)	48.13 (0.09)	48.17 (0.08)					
B12_§13	2.3895 (0.0023)	118.46 (0.11)	149.96 (0.05)	149.96 (0.05)				
B1	2.4028 (0.0017)	129.02 (0.09)	99.77 (0.06)	80.92 (0.06)	106.55 (0.06)			
B1_§6	2.4028 (0.0018)	129.02 (0.09)	80.92 (0.06)	99.77 (0.06)	106.55 (0.07)	47.32 (0.08)		
B2_§6	2.4260 (0.0016)	87.98 (0.07)	42.95 (0.05)	84.40 (0.06)	124.68 (0.04)	85.20 (0.06)	44.96 (0.05)	
B2	2.4260 (0.0016)	87.98 (0.07)	84.40 (0.06)	42.94 (0.05)	124.68 (0.04)	44.96 (0.05)	85.20 (0.06)	102.03 (0.08)
B2_§7	2.4277 (0.0016)	118.57 (0.04)	129.05 (0.06)	85.17 (0.05)	80.65 (0.05)	45.43 (0.05)	90.03 (0.06)	130.57 (0.06)
B2_§10	2.4277 (0.0016)	118.57 (0.04)	85.17 (0.05)	129.05 (0.06)	80.65 (0.05)	90.03 (0.06)	45.43 (0.05)	44.76 (0.07)
B13_§14	2.4484 (0.0018)	78.80 (0.15)	126.04 (0.09)	106.30 (0.08)	45.28 (0.08)	125.00 (0.09)	151.16 (0.08)	148.76 (0.09)
B13_§25	2.4484 (0.0017)	78.80 (0.15)	106.30 (0.08)	126.04 (0.09)	45.28 (0.08)	151.16 (0.08)	125.00 (0.09)	105.61 (0.08)
	Mn2 -	B13_§13	B3_§15	B3_§14	B12_§13	B1	B1_§6	B2_§6

Mn3 -	Distance	Angles						
B1	2.3628 (0.0016)							
B1_\$5	2.3628 (0.0016)	108.38 (0.08)						
B1_\$2	2.3628 (0.0016)	89.23 (0.06)	47.52 (0.08)					
B1_\$1	2.3628 (0.0016)	89.23 (0.06)	48.17 (0.08)	89.23 (0.06)				
B1_\$8	2.3628 (0.0016)	47.52 (0.08)	89.23 (0.06)	48.17 (0.08)	108.38 (0.08)			
B1_\$6	2.3628 (0.0016)	48.17 (0.08)	89.23 (0.06)	108.38 (0.08)	47.52 (0.08)	89.23 (0.06)		
Mn1	2.3800 (0.0026)	54.19 (0.04)	54.19 (0.04)	54.19 (0.04)	54.19 (0.04)	54.19 (0.04)	54.19 (0.04)	
B9_\$19	2.4713 (0.0022)	45.33 (0.06)	134.56 (0.06)	90.22 (0.05)	134.56 (0.06)	45.33 (0.06)	90.21 (0.05)	90.08 (0.05)
B9_\$18	2.4713 (0.0022)	134.56 (0.06)	45.33 (0.06)	45.33 (0.06)	90.21 (0.05)	90.22 (0.05)	134.56 (0.06)	90.08 (0.05)
B9_\$3	2.4713 (0.0022)	90.21 (0.05)	90.21 (0.05)	134.56 (0.06)	45.33 (0.06)	134.56 (0.06)	45.33 (0.06)	90.08 (0.05)
B11	2.5166 (0.0022)	102.87 (0.06)	146.37 (0.05)	146.37 (0.05)	121.72 (0.04)	121.72 (0.04)	102.87 (0.06)	154.27 (0.05)
B11_\$1	2.5166 (0.0022)	146.37 (0.05)	102.87 (0.06)	121.72 (0.04)	102.87 (0.06)	146.37 (0.05)	121.72 (0.04)	154.27 (0.05)
	Mn3 -	B1	B1_\$5	B1_\$2	B1_\$1	B1_\$8	B1_\$6	Mn1

A.2 Ausgewählte Bindungswinkel und -längen in $Zr_{5.63}B_{311.45}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 -	Distance	Angles						
B16_\$5	1.8252 (0.0172)							
B03_\$5	1.8384 (0.0024)	58.81 (0.33)						
B04_\$25	1.8462 (0.0023)	147.23 (0.62)	104.35 (0.10)					
B01_\$10	1.8737 (0.0031)	88.45 (0.57)	59.36 (0.06)	59.51 (0.06)				
B02_\$17	1.8803 (0.0021)	89.61 (0.56)	58.01 (0.08)	105.12 (0.11)	106.59 (0.07)			
B02_\$16	1.8807 (0.0021)	146.96 (0.61)	103.38 (0.11)	59.09 (0.08)	106.59 (0.07)	58.18 (0.09)		
B01_\$7	1.8910 (0.0031)	58.80 (0.33)	117.60 (0.08)	129.37 (0.08)	120.00 (0.00)	120.30 (0.07)	128.72 (0.07)	
Zr2_\$1	2.1320 (0.0191)	31.53 (1.06)	64.69 (0.76)	117.49 (0.65)	63.93 (0.25)	114.60 (0.95)	167.18 (0.49)	63.67 (0.26)
Zr1_\$1	2.3437 (0.0024)	91.82 (0.59)	117.14 (0.10)	70.23 (0.09)	66.44 (0.04)	172.83 (0.10)	121.07 (0.10)	66.21 (0.04)
Zr3_\$5	2.3973 (0.0017)	95.58 (0.59)	118.40 (0.08)	117.00 (0.08)	173.23 (0.04)	68.09 (0.07)	67.22 (0.07)	66.77 (0.04)
	B01 -	B16_\$5	B03_\$5	B04_\$25	B01_\$10	B02_\$17	B02_\$16	B01_\$7

B02 -	Distance	Angles						
B07_\$20	1.7666 (0.0021)							
B03_\$14	1.8035 (0.0019)	114.90 (0.11)						
B02_\$11	1.8285 (0.0028)	128.26 (0.07)	106.94 (0.09)					
B04_\$13	1.8379 (0.0020)	118.56 (0.11)	60.84 (0.09)	107.62 (0.10)				
B01_\$8	1.8803 (0.0021)	117.52 (0.10)	59.84 (0.09)	60.92 (0.09)	110.10 (0.10)			
B01_\$4	1.8806 (0.0021)	125.90 (0.11)	108.60 (0.10)	60.90 (0.09)	59.52 (0.09)	111.36 (0.10)		
Zr3_\$21	2.4069 (0.0015)	70.57 (0.07)	174.52 (0.10)	68.55 (0.06)	116.91 (0.09)	118.54 (0.08)	66.69 (0.07)	
Zr3_\$35	2.4326 (0.0015)	67.03 (0.07)	118.22 (0.09)	67.05 (0.06)	174.38 (0.10)	66.10 (0.07)	117.30 (0.08)	63.47 (0.05)
	B02 -	B07_\$20	B03_\$14	B02_\$11	B04_\$13	B01_\$8	B01_\$4	Zr3_\$21

B03 -	Distance	Angles						
B05_\$3	1.7098 (0.0030)							
B16_\$23	1.7989 (0.0021)	60.24 (0.64)						
B16	1.7989 (0.0021)	60.24 (0.64)	59.13 (1.33)					
B02_\$19	1.8033 (0.0019)	119.86 (0.08)	149.06 (0.67)	92.93 (0.67)				
B02_\$14	1.8034 (0.0019)	119.86 (0.08)	92.93 (0.67)	149.06 (0.66)	109.62 (0.14)			
B01_\$6	1.8384 (0.0023)	120.45 (0.13)	60.23 (0.64)	90.36 (0.65)	111.47 (0.12)	62.16 (0.08)		
B01_\$3	1.8384 (0.0023)	120.45 (0.13)	90.36 (0.65)	60.23 (0.64)	62.16 (0.08)	111.47 (0.12)	61.28 (0.11)	
B04_\$12	1.8439 (0.0030)	118.44 (0.15)	149.82 (0.66)	149.82 (0.66)	60.51 (0.08)	60.51 (0.08)	111.72 (0.12)	111.72 (0.12)
Zr2	2.1388 (0.0100)	66.34 (1.05)	31.41 (0.75)	31.41 (0.75)	117.75 (0.41)	117.75 (0.41)	64.31 (0.87)	64.31 (0.87)
	B03 -	B05_\$3	B16_\$23	B16	B02_\$19	B02_\$14	B01_\$6	B01_\$3

B04 -	Distance	Angles						
B10_\$41	1.7173 (0.0029)							
B02_\$13	1.8379 (0.0020)	119.52 (0.08)						
B02_\$11	1.8379 (0.0020)	119.52 (0.08)	106.62 (0.14)					
B03_\$21	1.8439 (0.0030)	116.10 (0.15)	58.66 (0.08)	58.65 (0.08)				
B01_\$8	1.8462 (0.0023)	125.57 (0.12)	109.57 (0.12)	61.39 (0.08)	108.36 (0.12)			
B01_\$2	1.8462 (0.0023)	125.57 (0.12)	61.39 (0.08)	109.57 (0.12)	108.36 (0.12)	60.99 (0.12)		
Zr1_\$14	2.4442 (0.0021)	72.47 (0.13)	118.07 (0.09)	118.07 (0.09)	171.43 (0.15)	64.47 (0.10)	64.47 (0.10)	
	B04 -	B10_\$41	B02_\$13	B02_\$11	B03_\$21	B01_\$8	B01_\$2	

B05 -	Distance	Angles						

A.2 Ausgewählte Bindungswinkel und -längen in $Zr_{5.63}B_{311.45}$

B03_\$5	1.7099 (0.0030)								
B06_\$29	1.7624 (0.0021)	122.95 (0.10)							
B06_\$31	1.7624 (0.0021)	122.95 (0.10)	105.70 (0.17)						
B16_\$5	1.7626 (0.0173)	62.38 (0.34)	92.41 (0.57)	147.66 (0.67)					
B16_\$3	1.7626 (0.0173)	62.38 (0.34)	147.66 (0.69)	92.41 (0.57)	60.48 (1.28)				
B06_\$4	1.7762 (0.0029)	122.88 (0.16)	58.95 (0.08)	58.96 (0.08)	149.76 (0.64)	149.76 (0.64)			
B05_\$22	1.7848 (0.0038)	121.95 (0.08)	59.58 (0.08)	106.90 (0.09)	59.58 (0.33)	89.85 (0.61)	106.76 (0.09)		
B05_\$23	1.7848 (0.0038)	121.95 (0.08)	106.90 (0.09)	59.58 (0.08)	89.85 (0.59)	59.58 (0.33)	106.76 (0.08)	60.00 (0.00)	
Zr2_\$1	2.1361 (0.0355)	66.50 (0.53)	117.23 (0.26)	117.23 (0.25)	31.42 (0.68)	31.42 (0.68)	170.61 (0.56)	65.31 (0.45)	
	B05 -	B03_\$5	B06_\$29	B06_\$31	B16_\$5	B16_\$3	B06_\$4	B05_\$22	
B06 -	Distance	Angles							
B09	1.6309 (0.0030)								
B06_\$30	1.7412 (0.0025)	122.11 (0.03)							
B06_\$26	1.7412 (0.0025)	122.11 (0.03)	107.56 (0.13)						
B05_\$28	1.7624 (0.0021)	119.37 (0.13)	109.32 (0.11)	60.91 (0.10)					
B05_\$27	1.7624 (0.0021)	119.37 (0.13)	60.91 (0.10)	109.32 (0.11)	60.84 (0.16)				
B05_\$16	1.7762 (0.0029)	121.53 (0.15)	60.14 (0.11)	60.14 (0.11)	110.37 (0.14)	110.37 (0.14)			
	B06 -	B09	B06_\$30	B06_\$26	B05_\$28	B05_\$27			
B07 -	Distance	Angles							
B02_\$20	1.7667 (0.0021)								
B11_\$25	1.7912 (0.0017)	123.73 (0.12)							
B09_\$39	1.7931 (0.0023)	122.53 (0.12)	105.22 (0.11)						
B08_\$38	1.8154 (0.0021)	120.21 (0.11)	61.83 (0.09)	57.64 (0.08)					
B13	1.8181 (0.0035)	122.54 (0.13)	62.45 (0.12)	104.95 (0.11)	111.48 (0.13)				
B07_\$10	1.9077 (0.0030)	122.16 (0.07)	107.14 (0.08)	57.87 (0.06)	106.30 (0.07)	58.36 (0.08)			
Zr3_\$14	2.3843 (0.0016)	69.95 (0.07)	112.35 (0.10)	119.40 (0.08)	169.75 (0.10)	58.83 (0.11)	66.42 (0.04)		
Zr3_\$25	2.4668 (0.0016)	66.94 (0.07)	66.06 (0.08)	170.45 (0.11)	117.91 (0.09)	68.00 (0.08)	119.60 (0.04)	63.28 (0.04)	
	B07 -	B02_\$20	B11_\$25	B09_\$39	B08_\$38	B13	B07_\$10	Zr3_\$14	
B08 -	Distance	Angles							
B08_\$33	1.6802 (0.0029)								
B09	1.7395 (0.0019)	121.07 (0.08)							
B07_\$34	1.8155 (0.0021)	121.20 (0.13)	60.54 (0.09)						
B10	1.8474 (0.0019)	119.45 (0.13)	62.10 (0.09)	111.03 (0.10)					
B12_\$15	1.8494 (0.0023)	124.01 (0.10)	106.03 (0.11)	107.00 (0.11)	58.05 (0.09)				
B11	1.8533 (0.0021)	125.96 (0.10)	104.82 (0.11)	58.44 (0.08)	105.92 (0.12)	58.83 (0.10)			
	B08 -	B08_\$33	B09	B07_\$34	B10	B12_\$15			
B09 -	Distance	Angles							
B06	1.6309 (0.0030)								
B08	1.7395 (0.0019)	116.80 (0.09)							
B08_\$36	1.7395 (0.0019)	116.80 (0.09)	114.53 (0.15)						
B07_\$34	1.7931 (0.0023)	120.31 (0.12)	61.83 (0.08)	115.01 (0.13)					
B07_\$32	1.7931 (0.0023)	120.31 (0.12)	115.01 (0.13)	61.83 (0.08)	64.27 (0.12)				
B10	1.8523 (0.0029)	117.36 (0.15)	61.81 (0.08)	61.81 (0.08)	111.83 (0.12)	111.83 (0.12)			
	B09 -	B06	B08	B08_\$36	B07_\$34	B07_\$32			
B10 -	Distance	Angles							
B04_\$24	1.7174 (0.0029)								
B12_\$15	1.7936 (0.0019)	123.39 (0.12)							
B12_\$46	1.7936 (0.0019)	123.39 (0.12)	62.92 (0.16)						
B08	1.8474 (0.0019)	121.05 (0.09)	61.03 (0.09)	110.03 (0.13)					
B08_\$36	1.8475 (0.0019)	121.05 (0.09)	110.03 (0.13)	61.03 (0.09)	104.75 (0.13)				
B09	1.8523 (0.0029)	123.69 (0.15)	103.71 (0.12)	103.71 (0.12)	56.09 (0.07)	56.09 (0.07)			
Zr1_\$14	2.5288 (0.0029)	67.17 (0.11)	67.23 (0.10)	67.23 (0.10)	120.08 (0.08)	120.08 (0.08)	169.14 (0.14)		
	B10 -	B04_\$24	B12_\$15	B12_\$46	B08	B08_\$36	B09		
B11 -	Distance	Angles							
B14_\$14	1.7371 (0.0022)								
B07_\$2	1.7912 (0.0017)	104.30 (0.09)							
B07_\$34	1.7913 (0.0017)	104.29 (0.09)	139.67 (0.15)						
B12_\$15	1.8186 (0.0030)	59.78 (0.16)	109.40 (0.08)	109.39 (0.08)					
B08_\$10	1.8533 (0.0021)	104.30 (0.13)	59.72 (0.07)	136.52 (0.13)	60.48 (0.09)				
B08	1.8533 (0.0021)	104.30 (0.13)	136.52 (0.13)	59.72 (0.07)	60.48 (0.09)	81.85 (0.12)			
B13_\$2	1.8712 (0.0027)	59.05 (0.15)	59.48 (0.13)	115.20 (0.15)	110.18 (0.14)	107.47 (0.12)	162.12 (0.16)		
B13_\$32	1.8712 (0.0027)	59.05 (0.15)	115.20 (0.15)	59.48 (0.13)	110.18 (0.14)	162.12 (0.16)	107.47 (0.12)	59.64 (0.23)	
Zr3	2.3891 (0.0022)	119.45 (0.16)	70.68 (0.08)	70.68 (0.08)	179.23 (0.15)	120.02 (0.09)	120.02 (0.09)	69.17 (0.10)	
	B11 -	B14_\$14	B07_\$2	B07_\$34	B12_\$15	B08_\$10	B08	B13_\$2	
B12 -	Distance	Angles							

B14_\$47	1.7734	(0.0036)							
B10_\$40	1.7937	(0.0020)	103.35	(0.09)					
B10_\$35	1.7937	(0.0020)	103.35	(0.09)	139.89	(0.17)			
B11_\$35	1.8186	(0.0030)	57.83	(0.12)	109.73	(0.09)	109.73	(0.09)	
B08_\$35	1.8495	(0.0023)	103.01	(0.11)	138.35	(0.13)	60.92	(0.07)	60.68 (0.09)
B08_\$37	1.8495	(0.0023)	103.01	(0.11)	60.92	(0.07)	138.35	(0.13)	60.68 (0.09) 82.05 (0.13)
B12_\$43	1.8722	(0.0038)	58.14	(0.08)	114.68	(0.08)	58.54	(0.08)	107.46 (0.08) 106.56 (0.07) 160.29 (0.07)
B12_\$45	1.8722	(0.0038)	58.14	(0.08)	58.54	(0.08)	114.68	(0.08)	107.46 (0.08) 160.29 (0.07) 106.56 (0.07) 60.00 (0.00)
Zr1_\$47	2.4700	(0.0035)	116.49	(0.13)	70.74	(0.09)	70.74	(0.09)	174.32 (0.14) 122.96 (0.09) 122.96 (0.09) 67.73 (0.05)
	B12 -		B14_\$47		B10_\$40		B10_\$35		B11_\$35 B08_\$35 B08_\$37 B12_\$43

B13 -		Distance	Angles						
B15	1.7233	(0.0034)							
B14_\$1	1.7820	(0.0046)	104.35	(0.20)					
B07_\$10	1.8181	(0.0035)	138.86	(0.14)	101.41	(0.16)			
B07	1.8181	(0.0035)	138.87	(0.14)	101.41	(0.16)	63.29	(0.15)	
B13_\$22	1.8609	(0.0064)	57.32	(0.09)	58.52	(0.11)	159.67	(0.11)	114.40 (0.09)
B13_\$23	1.8609	(0.0064)	57.32	(0.09)	58.52	(0.11)	114.40	(0.08)	159.67 (0.11) 60.00
B11_\$39	1.8711	(0.0027)	113.31	(0.14)	56.72	(0.11)	58.07	(0.09)	107.58 (0.17) 107.13 (0.12) 60.18 (0.12)
B11_\$25	1.8713	(0.0027)	113.31	(0.14)	56.72	(0.11)	107.58	(0.17)	58.07 (0.09) 60.18 (0.12) 107.14 (0.12) 104.72 (0.20)
Zr3_\$14	2.1222	(0.0035)	81.08	(0.13)	174.57	(0.22)	74.02	(0.13)	74.02 (0.13) 125.82 (0.08) 125.82 (0.08) 121.39 (0.13)
Zr3_\$39	2.4556	(0.0016)	71.68	(0.08)	114.30	(0.09)	68.65	(0.07)	124.35 (0.17) 120.38 (0.09) 67.73 (0.08) 65.42 (0.07)
Zr3_\$25	2.4557	(0.0016)	71.68	(0.08)	114.30	(0.09)	124.35	(0.17)	68.65 (0.07) 67.73 (0.08) 120.38 (0.09) 170.09 (0.16)
	B13 -		B15		B14_\$1		B07_\$10		B07 B13_\$22 B13_\$23 B11_\$39

B14 -		Distance	Angles						
B11_\$14	1.7371	(0.0022)							
B11_\$15	1.7371	(0.0022)	117.08	(0.08)					
B11_\$26	1.7372	(0.0022)	117.07	(0.08)	117.07	(0.08)			
B12_\$44	1.7734	(0.0036)	115.93	(0.13)	62.40	(0.11)	115.92	(0.13)	
B12_\$42	1.7734	(0.0036)	115.92	(0.13)	115.92	(0.13)	62.40	(0.11)	63.72 (0.16)
B12_\$24	1.7734	(0.0036)	62.40	(0.11)	115.93	(0.13)	115.92	(0.13)	63.72 (0.16) 63.72 (0.16)
B13_\$3	1.7820	(0.0046)	64.22	(0.10)	117.13	(0.23)	64.23	(0.10)	179.52 (0.19) 116.66 (0.11) 116.66 (0.11)
B13_\$5	1.7820	(0.0046)	64.23	(0.10)	64.23	(0.10)	117.13	(0.23)	116.66 (0.11) 179.52 (0.20) 116.66 (0.11) 62.95 (0.22)
B13_\$1	1.7820	(0.0046)	117.13	(0.23)	64.22	(0.10)	64.23	(0.10)	116.66 (0.11) 116.66 (0.11) 179.52 (0.20) 62.95 (0.22)
	B14 -		B11_\$14		B11_\$15		B11_\$26		B12_\$44 B12_\$42 B12_\$24 B13_\$3

B15 -		Distance	Angles						
B13_\$23	1.7233	(0.0034)							
B13_\$22	1.7233	(0.0034)	65.36	(0.19)					
B13	1.7233	(0.0034)	65.36	(0.19)	65.36	(0.19)			
B13_\$1	1.7234	(0.0034)	114.64	(0.19)	114.64	(0.19)	180.00	(0.00)	
B13_\$5	1.7234	(0.0034)	180.00		114.64	(0.19)	114.64	(0.19)	65.35 (0.19)
B13_\$3	1.7234	(0.0034)	114.64	(0.19)	180.00	(0.00)	114.64	(0.19)	65.35 (0.19) 65.35 (0.19)
Zr3_\$39	2.5179	(0.0008)	67.80	(0.04)	123.63	(0.12)	67.80	(0.04)	112.20 (0.04) 112.20 (0.04) 56.37 (0.12)
Zr3_\$49	2.5179	(0.0008)	67.80	(0.04)	67.80	(0.04)	123.63	(0.12)	56.37 (0.12) 112.20 (0.04) 112.20 (0.04) 119.27 (0.00)
Zr3_\$15	2.5179	(0.0008)	112.20	(0.04)	56.37	(0.12)	112.20	(0.04)	67.80 (0.04) 123.63 (0.12) 180.00 (0.02)
Zr3_\$14	2.5179	(0.0008)	112.20	(0.04)	112.21	(0.04)	56.37	(0.12)	123.63 (0.12) 67.80 (0.04) 67.80 (0.04) 60.73 (0.00)
Zr3_\$25	2.5179	(0.0008)	123.63	(0.12)	67.80	(0.04)	67.80	(0.04)	112.20 (0.04) 56.37 (0.12) 112.20 (0.04) 119.27 (0.00)
Zr3_\$26	2.5179	(0.0008)	56.37	(0.12)	112.20	(0.04)	112.21	(0.04)	67.80 (0.04) 123.63 (0.12) 67.80 (0.04) 60.73 (0.00)
	B15 -		B13_\$23		B13_\$22		B13		B13_\$1 B13_\$5 B13_\$3 Zr3_\$39

B16 -		Distance	Angles						
Zr2	1.1151	(0.0266)							
B05_\$5	1.7625	(0.0173)	93.10	(1.98)					
B05_\$3	1.7625	(0.0173)	93.10	(1.98)	60.84	(0.66)			
B16_\$22	1.7753	(0.0361)	37.25	(1.22)	59.76	(0.64)	90.15	(0.59)	
B16_\$23	1.7753	(0.0360)	37.25	(1.22)	90.15	(0.59)	59.76	(0.64)	60.00 (0.00)
B03	1.7989	(0.0021)	91.35	(0.66)	118.19	(0.96)	57.37	(0.32)	120.37 (0.66) 60.43 (0.66)
B03_\$22	1.7990	(0.0021)	91.35	(0.66)	57.37	(0.32)	118.20	(0.96)	60.43 (0.66) 120.37 (0.67) 174.94 (1.27)
B01_\$11	1.8252	(0.0171)	89.58	(1.97)	118.31	(0.10)	177.22	(1.26)	91.55 (0.56) 123.02 (0.62) 123.34 (0.96) 60.96 (0.33)
B01_\$3	1.8252	(0.0171)	89.58	(1.97)	177.22	(1.32)	118.31	(0.10)	123.02 (0.62) 91.55 (0.56) 60.96 (0.32) 123.34 (0.96)
	B16 -		Zr2		B05_\$5		B05_\$3		B16_\$22 B16_\$23 B03 B03_\$22

Zr1 -		Distance	Angles						
B01_\$9	2.3438	(0.0024)							
B01_\$1	2.3438	(0.0024)	47.12	(0.09)					
B01_\$5	2.3438	(0.0024)	47.58	(0.08)	88.14	(0.10)			
B01_\$3	2.3438	(0.0024)	106.86	(0.14)	88.14	(0.10)	88.14	(0.10)	
B01_\$11	2.3438	(0.0024)	88.14	(0.10)	106.86	(0.14)	47.12	(0.09)	47.58 (0.08)
B01_\$6	2.3438	(0.0024)	88.14	(0.10)	47.58	(0.08)	106.86	(0.14)	47.12 (0.09) 88.14 (0.10)
Zr2	2.3975	(0.0405)	53.43	(0.07)	53.43	(0.07)	53.43	(0.07)	53.43 (0.07) 53.43 (0.07) 53.43 (0.07)

A.3 Ausgewählte Bindungswinkel und -längen in $Al_6Cu_{5.40}B_{319.64}$

B04_\$15	2.4441 (0.0021)	89.73 (0.06)	133.44 (0.12)	45.30 (0.06)	89.73 (0.06)	45.30 (0.06)	133.44 (0.12)	89.34 (0.09)
B04_\$26	2.4442 (0.0021)	45.30 (0.06)	45.30 (0.06)	89.73 (0.06)	133.44 (0.12)	133.44 (0.12)	89.73 (0.06)	89.34 (0.09)
B04_\$14	2.4442 (0.0021)	133.44 (0.12)	89.73 (0.06)	133.44 (0.12)	45.30 (0.06)	89.73 (0.06)	45.30 (0.06)	89.34 (0.09)
B12_\$24	2.4698 (0.0035)	147.20 (0.09)	147.20 (0.09)	122.33 (0.06)	103.40 (0.07)	103.40 (0.07)	122.33 (0.06)	154.05 (0.06)
B12_\$42	2.4698 (0.0035)	122.33 (0.06)	103.40 (0.07)	147.20 (0.09)	122.33 (0.06)	147.20 (0.09)	103.40 (0.07)	154.05 (0.06)
Zr1 -		B01_\$9	B01_\$1	B01_\$5	B01_\$3	B01_\$11	B01_\$6	Zr2
Zr2 -	Distance	Angles						
B16_\$22	1.1151 (0.0267)							
B16_\$23	1.1151 (0.0267)	105.50 (2.44)						
B16	1.1151 (0.0267)	105.50 (2.44)	105.50 (2.44)					
B01_\$3	2.1320 (0.0190)	152.73 (0.69)	100.53 (0.68)	58.88 (1.21)				
B01_\$11	2.1320 (0.0190)	100.53 (0.68)	152.73 (0.69)	58.88 (1.20)	52.65 (0.51)			
B01_\$6	2.1320 (0.0190)	152.73 (0.68)	58.88 (1.20)	100.53 (0.68)	52.13 (0.51)	99.75 (1.21)		
B01_\$9	2.1320 (0.0190)	58.88 (1.20)	100.53 (0.68)	152.73 (0.69)	123.99 (1.92)	99.75 (1.21)	99.75 (1.21)	
B01_\$1	2.1320 (0.0190)	100.53 (0.68)	58.88 (1.20)	152.73 (0.69)	99.75 (1.21)	123.99 (1.92)	52.65 (0.51)	52.13 (0.51)
B01_\$5	2.1320 (0.0190)	58.88 (1.20)	152.73 (0.68)	100.53 (0.68)	99.75 (1.21)	52.13 (0.51)	123.99 (1.92)	52.65 (0.51)
B05_\$1	2.1360 (0.0354)	55.48 (1.75)	55.48 (1.75)	95.65 (2.64)	141.22 (1.26)	141.22 (1.26)	114.36 (0.69)	92.40 (0.47)
B05_\$5	2.1360 (0.0354)	55.48 (1.75)	95.65 (2.64)	55.48 (1.75)	114.36 (0.69)	92.40 (0.47)	141.22 (1.26)	114.36 (0.69)
B05_\$3	2.1360 (0.0354)	95.65 (2.64)	55.48 (1.75)	55.48 (1.75)	92.40 (0.47)	114.36 (0.69)	92.40 (0.47)	141.22 (1.26)
Zr2 -		B16_\$22	B16_\$23	B16	B01_\$3	B01_\$11	B01_\$6	B01_\$9
Zr3 -	Distance	Angles						
B13_\$14	2.1222 (0.0035)							
B07_\$33	2.3843 (0.0016)	47.15 (0.09)						
B07_\$14	2.3843 (0.0016)	47.15 (0.09)	47.16 (0.07)					
B11	2.3891 (0.0022)	117.99 (0.11)	149.50 (0.05)	149.50 (0.05)				
B01_\$11	2.3973 (0.0017)	128.52 (0.09)	81.42 (0.05)	99.57 (0.05)	107.72 (0.06)			
B01_\$3	2.3973 (0.0017)	128.52 (0.09)	99.57 (0.05)	81.42 (0.05)	107.72 (0.06)	46.46 (0.07)		
B02_\$18	2.4068 (0.0015)	117.68 (0.04)	84.94 (0.05)	128.11 (0.05)	81.72 (0.04)	46.09 (0.05)	90.11 (0.06)	
B02_\$12	2.4068 (0.0015)	117.67 (0.04)	128.11 (0.05)	84.94 (0.05)	81.72 (0.04)	90.11 (0.05)	46.09 (0.05)	123.68 (0.08)
B02_\$15	2.4327 (0.0015)	87.00 (0.07)	43.02 (0.05)	83.79 (0.05)	125.22 (0.04)	45.81 (0.05)	85.25 (0.05)	44.40 (0.07)
B02_\$19	2.4327 (0.0015)	87.00 (0.07)	83.79 (0.05)	43.01 (0.05)	125.22 (0.04)	85.25 (0.05)	45.81 (0.05)	131.18 (0.05)
B13_\$2	2.4556 (0.0016)	78.28 (0.15)	105.36 (0.08)	124.62 (0.09)	45.41 (0.08)	125.95 (0.09)	152.38 (0.08)	80.55 (0.09)
B13_\$32	2.4556 (0.0016)	78.28 (0.16)	124.62 (0.09)	105.36 (0.08)	45.42 (0.08)	152.38 (0.08)	125.95 (0.09)	120.26 (0.09)
Zr3 -		B13_\$14	B07_\$33	B07_\$14	B11	B01_\$11	B01_\$3	B02_\$18

A.3 Ausgewählte Bindungswinkel und -längen in $Al_6Cu_{5.40}B_{319.64}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 -	Distance	Angles							
B02	1.8298 (0.0023)								
B04	1.8339 (0.0026)	61.02 (0.09)							
B02_\$5	1.8686 (0.0023)	60.43 (0.10)	108.36 (0.12)						
B03	1.8891 (0.0025)	104.29 (0.12)	104.26 (0.11)	57.24 (0.09)					
B01_\$6	1.9390 (0.0034)	106.78 (0.07)	58.09 (0.06)	106.42 (0.07)	59.12 (0.06)				
B01_\$4	1.9780 (0.0033)	128.53 (0.07)	128.66 (0.09)	118.99 (0.07)	116.98 (0.09)	120.00			
Al1	2.2200 (0.0017)	167.44 (0.11)	115.88 (0.10)	112.38 (0.09)	63.94 (0.09)	64.10 (0.04)	63.54 (0.04)		
Cu1	2.3962 (0.0020)	66.97 (0.07)	116.64 (0.09)	71.33 (0.08)	121.94 (0.09)	173.73 (0.04)	65.62 (0.04)	122.14 (0.07)	
		B01 -	B02	B04	B02_\$5	B03	B01_\$6	B01_\$4	Al1
B02 -	Distance	Angles							
B07	1.7449 (0.0023)								
B03_\$7	1.8001 (0.0021)	116.54 (0.12)							
B01	1.8298 (0.0023)	126.02 (0.12)	106.90 (0.12)						
B04	1.8602 (0.0022)	119.47 (0.12)	59.09 (0.10)	59.60 (0.10)					
B02_\$5	1.8615 (0.0032)	127.46 (0.08)	106.63 (0.10)	60.82 (0.10)	107.56 (0.10)				
B01_\$5	1.8685 (0.0023)	118.48 (0.12)	61.95 (0.10)	109.29 (0.11)	109.92 (0.11)	58.76 (0.10)			
Cu1	2.3789 (0.0017)	67.40 (0.08)	174.81 (0.11)	67.97 (0.08)	116.33 (0.10)	71.86 (0.07)	119.85 (0.09)		
Cu1_\$24	2.5231 (0.0018)	69.53 (0.08)	119.64 (0.11)	114.72 (0.09)	170.88 (0.11)	63.63 (0.06)	64.12 (0.07)	64.43 (0.06)	
		B02 -	B07	B03_\$7	B01	B04	B02_\$5	B01_\$5	Cu1
B03 -	Distance	Angles							

B05_\$7	1.7458 (0.0034)							
B02_\$7	1.8001 (0.0021)	118.93 (0.09)						
B02_\$5	1.8001 (0.0021)	118.93 (0.09)	112.63 (0.16)					
B04_\$7	1.8055 (0.0034)	118.19 (0.16)	62.11 (0.09)	62.11 (0.09)				
B01_\$6	1.8890 (0.0025)	120.80 (0.14)	60.81 (0.09)	111.49 (0.13)	111.42 (0.13)			
B01	1.8891 (0.0025)	120.80 (0.14)	111.49 (0.13)	60.81 (0.09)	111.42 (0.13)	61.76 (0.12)		
A11	2.1936 (0.0024)	65.65 (0.11)	116.53 (0.09)	116.53 (0.09)	176.15 (0.15)	65.39 (0.09)	65.39 (0.09)	
	B03 -	B05_\$7	B02_\$7	B02_\$5	B04_\$7	B01_\$6	B01	
B04 -	Distance	Angles						
B08_\$13	1.7129 (0.0033)							
B03_\$7	1.8055 (0.0034)	117.24 (0.17)						
B01	1.8339 (0.0026)	125.54 (0.13)	106.50 (0.13)					
B01_\$6	1.8340 (0.0026)	125.53 (0.14)	106.50 (0.13)	63.83 (0.13)				
B02_\$6	1.8601 (0.0022)	119.58 (0.09)	58.80 (0.08)	110.00 (0.13)	59.38 (0.09)			
B02	1.8602 (0.0022)	119.58 (0.09)	58.80 (0.08)	59.38 (0.09)	110.00 (0.13)	107.27 (0.15)		
	B04 -	B08_\$13	B03_\$7	B01	B01_\$6	B02_\$6		
B05 -	Distance	Angles						
B03_\$7	1.7459 (0.0034)							
B06_\$13	1.7474 (0.0032)	122.06 (0.18)						
B06_\$10	1.7621 (0.0024)	121.91 (0.11)	60.66 (0.09)					
B06	1.7621 (0.0024)	121.91 (0.11)	60.67 (0.09)	108.62 (0.19)				
B05_\$10	1.8301 (0.0043)	122.22 (0.09)	107.18 (0.09)	58.72 (0.09)	107.03 (0.10)			
B05_\$11	1.8302 (0.0043)	122.22 (0.09)	107.18 (0.09)	107.03 (0.10)	58.71 (0.09)	60.00		
A11_\$7	2.1686 (0.0025)	67.16 (0.11)	170.78 (0.16)	115.65 (0.10)	115.65 (0.10)	65.04 (0.05)	65.04 (0.05)	
	B05 -	B03_\$7	B06_\$13	B06_\$10	B06	B05_\$10	B05_\$11	
B06 -	Distance	Angles						
B09	1.6318 (0.0034)							
B05_\$9	1.7474 (0.0032)	122.20 (0.17)						
B05	1.7621 (0.0024)	120.18 (0.14)	108.48 (0.16)					
B05_\$11	1.7621 (0.0024)	120.18 (0.14)	108.48 (0.16)	62.57 (0.18)				
B06_\$9	1.7724 (0.0027)	122.16 (0.03)	60.08 (0.12)	109.11 (0.12)	59.26 (0.10)			
B06_\$13	1.7724 (0.0027)	122.16 (0.03)	60.08 (0.12)	59.26 (0.10)	109.11 (0.12)	107.69 (0.14)		
	B06 -	B09	B05_\$9	B05	B05_\$11	B06_\$9		
B07 -	Distance	Angles						
B02	1.7449 (0.0023)							
B09	1.7971 (0.0025)	122.12 (0.13)						
B11	1.7988 (0.0018)	123.87 (0.13)	105.02 (0.13)					
B13	1.8082 (0.0037)	124.00 (0.15)	104.23 (0.13)	62.30 (0.13)				
B10	1.8241 (0.0023)	119.27 (0.12)	57.68 (0.09)	61.83 (0.10)	111.10 (0.15)			
B07_\$14	1.9141 (0.0034)	122.51 (0.08)	57.82 (0.06)	107.14 (0.09)	58.04 (0.08)	106.48 (0.08)		
B16_\$24	2.1325 (0.0022)	72.81 (0.13)	147.58 (0.12)	83.67 (0.12)	51.67 (0.15)	144.71 (0.12)	89.76 (0.07)	
Cu1	2.3481 (0.0017)	69.28 (0.08)	167.98 (0.12)	63.27 (0.09)	68.65 (0.09)	114.80 (0.10)	121.11 (0.05)	34.28 (0.04)
Cu1_\$24	2.5163 (0.0019)	69.95 (0.08)	120.67 (0.09)	111.90 (0.10)	59.59 (0.12)	170.50 (0.11)	67.65 (0.04)	32.08 (0.04)
	B07 -	B02	B09	B11	B13	B10	B07_\$14	B16_\$24
B08 -	Distance	Angles						
B04_\$9	1.7130 (0.0033)							
B12	1.7947 (0.0022)	123.47 (0.14)						
B12_\$18	1.7947 (0.0022)	123.47 (0.14)	62.83 (0.18)					
B09	1.8465 (0.0033)	122.98 (0.17)	104.25 (0.13)	104.25 (0.13)				
B10	1.8513 (0.0022)	120.36 (0.10)	61.47 (0.10)	110.65 (0.14)	56.38 (0.08)			
B10_\$14	1.8513 (0.0022)	120.36 (0.10)	110.65 (0.14)	61.47 (0.10)	56.38 (0.08)	105.58 (0.15)		
	B08 -	B04_\$9	B12	B12_\$18	B09	B10		
B09 -	Distance	Angles						
B06	1.6318 (0.0034)							
B10_\$14	1.7469 (0.0021)	116.42 (0.10)						
B10	1.7469 (0.0021)	116.42 (0.10)	115.14 (0.17)					
B07_\$14	1.7971 (0.0025)	120.30 (0.14)	61.93 (0.09)	115.37 (0.14)				
B07	1.7971 (0.0025)	120.30 (0.14)	115.37 (0.14)	61.93 (0.09)	64.35 (0.13)			
B08	1.8465 (0.0033)	117.33 (0.16)	61.95 (0.09)	61.95 (0.09)	111.84 (0.14)	111.84 (0.14)		
	B09 -	B06	B10_\$14	B10	B07_\$14	B07		
B10 -	Distance	Angles						
B10_\$16	1.6904 (0.0033)							
B09	1.7469 (0.0021)	121.39 (0.09)						
B07	1.8241 (0.0023)	121.72 (0.15)	60.38 (0.10)					
B08	1.8513 (0.0022)	119.60 (0.15)	61.67 (0.10)	110.40 (0.12)				

A.3 Ausgewählte Bindungswinkel und -längen in $Al_6Cu_{5.40}B_{319.64}$

B11	1.8614 (0.0024)	126.34 (0.11)	104.46 (0.12)	58.42 (0.09)	105.34 (0.13)				
B12	1.8639 (0.0026)	124.04 (0.11)	105.46 (0.12)	106.68 (0.12)	57.77 (0.10)	58.66 (0.11)			
	B10 -	B10_\$16	B09	B07	B08	B11			
B11 - Distance Angles									
B14_\$17	1.7440 (0.0025)								
B07_\$4	1.7988 (0.0018)	104.34 (0.10)							
B07	1.7988 (0.0018)	104.33 (0.10)	139.58 (0.17)						
B12	1.8247 (0.0033)	59.48 (0.18)	109.47 (0.08)	109.47 (0.08)					
B10_\$4	1.8613 (0.0024)	104.41 (0.15)	59.75 (0.08)	136.43 (0.14)	60.74 (0.10)				
B10	1.8614 (0.0024)	104.41 (0.15)	136.43 (0.14)	59.75 (0.08)	60.74 (0.10)	81.76 (0.14)			
B13	1.8659 (0.0030)	58.99 (0.16)	115.80 (0.16)	59.09 (0.13)	109.56 (0.16)	162.41 (0.17)	106.95 (0.13)		
B13_\$15	1.8659 (0.0030)	59.00 (0.16)	59.09 (0.13)	115.80 (0.16)	109.55 (0.15)	106.95 (0.12)	162.40 (0.17)	60.73 (0.24)	
Cu1	2.2248 (0.0025)	120.85 (0.18)	70.50 (0.08)	70.50 (0.08)	179.67 (0.18)	119.03 (0.10)	119.04 (0.10)	70.73 (0.12)	
	B11 -	B14_\$17	B07_\$4	B07	B12	B10_\$4	B10	B13	
B12 - Distance Angles									
B14_\$17	1.7718 (0.0041)								
B08	1.7947 (0.0022)	103.12 (0.10)							
B08_\$15	1.7948 (0.0022)	103.12 (0.10)	140.71 (0.19)						
B11	1.8247 (0.0033)	57.99 (0.14)	109.30 (0.10)	109.30 (0.10)					
B10	1.8639 (0.0025)	103.20 (0.12)	60.76 (0.08)	137.95 (0.15)	60.60 (0.10)				
B10_\$4	1.8639 (0.0026)	103.20 (0.12)	137.95 (0.15)	60.76 (0.08)	60.60 (0.10)	81.62 (0.14)			
B12_\$15	1.8709 (0.0043)	58.13 (0.09)	114.87 (0.09)	58.58 (0.09)	107.60 (0.09)	160.52 (0.08)	106.81 (0.07)		
B12_\$18	1.8709 (0.0043)	58.13 (0.09)	58.59 (0.09)	114.87 (0.09)	107.60 (0.09)	106.81 (0.07)	160.51 (0.08)	60.00	
	B12 -	B14_\$17	B08	B08_\$15	B11	B10	B10_\$4	B12_\$15	
B13 - Distance Angles									
B15_\$23	1.7368 (0.0036)								
B16_\$24	1.7420 (0.0038)	66.05 (0.16)							
B16_\$18	1.7420 (0.0038)	66.05 (0.16)	65.94 (0.14)						
B14_\$17	1.7806 (0.0050)	103.46 (0.21)	143.95 (0.12)	143.95 (0.12)					
B07	1.8082 (0.0037)	138.39 (0.15)	73.81 (0.16)	107.29 (0.22)	102.47 (0.18)				
B07_\$14	1.8082 (0.0037)	138.39 (0.15)	107.29 (0.22)	73.81 (0.16)	102.47 (0.18)	63.91 (0.17)			
B11	1.8659 (0.0030)	112.52 (0.14)	93.71 (0.09)	158.77 (0.18)	57.09 (0.12)	58.60 (0.10)	108.82 (0.19)		
B11_\$18	1.8660 (0.0030)	112.52 (0.14)	158.77 (0.18)	93.71 (0.09)	57.09 (0.12)	108.82 (0.19)	58.60 (0.10)	105.68 (0.22)	
B13_\$15	1.8865 (0.0065)	57.11 (0.10)	90.15 (0.13)	123.16 (0.16)	58.01 (0.12)	114.33 (0.09)	160.25 (0.12)	59.63 (0.12)	
B13_\$18	1.8865 (0.0065)	57.11 (0.10)	123.15 (0.16)	90.16 (0.13)	58.01 (0.12)	160.25 (0.12)	114.33 (0.09)	106.94 (0.12)	
Cu1_\$24	2.2349 (0.0037)	78.17 (0.13)	36.70 (0.08)	36.69 (0.08)	178.38 (0.23)	76.16 (0.14)	76.16 (0.14)	122.39 (0.13)	
Cu1	2.3856 (0.0017)	73.98 (0.09)	33.39 (0.03)	98.93 (0.15)	111.47 (0.09)	66.45 (0.07)	124.29 (0.17)	61.68 (0.07)	
	B13 -	B15_\$23	B16_\$24	B16_\$18	B14_\$17	B07	B07_\$14	B11	
B14 - Distance Angles									
B11_\$17	1.7440 (0.0025)								
B11_\$19	1.7440 (0.0025)	117.00 (0.09)							
B11_\$13	1.7441 (0.0025)	117.00 (0.09)	117.00 (0.09)						
B12_\$19	1.7717 (0.0041)	116.04 (0.15)	62.52 (0.12)	116.03 (0.15)					
B12_\$17	1.7717 (0.0041)	62.52 (0.12)	116.04 (0.15)	116.04 (0.15)	63.74 (0.18)				
B12_\$13	1.7718 (0.0041)	116.04 (0.15)	116.04 (0.15)	62.52 (0.12)	63.74 (0.18)	63.74 (0.18)			
B13_\$13	1.7807 (0.0050)	63.92 (0.11)	117.62 (0.25)	63.92 (0.11)	179.85 (0.21)	116.14 (0.11)			
B13_\$17	1.7807 (0.0050)	63.92 (0.11)	63.92 (0.11)	117.62 (0.25)	116.15 (0.11)	116.14 (0.11)	179.86 (0.22)	63.97 (0.23)	
B13_\$19	1.7807 (0.0050)	117.62 (0.25)	63.92 (0.11)	63.92 (0.11)	116.14 (0.12)	179.85 (0.21)	116.14 (0.11)	63.97 (0.23)	
	B14 -	B11_\$17	B11_\$19	B11_\$13	B12_\$19	B12_\$17	B12_\$13	B13_\$13	
B15 - Distance Angles									
B13_\$19	1.7370 (0.0036)								
B13_\$21	1.7370 (0.0037)	180.00 (0.00)							
B13_\$20	1.7370 (0.0036)	114.22 (0.19)	65.78 (0.19)						
B13_\$17	1.7370 (0.0036)	65.78 (0.19)	114.22 (0.19)	180.00 (0.14)					
B13_\$13	1.7370 (0.0037)	65.78 (0.19)	114.22 (0.20)	114.22 (0.19)	65.78 (0.19)				
B13_\$22	1.7370 (0.0036)	114.22 (0.20)	65.78 (0.19)	65.78 (0.19)	114.22 (0.19)	180.00 (0.00)			
B16_\$17	1.8960 (0.0044)	122.89 (0.10)	57.11 (0.10)	90.00	90.00	57.11 (0.10)	122.89 (0.10)		
B16_\$20	1.8960 (0.0044)	57.11 (0.10)	122.89 (0.10)	90.00	90.00	122.89 (0.10)	57.11 (0.10)	180.00 (0.23)	
B16_\$13	1.8960 (0.0043)	57.11 (0.10)	122.89 (0.10)	57.11 (0.10)	122.89 (0.10)	90.00	90.00 (0.00)	120.00 (0.00)	
B16_\$21	1.8960 (0.0043)	90.00	90.00 (0.00)	57.11 (0.10)	122.89 (0.10)	57.11 (0.10)	122.89 (0.10)	60.00 (0.00)	
B16_\$19	1.8960 (0.0043)	90.00 (0.00)	90.00	122.89 (0.10)	57.11 (0.10)	122.89 (0.10)	57.11 (0.10)	120.00 (0.00)	
B16_\$22	1.8960 (0.0043)	122.89 (0.10)	57.11 (0.10)	122.89 (0.10)	57.11 (0.10)	90.00 (0.00)	90.00	60.00 (0.00)	
	B15 -	B13_\$19	B13_\$21	B13_\$20	B13_\$17	B13_\$13	B13_\$22	B16_\$17	
B16 - Distance Angles									
Cu1	1.3365 (0.0011)								
Cu1_\$8	1.3366 (0.0011)	156.33 (0.37)							

B13_§8	1.7420 (0.0038)	92.15 (0.12)	100.77 (0.11)						
B13_§15	1.7421 (0.0038)	100.77 (0.11)	92.14 (0.12)	113.69 (0.33)					
B16_§24	1.8959 (0.0043)	44.82 (0.17)	156.13 (0.15)	57.03 (0.07)	89.84 (0.13)				
B15_§23	1.8960 (0.0043)	101.83 (0.18)	101.84 (0.18)	56.84 (0.16)	56.84 (0.16)	60.00			
B16_§8	1.8961 (0.0043)	156.12 (0.14)	44.82 (0.17)	89.84 (0.13)	57.03 (0.07)	120.00 (0.00)	60.00 (0.00)		
B07_§8	2.1324 (0.0022)	89.99 (0.11)	81.73 (0.10)	54.52 (0.12)	164.73 (0.21)	90.25 (0.07)	110.57 (0.12)	110.31 (0.07)	
B07_§4	2.1325 (0.0022)	81.73 (0.10)	89.98 (0.11)	164.73 (0.21)	54.52 (0.12)	110.31 (0.07)	110.57 (0.12)	90.24 (0.07)	
	B16 -	Cu1	Cu1_§8	B13_§8	B13_§15	B16_§24	B15_§23	B16_§8	
A11 - Distance Angles									
B05_§12	2.1685 (0.0025)								
B05_§8	2.1685 (0.0025)	49.92 (0.11)							
B05_§7	2.1685 (0.0025)	49.92 (0.11)	49.92 (0.11)						
B03_§2	2.1936 (0.0024)	47.18 (0.09)	91.75 (0.07)	91.75 (0.07)					
B03	2.1936 (0.0024)	91.75 (0.07)	91.75 (0.07)	47.18 (0.09)	114.61 (0.05)				
B03_§1	2.1936 (0.0024)	91.75 (0.07)	47.18 (0.09)	91.75 (0.07)	114.61 (0.05)	114.61 (0.05)			
B01_§4	2.2200 (0.0017)	141.46 (0.07)	92.16 (0.07)	114.43 (0.05)	148.33 (0.06)	96.67 (0.05)	50.68 (0.06)		
B01_§6	2.2200 (0.0017)	114.43 (0.05)	141.46 (0.07)	92.16 (0.07)	96.67 (0.05)	50.68 (0.06)	148.33 (0.06)	99.64 (0.06)	
B01_§3	2.2200 (0.0017)	92.16 (0.07)	114.43 (0.05)	141.46 (0.07)	50.68 (0.06)	148.33 (0.06)	96.67 (0.05)	99.64 (0.06)	
B01_§2	2.2200 (0.0017)	92.16 (0.07)	141.46 (0.07)	114.43 (0.05)	50.68 (0.06)	96.67 (0.05)	148.33 (0.06)	123.82 (0.09)	
B01_§1	2.2200 (0.0017)	114.43 (0.05)	92.16 (0.07)	141.46 (0.07)	96.67 (0.05)	148.33 (0.06)	50.68 (0.06)	51.79 (0.09)	
B01	2.2200 (0.0017)	141.47 (0.07)	114.43 (0.05)	92.16 (0.07)	148.33 (0.06)	50.68 (0.06)	96.67 (0.05)	52.91 (0.09)	
	A11 -	B05_§12	B05_§8	B05_§7	B03_§2	B03	B03_§1	B01_§4	
Cu1 - Distance Angles									
B16_§24	1.3365 (0.0011)								
B16	1.3365 (0.0011)	90.35 (0.34)							
B11	2.2248 (0.0025)	91.93 (0.08)	91.94 (0.08)						
B13_§8	2.2351 (0.0037)	51.16 (0.11)	51.15 (0.11)	119.90 (0.12)					
B07	2.3481 (0.0017)	63.99 (0.08)	125.54 (0.16)	46.23 (0.04)	113.83 (0.08)				
B07_§4	2.3481 (0.0017)	125.54 (0.16)	63.99 (0.08)	46.23 (0.04)	113.82 (0.08)	91.93 (0.08)			
B02	2.3789 (0.0017)	71.17 (0.17)	161.22 (0.19)	85.50 (0.05)	114.83 (0.05)	43.32 (0.06)	124.00 (0.07)		
B02_§4	2.3789 (0.0017)	161.21 (0.19)	71.17 (0.17)	85.50 (0.05)	114.83 (0.05)	123.99 (0.07)	43.32 (0.06)	126.99 (0.09)	
B13	2.3856 (0.0017)	45.84 (0.13)	82.20 (0.19)	47.59 (0.09)	78.21 (0.16)	44.90 (0.10)	81.96 (0.09)	82.37 (0.10)	
B13_§15	2.3856 (0.0017)	82.19 (0.19)	45.84 (0.13)	47.59 (0.09)	78.21 (0.16)	81.96 (0.09)	44.90 (0.10)	125.09 (0.10)	
B01_§4	2.3961 (0.0020)	150.08 (0.16)	106.33 (0.19)	111.64 (0.07)	122.55 (0.10)	119.67 (0.07)	84.35 (0.06)	91.86 (0.06)	
B01	2.3962 (0.0020)	106.34 (0.19)	150.08 (0.16)	111.64 (0.07)	122.56 (0.10)	84.35 (0.06)	119.67 (0.07)	45.06 (0.06)	
	Cu1 -	B16_§24	B16	B11	B13_§8	B07	B07_§4	B02	

A.4 Ausgewählte Bindungswinkel und -längen in $\text{Si}_{3.28}\text{B}_{311.15}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 - Distance Angles									
B01_§6	1.8631 (0.0062)								
B02_§9	1.8751 (0.0041)	129.48 (0.13)							
B04_§2	1.8755 (0.0047)	130.00 (0.15)	59.67 (0.16)						
B02_§13	1.8803 (0.0042)	120.11 (0.13)	58.72 (0.18)	105.60 (0.22)					
B03	1.8835 (0.0045)	118.33 (0.15)	102.26 (0.21)	102.30 (0.20)	57.30 (0.16)				
B01_§8	1.9677 (0.0059)	120.00 (0.00)	106.05 (0.13)	58.36 (0.11)	106.01 (0.13)	58.51 (0.11)			
Si2	2.0839 (0.0432)	63.45 (0.60)	117.52 (1.10)	165.78 (0.72)	64.58 (0.81)	63.98 (0.85)	112.85 (1.16)		
Si1	2.1823 (0.0033)	64.73 (0.08)	165.23 (0.19)	116.34 (0.17)	112.70 (0.17)	63.83 (0.16)	63.20 (0.08)	62.39 (1.20)	
	B01 -	B01_§6	B02_§9	B04_§2	B02_§13	B03	B01_§8	Si2	
B02 - Distance Angles									
B07_§14	1.7235 (0.0041)								
B03_§2	1.8048 (0.0039)	116.81 (0.23)							
B02_§12	1.8413 (0.0057)	127.51 (0.14)	106.76 (0.19)						
B04_§10	1.8660 (0.0039)	119.10 (0.22)	58.93 (0.19)	107.60 (0.19)					
B01_§1	1.8751 (0.0041)	124.81 (0.22)	107.59 (0.20)	60.78 (0.18)	60.18 (0.18)				
B01_§7	1.8804 (0.0042)	117.58 (0.21)	61.43 (0.18)	60.50 (0.17)	110.36 (0.20)	111.51 (0.20)			
Si2_§32	2.1246 (0.0218)	63.63 (1.26)	64.30 (1.12)	117.10 (1.27)	114.91 (1.11)	171.26 (1.19)	62.35 (1.30)		
	B02 -	B07_§14	B03_§2	B02_§12	B04_§10	B01_§1	B01_§7		
B03 - Distance Angles									
B05_§20	1.7353 (0.0060)								

A.4 Ausgewählte Bindungswinkel und -längen in $Si_{3.28}B_{311.15}$

B02_\$13	1.8047 (0.0039)	118.80 (0.17)						
B02_\$2	1.8048 (0.0039)	118.79 (0.17)	112.71 (0.28)					
B04_\$9	1.8063 (0.0060)	117.62 (0.31)	62.23 (0.15)	62.23 (0.15)				
B01_\$8	1.8835 (0.0044)	119.45 (0.24)	112.88 (0.25)	61.26 (0.15)	112.92 (0.24)			
B01	1.8835 (0.0045)	119.45 (0.24)	61.26 (0.15)	112.88 (0.25)	112.92 (0.24)	62.98 (0.23)		
Si2_\$4	2.1086 (0.0228)	65.22 (1.25)	175.50 (1.32)	65.23 (1.10)	118.43 (1.07)	62.63 (1.30)	115.39 (1.23)	
Si2	2.1086 (0.0228)	65.22 (1.25)	65.23 (1.10)	175.50 (1.32)	118.43 (1.08)	115.39 (1.23)	62.63 (1.30)	116.52 (2.18)
Si1	2.1644 (0.0041)	65.15 (0.21)	116.80 (0.16)	116.80 (0.16)	177.23 (0.30)	64.81 (0.17)	64.81 (0.17)	62.31 (1.08)
	B03 -	B05_\$20	B02_\$13	B02_\$2	B04_\$9	B01_\$8	B01	Si2_\$4
B04 -	Distance	Angles						
B11_\$38	1.7078 (0.0057)							
B03_\$1	1.8063 (0.0060)	118.11 (0.33)						
B02_\$10	1.8659 (0.0039)	119.96 (0.17)	58.85 (0.15)					
B02_\$12	1.8659 (0.0039)	119.96 (0.17)	58.84 (0.15)	107.25 (0.28)				
B01_\$7	1.8755 (0.0047)	124.11 (0.25)	107.51 (0.24)	110.31 (0.23)	60.16 (0.15)			
B01_\$2	1.8755 (0.0047)	124.11 (0.25)	107.51 (0.24)	60.16 (0.15)	110.31 (0.23)	63.28 (0.22)		
	B04 -	B11_\$38	B03_\$1	B02_\$10	B02_\$12	B01_\$7		
B05 -	Distance	Angles						
B03_\$15	1.7354 (0.0060)							
B06_\$22	1.7632 (0.0041)	122.24 (0.19)						
B06_\$26	1.7633 (0.0041)	122.24 (0.19)	107.28 (0.33)					
B06_\$24	1.7662 (0.0053)	122.14 (0.31)	59.81 (0.16)	59.82 (0.16)				
B05_\$4	1.8003 (0.0072)	122.21 (0.16)	107.14 (0.16)	59.30 (0.15)	107.12 (0.16)			
B05_\$3	1.8003 (0.0073)	122.21 (0.16)	59.30 (0.15)	107.15 (0.16)	107.12 (0.17)	60.00 (0.00)		
Si2_\$20	2.0953 (0.0411)	66.02 (0.84)	171.41 (0.69)	67.07 (1.24)	119.16 (1.33)	64.56 (0.54)	115.23 (0.85)	
Si2_\$15	2.0953 (0.0412)	66.02 (0.84)	67.07 (1.24)	171.41 (0.70)	119.15 (1.30)	115.23 (0.86)	64.55 (0.55)	117.70 (2.54)
Si1_\$18	2.1306 (0.0049)	67.19 (0.19)	116.44 (0.17)	116.43 (0.17)	170.67 (0.29)	65.01 (0.10)	65.01 (0.10)	63.10 (1.26)
	B05 -	B03_\$15	B06_\$22	B06_\$26	B06_\$24	B05_\$4	B05_\$3	Si2_\$20
B06 -	Distance	Angles						
B09	1.6347 (0.0057)							
B06_\$25	1.7597 (0.0047)	122.23 (0.05)						
B06_\$27	1.7597 (0.0047)	122.23 (0.05)	107.59 (0.25)					
B05_\$17	1.7632 (0.0041)	119.65 (0.25)	60.17 (0.18)	109.06 (0.21)				
B05_\$19	1.7632 (0.0041)	119.65 (0.25)	109.06 (0.21)	60.17 (0.18)	61.40 (0.30)			
B05_\$21	1.7663 (0.0053)	122.35 (0.30)	60.01 (0.21)	60.01 (0.21)	109.23 (0.28)	109.23 (0.28)		
Si2_\$45	2.1495 (0.0481)	65.95 (1.21)	116.69 (0.57)	116.69 (0.57)	63.86 (1.00)	63.86 (1.00)	171.70 (1.23)	
	B06 -	B09	B06_\$25	B06_\$27	B05_\$17	B05_\$19	B05_\$21	
B07 -	Distance	Angles						
B02_\$14	1.7235 (0.0041)							
B10_\$36	1.7916 (0.0032)	124.05 (0.23)						
B13	1.8001 (0.0058)	122.40 (0.24)	63.26 (0.23)					
B09_\$35	1.8036 (0.0047)	122.15 (0.24)	104.89 (0.23)	105.26 (0.22)				
B08_\$34	1.8380 (0.0038)	119.57 (0.21)	62.08 (0.18)	112.65 (0.26)	57.21 (0.16)			
B07_\$6	1.9074 (0.0060)	122.31 (0.14)	107.00 (0.15)	58.01 (0.14)	58.08 (0.12)	106.29 (0.13)		
Si2_\$2	2.0571 (0.0409)	67.72 (0.88)	168.21 (0.85)	111.15 (0.88)	65.68 (1.27)	114.29 (1.35)	62.38 (0.60)	
	B07 -	B02_\$14	B10_\$36	B13	B09_\$35	B08_\$34	B07_\$6	
B08 -	Distance	Angles						
B08_\$30	1.6924 (0.0056)							
B09	1.7436 (0.0037)	121.31 (0.16)						
B07_\$31	1.8378 (0.0038)	121.78 (0.26)	60.41 (0.19)					
B11	1.8488 (0.0038)	119.01 (0.26)	61.80 (0.19)	110.79 (0.20)				
B12_\$11	1.8525 (0.0042)	123.93 (0.19)	105.53 (0.21)	106.81 (0.21)	57.98 (0.17)			
B10	1.8719 (0.0041)	126.62 (0.20)	104.00 (0.21)	57.75 (0.15)	106.00 (0.23)	59.31 (0.18)		
	B08 -	B08_\$30	B09	B07_\$31	B11	B12_\$11		
B09 -	Distance	Angles						
B06	1.6347 (0.0057)							
B08	1.7436 (0.0036)	116.43 (0.17)						
B08_\$33	1.7436 (0.0036)	116.43 (0.17)	114.85 (0.30)					
B07_\$31	1.8036 (0.0047)	120.32 (0.25)	62.39 (0.15)	115.32 (0.25)				
B07_\$29	1.8036 (0.0047)	120.32 (0.25)	115.32 (0.25)	62.39 (0.15)	63.84 (0.23)			
B11	1.8470 (0.0059)	116.77 (0.30)	61.90 (0.16)	61.90 (0.16)	112.44 (0.24)	112.44 (0.24)		
Si2_\$45	2.1043 (0.0478)	68.87 (1.25)	116.30 (0.45)	116.30 (0.45)	62.97 (1.01)	62.97 (1.01)	174.36 (1.27)	
	B09 -	B06	B08	B08_\$33	B07_\$31	B07_\$29	B11	
B10 -	Distance	Angles						
B14_\$2	1.7380 (0.0043)							

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B07_28	1.7915 (0.0032)	104.68 (0.17)							
B07_31	1.7916 (0.0032)	104.68 (0.17)	139.82 (0.30)						
B12_11	1.8427 (0.0055)	59.00 (0.29)	109.22 (0.15)	109.22 (0.15)					
B08	1.8719 (0.0041)	103.51 (0.25)	135.72 (0.25)	60.17 (0.13)	59.82 (0.17)				
B08_36	1.8720 (0.0041)	103.51 (0.25)	60.17 (0.13)	135.72 (0.25)	59.82 (0.17)	80.48 (0.23)			
B13_28	1.8834 (0.0050)	61.01 (0.28)	58.60 (0.22)	115.94 (0.27)	111.06 (0.25)	163.56 (0.29)	107.45 (0.20)		
B13_29	1.8834 (0.0050)	61.01 (0.28)	115.94 (0.27)	58.59 (0.22)	111.05 (0.25)	107.45 (0.20)	163.56 (0.29)	61.36 (0.38)	
	B10 -	B14_2	B07_28	B07_31	B12_11	B08	B08_36	B13_28	
B11 - Distance Angles									
B04_16	1.7077 (0.0057)								
B12_11	1.7939 (0.0037)	124.01 (0.25)							
B12_43	1.7940 (0.0037)	124.01 (0.25)	62.56 (0.30)						
B09	1.8470 (0.0059)	123.01 (0.31)	103.72 (0.24)	103.72 (0.24)					
B08_33	1.8487 (0.0038)	120.57 (0.17)	110.01 (0.25)	61.11 (0.17)	56.30 (0.15)				
B08	1.8488 (0.0038)	120.57 (0.17)	61.11 (0.17)	110.01 (0.25)	56.30 (0.15)	105.26 (0.27)			
	B11 -	B04_16	B12_11	B12_43	B09	B08_33			
B12 - Distance Angles									
B14_44	1.7655 (0.0072)								
B11_37	1.7939 (0.0038)	103.41 (0.16)							
B11_32	1.7939 (0.0038)	103.41 (0.16)	140.16 (0.34)						
B10_32	1.8427 (0.0055)	57.55 (0.23)	109.58 (0.17)	109.58 (0.17)					
B08_32	1.8526 (0.0042)	103.21 (0.21)	137.81 (0.25)	60.90 (0.15)	60.87 (0.17)				
B08_7	1.8526 (0.0042)	103.21 (0.21)	60.90 (0.15)	137.81 (0.25)	60.87 (0.17)	81.49 (0.24)			
B12_40	1.8629 (0.0071)	58.16 (0.16)	114.89 (0.15)	58.72 (0.15)	107.24 (0.15)	106.88 (0.13)	160.56 (0.14)		
B12_42	1.8629 (0.0071)	58.16 (0.16)	58.72 (0.15)	114.89 (0.15)	107.24 (0.15)	160.56 (0.14)	106.88 (0.13)	60.00 (0.00)	
	B12 -	B14_44	B11_37	B11_32	B10_32	B08_32	B08_7	B12_40	
B13 - Distance Angles									
B15	1.6962 (0.0056)								
B07_36	1.8001 (0.0058)	140.71 (0.22)							
B07	1.8001 (0.0058)	140.71 (0.22)	63.98 (0.27)						
B14_18	1.8425 (0.0085)	102.10 (0.33)	100.19 (0.28)	100.19 (0.28)					
B10_35	1.8834 (0.0050)	111.62 (0.23)	58.15 (0.16)	107.67 (0.29)	55.60 (0.20)				
B10_36	1.8835 (0.0050)	111.62 (0.23)	107.67 (0.29)	58.15 (0.16)	55.60 (0.20)	103.35 (0.36)			
B13_4	1.9221 (0.0104)	55.49 (0.16)	113.63 (0.16)	158.53 (0.20)	58.56 (0.18)	59.32 (0.19)	105.92 (0.20)		
B13_3	1.9221 (0.0105)	55.49 (0.16)	158.53 (0.20)	113.63 (0.16)	58.56 (0.18)	105.92 (0.20)	59.32 (0.19)	60.00 (0.00)	
	B13 -	B15	B07_36	B07	B14_18	B10_35	B10_36	B13_4	
B14 - Distance Angles									
B10_2	1.7380 (0.0043)								
B10_11	1.7380 (0.0043)	116.46 (0.17)							
B10_27	1.7381 (0.0042)	116.45 (0.17)	116.45 (0.17)						
B12_41	1.7655 (0.0072)	116.76 (0.26)	63.46 (0.20)	116.76 (0.26)					
B12_39	1.7655 (0.0072)	116.76 (0.26)	116.76 (0.26)	63.46 (0.20)	63.69 (0.32)				
B12_16	1.7655 (0.0072)	63.46 (0.20)	116.76 (0.26)	116.76 (0.26)	63.69 (0.32)	63.69 (0.32)			
B13_20	1.8425 (0.0085)	63.39 (0.19)	116.04 (0.43)	63.40 (0.19)	179.50 (0.36)	116.72 (0.18)	116.72 (0.18)		
B13_15	1.8425 (0.0085)	63.40 (0.19)	63.40 (0.19)	116.05 (0.43)	116.72 (0.18)	179.50 (0.37)	116.72 (0.18)	62.88 (0.37)	
B13_18	1.8425 (0.0085)	116.04 (0.43)	63.39 (0.19)	63.40 (0.19)	116.72 (0.18)	116.72 (0.18)	179.50 (0.37)	62.88 (0.37)	
	B14 -	B10_2	B10_11	B10_27	B12_41	B12_39	B12_16	B13_20	
B15 - Distance Angles									
B13	1.6962 (0.0056)								
B13_4	1.6962 (0.0056)	69.03 (0.32)							
B13_3	1.6962 (0.0056)	69.03 (0.32)	69.03 (0.32)						
B13_18	1.6962 (0.0056)	180.00 (0.00)	110.97 (0.32)	110.97 (0.32)					
B13_15	1.6962 (0.0056)	110.98 (0.32)	180.00 (0.00)	110.97 (0.32)	69.02 (0.32)				
B13_20	1.6962 (0.0056)	110.97 (0.32)	110.97 (0.32)	180.00 (0.24)	69.02 (0.32)	69.02 (0.32)			
	B15 -	B13	B13_4	B13_3	B13_18	B13_15			
S11 - Distance Angles									
B05_15	2.1305 (0.0049)								
B05_18	2.1306 (0.0049)	49.98 (0.20)							
B05_20	2.1306 (0.0049)	49.99 (0.20)	49.98 (0.20)						
B03_4	2.1644 (0.0041)	92.23 (0.16)	47.65 (0.17)	92.23 (0.16)					
B03_3	2.1644 (0.0041)	47.65 (0.17)	92.24 (0.16)	92.24 (0.16)	114.99 (0.11)				
B03	2.1644 (0.0041)	92.23 (0.16)	92.23 (0.16)	47.65 (0.17)	114.99 (0.11)	114.99 (0.11)			
B01_36	2.1822 (0.0033)	92.91 (0.13)	142.41 (0.15)	114.29 (0.10)	148.86 (0.13)	51.35 (0.12)	95.48 (0.10)		
B01_8	2.1822 (0.0033)	142.40 (0.15)	114.29 (0.10)	92.90 (0.13)	95.48 (0.10)	148.86 (0.13)	51.35 (0.12)	98.97 (0.14)	
B01_5	2.1822 (0.0033)	114.29 (0.10)	92.90 (0.13)	142.40 (0.15)	51.35 (0.12)	95.48 (0.10)	148.86 (0.13)	98.97 (0.14)	
B01_4	2.1822 (0.0033)	142.40 (0.15)	92.90 (0.13)	114.29 (0.10)	51.35 (0.12)	148.86 (0.13)	95.48 (0.10)	122.73 (0.22)	

A.5 Ausgewählte Bindungswinkel und -längen in $Ni_{3.38}B_{316.11}$

B01_\$3	2.1822 (0.0033)	92.91 (0.13)	114.29 (0.10)	142.40 (0.15)	95.48 (0.10)	51.35 (0.12)	148.86 (0.13)	53.59 (0.16)
B01	2.1823 (0.0033)	114.29 (0.10)	142.40 (0.15)	92.90 (0.13)	148.86 (0.13)	95.48 (0.10)	51.35 (0.12)	50.54 (0.17)
	Si1 -	B05_\$15	B05_\$18	B05_\$20	B03_\$4	B03_\$3	B03	B01_\$6
Si2 -	Distance	Angles						
B07_\$30	2.0571 (0.0400)							
B07_\$2	2.0571 (0.0401)	55.24 (1.17)						
B01_\$6	2.0839 (0.0432)	96.24 (1.39)	121.55 (2.22)					
B01	2.0839 (0.0432)	121.54 (2.22)	96.24 (1.39)	53.11 (1.20)				
B05_\$15	2.0953 (0.0409)	110.81 (1.36)	138.89 (2.49)	96.84 (1.41)	120.21 (2.16)			
B05_\$20	2.0953 (0.0409)	138.90 (2.49)	110.80 (1.36)	120.21 (2.17)	96.84 (1.41)	50.89 (1.09)		
B09_\$23	2.1043 (0.0478)	51.35 (1.08)	51.35 (1.08)	146.43 (1.48)	146.44 (1.49)	88.80 (1.75)	88.80 (1.75)	
B03_\$3	2.1086 (0.0227)	92.35 (0.49)	147.52 (1.64)	53.39 (0.80)	100.23 (1.89)	48.76 (0.72)	94.85 (1.70)	112.27 (1.38)
B03	2.1086 (0.0228)	147.52 (1.64)	92.35 (0.49)	100.23 (1.89)	53.39 (0.80)	94.85 (1.70)	48.76 (0.72)	112.28 (1.38)
B02_\$11	2.1246 (0.0217)	48.65 (0.67)	99.06 (1.75)	53.06 (0.78)	100.84 (1.90)	92.45 (0.57)	143.23 (1.62)	93.78 (1.39)
B02_\$13	2.1247 (0.0217)	99.06 (1.75)	48.65 (0.67)	100.84 (1.90)	53.06 (0.78)	143.22 (1.62)	92.45 (0.57)	93.78 (1.39)
B06_\$23	2.1495 (0.0481)	90.32 (1.75)	90.32 (1.75)	144.89 (1.56)	144.90 (1.55)	49.07 (1.03)	49.07 (1.03)	45.19 (1.01)
	Si2 -	B07_\$30	B07_\$2	B01_\$6	B01	B05_\$15	B05_\$20	B09_\$23

A.5 Ausgewählte Bindungswinkel und -längen in $Ni_{3.38}B_{316.11}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 -	Distance	Angles						
B16_\$24	1.8221 (0.0216)							
B03_\$24	1.8355 (0.0052)	59.19 (0.44)						
B04_\$27	1.8410 (0.0054)	146.32 (0.82)	103.56 (0.24)					
B02_\$15	1.8576 (0.0049)	146.96 (0.80)	103.29 (0.25)	60.06 (0.19)				
B02_\$16	1.8579 (0.0048)	89.18 (0.73)	58.12 (0.19)	106.27 (0.26)	58.60 (0.21)			
B01_\$7	1.9031 (0.0071)	58.52 (0.42)	117.70 (0.18)	129.27 (0.18)	128.91 (0.15)	119.80 (0.15)		
B01_\$10	1.9081 (0.0070)	88.39 (0.74)	58.68 (0.13)	58.79 (0.13)	106.57 (0.16)	106.57 (0.15)	120.00 (0.00)	
Ni1_\$1	2.1383 (0.0043)	32.20 (0.85)	65.05 (0.21)	115.89 (0.22)	167.22 (0.24)	114.82 (0.23)	63.58 (0.10)	63.50 (0.10)
	B01 -	B16_\$24	B03_\$24	B04_\$27	B02_\$15	B02_\$16	B01_\$7	B01_\$10
B02 -	Distance	Angles						
B07_\$19	1.7279 (0.0049)							
B03_\$13	1.7942 (0.0045)	116.51 (0.26)						
B02_\$17	1.8181 (0.0065)	127.57 (0.16)	106.59 (0.21)					
B04_\$12	1.8509 (0.0045)	118.99 (0.25)	60.09 (0.23)	107.51 (0.23)				
B01_\$4	1.8576 (0.0049)	125.39 (0.25)	107.64 (0.24)	60.71 (0.21)	59.53 (0.21)			
B01_\$8	1.8578 (0.0048)	117.90 (0.25)	60.31 (0.21)	60.70 (0.20)	110.14 (0.24)	111.00 (0.23)		
B17_\$43	2.0078 (0.0173)	54.30 (1.33)	107.74 (1.32)	85.86 (1.31)	163.68 (1.31)	136.78 (1.28)	67.74 (1.33)	
Ni2_\$43	2.4995 (0.0061)	59.32 (0.22)	125.59 (0.27)	71.96 (0.18)	174.31 (0.28)	116.38 (0.23)	74.72 (0.23)	20.58 (1.29)
	B02 -	B07_\$19	B03_\$13	B02_\$17	B04_\$12	B01_\$4	B01_\$8	B17_\$43
B03 -	Distance	Angles						
B05_\$31	1.7263 (0.0069)							
B02_\$18	1.7941 (0.0045)	118.82 (0.19)						
B02_\$13	1.7942 (0.0045)	118.82 (0.19)	111.59 (0.34)					
B16_\$22	1.8063 (0.0044)	60.52 (0.82)	148.95 (0.89)	91.71 (0.87)				
B16	1.8063 (0.0044)	60.53 (0.82)	91.71 (0.86)	148.95 (0.89)	60.00 (1.72)			
B04_\$25	1.8256 (0.0071)	117.14 (0.34)	61.50 (0.18)	61.50 (0.18)	149.16 (0.86)	149.17 (0.86)		
B01_\$3	1.8355 (0.0052)	120.53 (0.29)	61.56 (0.18)	112.56 (0.28)	91.16 (0.86)	60.03 (0.81)	112.31 (0.28)	
B01_\$6	1.8355 (0.0052)	120.53 (0.29)	112.55 (0.28)	61.56 (0.18)	60.04 (0.81)	91.16 (0.86)	112.31 (0.28)	62.64 (0.26)
Ni1	2.1519 (0.0050)	67.01 (0.28)	117.03 (0.20)	117.03 (0.20)	31.98 (0.86)	31.98 (0.86)	175.86 (0.35)	64.29 (0.22)
	B03 -	B05_\$31	B02_\$18	B02_\$13	B16_\$22	B16	B04_\$25	B01_\$3
B04 -	Distance	Angles						
B11_\$48	1.6997 (0.0066)							
B03_\$20	1.8256 (0.0071)	117.46 (0.35)						
B01_\$8	1.8409 (0.0054)	125.31 (0.29)	107.02 (0.27)					
B01_\$2	1.8410 (0.0054)	125.31 (0.29)	107.02 (0.27)	62.43 (0.26)				
B02_\$17	1.8509 (0.0045)	119.82 (0.20)	58.41 (0.18)	60.42 (0.18)	109.71 (0.27)			
B02_\$12	1.8510 (0.0045)	119.82 (0.20)	58.41 (0.18)	109.71 (0.27)	60.42 (0.18)	106.57 (0.32)		
	B04 -	B11_\$48	B03_\$20	B01_\$8	B01_\$2	B02_\$17		
B05 -	Distance	Angles						

B03_23	1.7263	(0.0069)							
B06_34	1.7558	(0.0066)	122.44	(0.37)					
B06_33	1.7645	(0.0050)	122.42	(0.23)	59.72	(0.18)			
B06_36	1.7645	(0.0050)	122.42	(0.23)	59.72	(0.19)	107.06	(0.40)	
B16_23	1.7817	(0.0221)	61.96	(0.45)	149.54	(0.83)	91.71	(0.75)	147.69 (0.88)
B16_31	1.7817	(0.0219)	61.96	(0.45)	149.54	(0.83)	147.69	(0.90)	91.71 (0.73)
B05_21	1.7918	(0.0087)	121.76	(0.19)	107.34	(0.20)	59.49	(0.18)	107.24 (0.20)
B05_22	1.7918	(0.0086)	121.76	(0.18)	107.34	(0.20)	107.25	(0.20)	59.49 (0.18)
Ni1_29	2.1699	(0.0070)	65.91	(0.23)	171.65	(0.35)	116.95	(0.20)	116.95 (0.20)
	B05 -		B03_23		B06_34		B06_33		B06_36
							B16_23		B16_31
									B05_21
B06 -	Distance	Angles							
B09	1.6220	(0.0071)							
B06_35	1.7526	(0.0059)	122.26	(0.06)					
B06_37	1.7526	(0.0059)	122.26	(0.06)	108.12	(0.31)			
B05_32	1.7558	(0.0066)	122.76	(0.37)	60.39	(0.26)	60.39	(0.26)	
B05_30	1.7646	(0.0050)	119.52	(0.31)	108.69	(0.25)	59.89	(0.22)	109.13 (0.33)
B05_28	1.7646	(0.0050)	119.52	(0.31)	59.89	(0.22)	108.69	(0.25)	109.13 (0.33)
	B06 -		B09		B06_35		B06_37		B05_32
									B05_30
B07 -	Distance	Angles							
B17_13	1.7228	(0.0385)							
B02_19	1.7279	(0.0049)	71.17	(1.03)					
B10_49	1.7865	(0.0038)	127.35	(1.60)	124.01	(0.27)			
B09_46	1.7949	(0.0052)	104.04	(1.17)	122.31	(0.28)	104.70	(0.27)	
B13	1.7969	(0.0076)	68.58	(1.50)	124.12	(0.30)	62.16	(0.28)	104.04 (0.26)
B08_45	1.8248	(0.0046)	161.04	(1.06)	119.79	(0.25)	61.67	(0.21)	57.25 (0.19)
B07_41	1.9030	(0.0069)	56.47	(0.85)	122.30	(0.16)	107.15	(0.19)	57.99 (0.13)
Ni2_13	2.1968	(0.0066)	24.06	(1.60)	78.11	(0.23)	103.99	(0.31)	120.68 (0.21)
Ni2_49	2.5274	(0.0061)	74.90	(1.36)	72.44	(0.23)	66.02	(0.20)	164.46 (0.29)
	B07 -		B17_13		B02_19		B10_49		B09_46
							B13		B08_45
									B07_41
B08 -	Distance	Angles							
B08_40	1.6893	(0.0069)							
B09	1.7344	(0.0045)	121.19	(0.19)					
B07_42	1.8248	(0.0046)	121.55	(0.30)	60.51	(0.21)			
B11	1.8406	(0.0044)	118.89	(0.30)	61.75	(0.22)	111.00	(0.24)	
B12_14	1.8486	(0.0053)	123.67	(0.23)	105.63	(0.25)	107.44	(0.25)	57.87 (0.21)
B10	1.8515	(0.0049)	126.30	(0.24)	104.47	(0.25)	58.15	(0.18)	106.34 (0.27)
	B08 -		B08_40		B09		B07_42		B11
									B12_14
B09 -	Distance	Angles							
B06	1.6220	(0.0071)							
B08_7	1.7344	(0.0045)	116.49	(0.21)					
B08	1.7344	(0.0045)	116.49	(0.21)	114.77	(0.36)			
B07_39	1.7950	(0.0052)	120.34	(0.29)	62.24	(0.18)	115.29	(0.30)	
B07_42	1.7950	(0.0052)	120.34	(0.29)	115.29	(0.30)	62.24	(0.18)	64.02 (0.26)
B11	1.8368	(0.0066)	116.54	(0.34)	61.97	(0.19)	61.97	(0.19)	112.56 (0.28)
	B09 -		B06		B08_7		B08		B07_39
									B07_42
B11 -	Distance	Angles							
B04_26	1.6997	(0.0066)							
B12_14	1.7849	(0.0044)	123.22	(0.29)					
B12_54	1.7849	(0.0044)	123.22	(0.29)	62.43	(0.36)			
B09	1.8368	(0.0066)	123.65	(0.36)	104.07	(0.27)	104.07	(0.27)	
B08_7	1.8405	(0.0044)	120.97	(0.20)	110.02	(0.29)	61.29	(0.21)	56.28 (0.17)
B08	1.8406	(0.0044)	120.97	(0.20)	61.29	(0.21)	110.02	(0.29)	56.28 (0.17)
	B11 -		B04_26		B12_14		B12_54		B09
									B08_7
B10 -	Distance	Angles							
B14_13	1.7354	(0.0050)							
B07_38	1.7865	(0.0038)	104.40	(0.20)					
B07_42	1.7866	(0.0038)	104.40	(0.21)	139.68	(0.35)			
B18	1.7892	(0.0622)	96.51	(2.10)	74.62	(0.49)	74.62	(0.50)	
B12_14	1.8416	(0.0066)	59.32	(0.36)	109.40	(0.18)	109.40	(0.18)	155.82 (2.09)
B13_38	1.8499	(0.0060)	59.05	(0.33)	59.20	(0.28)	115.93	(0.34)	50.95 (1.57)
B13_39	1.8500	(0.0060)	59.05	(0.33)	115.93	(0.34)	59.19	(0.28)	50.95 (1.59)
B08	1.8515	(0.0049)	103.79	(0.31)	136.32	(0.30)	60.18	(0.16)	133.62 (0.92)
B08_41	1.8515	(0.0049)	103.79	(0.31)	60.18	(0.16)	136.32	(0.30)	133.62 (0.91)
Ni2	2.4308	(0.0080)	111.19	(0.41)	71.80	(0.18)	71.80	(0.18)	14.68 (2.07)
	B10 -		B14_13		B07_38		B07_42		B18
									B12_14
									B13_38
									B13_39

A.5 Ausgewählte Bindungswinkel und -längen in $Ni_{3.38}B_{316.11}$

B12 -	Distance	Angles							
B14_\$55	1.7723 (0.0086)								
B11_\$43	1.7850 (0.0044)	103.32 (0.19)							
B11_\$47	1.7850 (0.0044)	103.32 (0.19)	140.96 (0.39)						
B10_\$43	1.8416 (0.0066)	57.36 (0.27)	109.15 (0.20)	109.15 (0.20)					
B08_\$43	1.8486 (0.0053)	102.45 (0.25)	60.84 (0.17)	137.74 (0.30)	60.23 (0.20)				
B08_\$44	1.8486 (0.0053)	102.45 (0.25)	137.74 (0.31)	60.84 (0.17)	60.23 (0.20)	81.25 (0.30)			
B12_\$51	1.8501 (0.0088)	58.53 (0.19)	58.79 (0.18)	115.11 (0.18)	107.48 (0.18)	106.85 (0.16)	160.21 (0.17)		
B12_\$53	1.8501 (0.0088)	58.53 (0.19)	115.11 (0.19)	58.79 (0.18)	107.48 (0.18)	160.21 (0.17)	106.85 (0.16)	60.00 (0.00)	
	B12 -	B14_\$55	B11_\$43	B11_\$47	B10_\$43	B08_\$43	B08_\$44	B12_\$51	

B13 -	Distance	Angles								
B18_\$49	1.5663 (0.0542)									
B18_\$46	1.5663 (0.0540)	122.53 (4.32)								
B15	1.7145 (0.0073)	62.57 (2.06)	62.57 (2.07)							
Ni2_\$13	1.7411 (0.0105)	76.46 (1.69)	76.45 (1.69)	77.48 (0.37)						
B14_\$29	1.7697 (0.0102)	103.90 (1.72)	103.90 (1.72)	103.33 (0.43)	179.18 (0.61)					
B07_\$41	1.7969 (0.0076)	138.90 (1.62)	79.92 (1.89)	138.38 (0.30)	76.74 (0.37)	102.57 (0.36)				
B07	1.7969 (0.0076)	79.92 (1.87)	138.90 (1.63)	138.38 (0.30)	76.75 (0.36)	102.57 (0.36)	63.95 (0.34)			
B10_\$46	1.8500 (0.0060)	160.02 (1.60)	62.52 (2.11)	112.33 (0.30)	122.50 (0.28)	57.24 (0.24)	58.64 (0.20)	109.02 (0.38)		
B10_\$49	1.8500 (0.0060)	62.52 (2.11)	160.02 (1.59)	112.33 (0.30)	122.50 (0.28)	57.25 (0.24)	109.02 (0.38)	58.64 (0.20)		
B13_\$21	1.8709 (0.0135)	53.33 (1.51)	106.24 (1.68)	56.93 (0.20)	122.57 (0.28)	58.09 (0.24)	160.43 (0.24)	114.38 (0.19)		
B13_\$22	1.8709 (0.0134)	106.24 (1.67)	53.33 (1.52)	56.93 (0.20)	122.57 (0.27)	58.09 (0.24)	114.38 (0.19)	160.43 (0.24)		
B17_\$13	1.9838 (0.0479)	89.57 (1.67)	89.57 (1.67)	105.74 (1.38)	28.26 (1.38)	150.93 (1.43)	53.94 (1.05)	53.94 (1.05)		
	B13 -	B18_\$49	B18_\$46	B15	Ni2_\$13	B14_\$29	B07_\$41	B07		

B14 -	Distance	Angles								
B10_\$13	1.7354 (0.0051)									
B10_\$14	1.7354 (0.0051)	116.82 (0.19)								
B10_\$37	1.7354 (0.0050)	116.82 (0.19)	116.82 (0.19)							
B13_\$31	1.7696 (0.0102)	63.70 (0.23)	117.23 (0.54)	63.70 (0.23)						
B13_\$23	1.7696 (0.0102)	63.70 (0.23)	63.70 (0.23)	117.23 (0.54)	63.82 (0.48)					
B13_\$29	1.7696 (0.0102)	117.23 (0.54)	63.70 (0.23)	63.70 (0.23)	63.82 (0.48)	63.82 (0.48)				
B12_\$52	1.7723 (0.0086)	116.13 (0.31)	63.33 (0.25)	116.12 (0.31)	179.45 (0.46)	116.63 (0.24)	116.63 (0.24)			
B12_\$50	1.7723 (0.0086)	116.12 (0.31)	116.12 (0.31)	63.33 (0.25)	116.63 (0.24)	179.45 (0.45)	116.63 (0.24)	62.93 (0.38)		
B12_\$26	1.7723 (0.0086)	63.33 (0.25)	116.12 (0.31)	116.12 (0.31)	116.63 (0.24)	116.63 (0.24)	179.45 (0.45)	62.93 (0.38)		
	B14 -	B10_\$13	B10_\$14	B10_\$37	B13_\$31	B13_\$23	B13_\$29	B12_\$52		

B15 -	Distance	Angles								
B18_\$46	1.7084 (0.0609)									
B18_\$57	1.7084 (0.0604)	107.01 (2.38)								
B18_\$49	1.7084 (0.0602)	107.01 (2.39)	107.01 (2.39)							
B18_\$14	1.7084 (0.0608)	180.00 (0.01)	72.99 (2.38)	72.99 (2.39)						
B18_\$13	1.7084 (0.0609)	72.99 (2.39)	180.00 (0.01)	72.99 (2.39)	107.01 (2.38)					
B18_\$37	1.7084 (0.0602)	72.99 (2.39)	72.99 (2.39)	180.00 (1.42)	107.01 (2.39)	107.01 (2.39)				
B13	1.7145 (0.0074)	54.47 (1.63)	107.22 (2.22)	54.47 (1.63)	125.53 (1.64)	72.78 (2.22)	125.53 (1.64)			
B13_\$22	1.7145 (0.0073)	54.47 (1.64)	54.47 (1.63)	107.22 (2.22)	125.53 (1.63)	125.53 (1.64)	72.78 (2.22)	66.13 (0.40)		
B13_\$21	1.7145 (0.0073)	107.22 (2.23)	54.47 (1.63)	54.47 (1.64)	72.78 (2.22)	125.53 (1.63)	125.53 (1.63)	66.13 (0.40)		
B13_\$29	1.7145 (0.0073)	125.53 (1.63)	72.78 (2.22)	125.53 (1.63)	54.47 (1.64)	107.22 (2.22)	54.47 (1.64)	180.00 (0.00)		
B13_\$23	1.7145 (0.0073)	125.53 (1.64)	125.53 (1.63)	72.78 (2.22)	54.47 (1.63)	54.47 (1.63)	107.22 (2.22)	113.87 (0.40)		
B13_\$31	1.7145 (0.0074)	72.78 (2.23)	125.53 (1.63)	125.53 (1.64)	107.22 (2.22)	54.47 (1.63)	54.47 (1.63)	113.87 (0.40)		
	B15 -	B18_\$46	B18_\$57	B18_\$49	B18_\$14	B18_\$13	B18_\$37	B13		

B16 -	Distance	Angles								
Ni1	1.1397 (0.0268)									
B05_\$31	1.7817 (0.0219)	93.32 (1.46)								
B05_\$23	1.7817 (0.0219)	93.32 (1.46)	60.38 (0.85)							
B16_\$22	1.8062 (0.0467)	37.59 (0.73)	59.54 (0.82)	89.77 (0.76)						
B16_\$21	1.8062 (0.0468)	37.59 (0.73)	89.77 (0.76)	59.54 (0.82)	60.00 (0.00)					
B03_\$21	1.8063 (0.0044)	90.96 (0.86)	117.88 (1.21)	57.51 (0.45)	119.94 (0.86)	60.00 (0.86)				
B03	1.8063 (0.0044)	90.96 (0.86)	57.51 (0.45)	117.88 (1.21)	60.00 (0.86)	119.94 (0.86)	175.12 (1.60)			
B01_\$11	1.8220 (0.0215)	89.36 (1.33)	177.05 (1.53)	118.26 (0.20)	123.38 (0.81)	91.60 (0.73)	60.78 (0.43)	123.74 (1.21)		
B01_\$3	1.8220 (0.0215)	89.36 (1.33)	118.26 (0.20)	177.05 (1.60)	91.60 (0.73)	123.39 (0.80)	123.74 (1.21)	60.78 (0.43)		
	B16 -	Ni1	B05_\$31	B05_\$23	B16_\$22	B16_\$21	B03_\$21	B03		

B17 -	Distance	Angles								
Ni2	0.9393 (0.0483)									
B07_\$40	1.7227 (0.0384)	107.55 (3.11)								
B07_\$13	1.7228 (0.0384)	107.55 (3.12)	67.05 (1.70)							
B18	1.7687 (0.0863)	3.87 (2.34)	110.69 (2.73)	110.69 (2.75)						
B13_\$13	1.9838 (0.0474)	61.36 (2.56)	57.48 (1.36)	57.48 (1.36)	65.23 (2.50)					
B02_\$14	2.0078 (0.0171)	110.72 (1.28)	54.54 (0.63)	116.83 (2.23)	110.44 (1.28)	102.55 (1.37)				

B02_18	2.0078 (0.0172)	110.72 (1.28)	116.82 (2.23)	54.54 (0.63)	110.44 (1.28)	102.54 (1.38)	138.06 (2.54)		
	B17 -	Ni2	B07_40	B07_13	B18	B13_13	B02_14		
B18 - Distance Angles									
Ni2	0.8340 (0.0666)								
B13_38	1.5663 (0.0539)	141.51 (2.22)							
B13_39	1.5664 (0.0540)	141.51 (2.22)	73.34 (2.98)						
B15_56	1.7083 (0.0603)	111.90 (5.16)	62.96 (2.23)	62.96 (2.22)					
B17	1.7687 (0.0862)	4.36 (2.65)	142.54 (1.68)	142.54 (1.68)	116.26 (3.68)				
B10	1.7892 (0.0622)	132.39 (5.58)	66.53 (2.36)	66.53 (2.36)	115.71 (3.73)	128.04 (3.82)			
B13_13	2.0306 (0.0608)	58.15 (3.54)	105.32 (2.74)	105.32 (2.74)	53.75 (1.68)	62.51 (2.47)	169.46 (3.88)		
B18_59	2.0319 (0.0866)	79.51 (4.38)	114.89 (2.00)	67.27 (1.64)	53.51 (1.19)	82.69 (3.32)	130.55 (3.71)	45.36 (2.61)	
B18_58	2.0320 (0.0865)	79.51 (4.38)	67.27 (1.64)	114.90 (1.99)	53.51 (1.19)	82.69 (3.32)	130.55 (3.69)	45.36 (2.62)	
Ni2_59	2.0511 (0.0247)	86.27 (2.43)	121.71 (3.37)	55.61 (0.83)	69.55 (1.59)	88.03 (2.10)	109.96 (1.86)	67.88 (1.59)	
Ni2_58	2.0512 (0.0247)	86.27 (2.43)	55.61 (0.83)	121.71 (3.36)	69.55 (1.59)	88.03 (2.09)	109.96 (1.86)	67.89 (1.59)	
	B18 -	Ni2	B13_38	B13_39	B15_56	B17	B10	B13_13	
Ni1 - Distance Angles									
B16_22	1.1397 (0.0268)								
B16	1.1397 (0.0269)	104.82 (1.46)							
B16_21	1.1398 (0.0268)	104.82 (1.46)	104.82 (1.46)						
B01_3	2.1382 (0.0043)	100.58 (0.54)	58.43 (1.07)	152.73 (0.31)					
B01_11	2.1382 (0.0043)	152.74 (0.31)	58.43 (1.07)	100.58 (0.54)	52.85 (0.20)				
B01_6	2.1382 (0.0043)	58.44 (1.07)	100.58 (0.54)	152.74 (0.31)	53.00 (0.20)	101.03 (0.21)			
B01_9	2.1382 (0.0043)	100.58 (0.54)	152.74 (0.31)	58.44 (1.07)	126.05 (0.34)	101.03 (0.21)	101.03 (0.21)		
B01_1	2.1382 (0.0043)	58.44 (1.07)	152.74 (0.31)	100.59 (0.53)	101.03 (0.21)	126.05 (0.34)	52.85 (0.20)	53.00 (0.20)	
B01_5	2.1382 (0.0043)	152.74 (0.31)	100.58 (0.54)	58.44 (1.07)	101.03 (0.21)	53.00 (0.20)	126.05 (0.34)	52.85 (0.20)	
B03_22	2.1519 (0.0051)	57.07 (0.09)	141.76 (1.32)	57.07 (0.09)	149.42 (0.17)	149.42 (0.17)	96.46 (0.12)	50.66 (0.14)	
B03_21	2.1519 (0.0050)	141.75 (1.32)	57.07 (0.09)	57.06 (0.09)	96.46 (0.12)	50.66 (0.14)	149.42 (0.17)	96.46 (0.12)	
B03	2.1519 (0.0051)	57.07 (0.09)	57.07 (0.09)	141.76 (1.32)	50.66 (0.14)	96.46 (0.12)	50.66 (0.14)	149.42 (0.17)	
	Ni1 -	B16_22	B16	B16_21	B01_3	B01_11	B01_6	B01_9	
Ni2 - Distance Angles									
B18	0.8340 (0.0668)								
B17	0.9393 (0.0483)	171.78 (4.98)							
B13_13	1.7412 (0.0105)	97.84 (4.09)	90.38 (2.84)						
B18_59	2.0512 (0.0248)	76.92 (4.42)	108.98 (2.50)	47.93 (1.88)					
B18_58	2.0513 (0.0247)	76.92 (4.39)	108.97 (2.50)	47.94 (1.88)	84.07 (3.66)				
B15_56	2.1626 (0.0082)	47.13 (4.05)	141.09 (2.85)	50.71 (0.32)	47.74 (1.61)	47.75 (1.62)			
Ni2_59	2.1633 (0.0082)	71.11 (1.65)	112.03 (1.05)	70.48 (0.27)	22.63 (1.85)	103.66 (1.79)	59.99 (0.00)		
Ni2_58	2.1634 (0.0082)	71.11 (1.65)	112.03 (1.05)	70.48 (0.27)	103.66 (1.77)	22.63 (1.86)	59.99 (0.00)	119.91 (0.04)	
B07_40	2.1968 (0.0066)	138.10 (3.11)	48.39 (2.30)	52.77 (0.29)	95.67 (1.81)	61.24 (1.54)	97.70 (0.30)	114.95 (0.45)	
B07_13	2.1968 (0.0066)	138.10 (3.14)	48.39 (2.30)	52.77 (0.28)	61.24 (1.54)	95.68 (1.81)	97.69 (0.30)	70.85 (0.32)	
B13_38	2.2790 (0.0078)	25.32 (1.17)	155.76 (0.22)	90.23 (0.48)	89.14 (1.54)	55.63 (1.61)	45.32 (0.23)	90.95 (0.29)	
B13_39	2.2790 (0.0078)	25.33 (1.15)	155.76 (0.22)	90.23 (0.48)	55.63 (1.61)	89.15 (1.55)	45.32 (0.23)	46.05 (0.26)	
	Ni2 -	B18	B17	B13_13	B18_59	B18_58	B15_56	Ni2_59	

A.6 Ausgewählte Bindungswinkel und -längen in $\text{Sc}_{10.37}\text{B}_{309.59}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 - Distance Angles									
B02_17	1.8238 (0.0056)								
B03_5	1.8273 (0.0058)	59.50 (0.22)							
B04_23	1.8732 (0.0062)	105.85 (0.30)	105.24 (0.27)						
B02_16	1.8800 (0.0055)	59.94 (0.24)	106.21 (0.29)	58.15 (0.22)					
B01_10	1.8947 (0.0084)	106.82 (0.18)	58.77 (0.15)	59.62 (0.15)	106.31 (0.18)				
B01_7	1.9316 (0.0080)	120.05 (0.18)	116.47 (0.21)	128.82 (0.21)	128.25 (0.17)	120.00 (0.00)			
Sc1_1	2.4215 (0.0042)	173.22 (0.26)	116.89 (0.23)	68.95 (0.21)	118.23 (0.20)	66.97 (0.10)	66.49 (0.10)		
Sc2_5	2.4323 (0.0052)	68.80 (0.19)	120.40 (0.22)	116.00 (0.21)	67.22 (0.18)	173.31 (0.10)	66.60 (0.10)	117.11 (0.17)	
	B01 -	B02_17	B03_5	B04_23	B02_16	B01_10	B01_7	Sc1_1	
B02 - Distance Angles									
B07_20	1.7544 (0.0056)								
B03_14	1.8118 (0.0051)	114.87 (0.29)							
B04_13	1.8236 (0.0052)	119.52 (0.30)	60.19 (0.25)						
B01_8	1.8239 (0.0056)	117.90 (0.28)	60.35 (0.24)	109.18 (0.27)					

A.6 Ausgewählte Bindungswinkel und -längen in $Sc_{10.37}B_{309.59}$

B02_\$11	1.8508 (0.0076)	127.76 (0.18)	108.10 (0.24)	106.79 (0.25)	61.54 (0.23)				
B01_\$4	1.8799 (0.0055)	126.27 (0.28)	109.18 (0.28)	60.74 (0.25)	109.78 (0.26)	58.53 (0.23)			
Sc2_\$21	2.4310 (0.0042)	69.19 (0.20)	175.93 (0.27)	118.15 (0.25)	118.37 (0.23)	68.48 (0.16)	67.29 (0.19)		
Sc2_\$35	2.4565 (0.0043)	66.53 (0.20)	119.89 (0.25)	173.73 (0.27)	67.39 (0.20)	67.02 (0.16)	114.84 (0.22)	61.29 (0.16)	
	B02 -	B07_\$20	B03_\$14	B04_\$13	B01_\$8	B02_\$11	B01_\$4	Sc2_\$21	
B03 - Distance Angles									
B05_\$3	1.6840 (0.0076)								
B02_\$19	1.8118 (0.0051)	120.65 (0.21)							
B02_\$14	1.8118 (0.0050)	120.65 (0.21)	109.02 (0.37)						
B04_\$12	1.8230 (0.0081)	120.21 (0.39)	60.23 (0.21)	60.23 (0.21)					
B01_\$3	1.8274 (0.0058)	121.24 (0.33)	60.15 (0.21)	110.28 (0.31)	109.07 (0.31)				
B01_\$6	1.8274 (0.0058)	121.24 (0.33)	110.28 (0.31)	60.15 (0.21)	109.06 (0.31)	62.45 (0.30)			
	B03 -	B05_\$3	B02_\$19	B02_\$14	B04_\$12	B01_\$3			
B04 - Distance Angles									
B10_\$41	1.7545 (0.0078)								
B03_\$21	1.8229 (0.0081)	115.80 (0.38)							
B02_\$13	1.8236 (0.0052)	119.30 (0.22)	59.58 (0.20)						
B02_\$11	1.8237 (0.0052)	119.30 (0.22)	59.58 (0.20)	107.98 (0.37)					
B01_\$8	1.8731 (0.0062)	125.27 (0.33)	109.00 (0.31)	109.59 (0.32)	61.12 (0.20)				
B01_\$2	1.8731 (0.0062)	125.27 (0.33)	109.00 (0.31)	61.11 (0.20)	109.59 (0.32)	60.77 (0.30)			
Sc1_\$14	2.4726 (0.0056)	70.08 (0.26)	174.12 (0.34)	118.23 (0.21)	118.23 (0.21)	66.06 (0.21)	66.06 (0.21)		
	B04 -	B10_\$41	B03_\$21	B02_\$13	B02_\$11	B01_\$8	B01_\$2		
B05 - Distance Angles									
B03_\$5	1.6840 (0.0076)								
B06_\$29	1.7548 (0.0057)	122.80 (0.26)							
B06_\$31	1.7548 (0.0056)	122.80 (0.27)	105.41 (0.44)						
B05_\$28	1.7616 (0.0102)	122.28 (0.21)	107.07 (0.23)	59.87 (0.21)					
B05_\$26	1.7617 (0.0103)	122.28 (0.22)	59.87 (0.21)	107.07 (0.23)	60.00 (0.00)				
B06_\$4	1.7767 (0.0075)	122.36 (0.43)	58.71 (0.20)	58.72 (0.20)	106.86 (0.22)	106.86 (0.22)			
	B05 -	B03_\$5	B06_\$29	B06_\$31	B05_\$28	B05_\$26			
B06 - Distance Angles									
B09	1.6287 (0.0078)								
B06_\$30	1.7314 (0.0064)	122.28 (0.07)							
B06_\$24	1.7314 (0.0064)	122.28 (0.07)	107.47 (0.36)						
B05_\$27	1.7548 (0.0056)	118.94 (0.35)	109.19 (0.28)	61.27 (0.26)					
B05_\$25	1.7548 (0.0056)	118.94 (0.35)	61.27 (0.26)	109.19 (0.28)	60.26 (0.42)				
B05_\$16	1.7767 (0.0075)	122.17 (0.40)	60.02 (0.30)	60.02 (0.30)	110.43 (0.36)	110.43 (0.36)			
	B06 -	B09	B06_\$30	B06_\$24	B05_\$27	B05_\$25			
B07 - Distance Angles									
B02_\$20	1.7544 (0.0056)								
B11_\$23	1.7873 (0.0044)	123.92 (0.32)							
B09_\$39	1.7984 (0.0062)	121.42 (0.30)	105.48 (0.30)						
B13	1.8009 (0.0094)	123.63 (0.36)	62.74 (0.32)	105.04 (0.30)					
B08_\$38	1.8136 (0.0057)	119.13 (0.29)	61.86 (0.25)	57.78 (0.22)	111.70 (0.36)				
B07_\$10	1.8962 (0.0079)	122.05 (0.18)	107.60 (0.22)	58.19 (0.15)	58.23 (0.21)	106.83 (0.18)			
Sc2_\$14	2.3832 (0.0048)	70.99 (0.19)	111.57 (0.26)	120.15 (0.22)	58.25 (0.30)	169.66 (0.27)	66.56 (0.10)		
Sc2_\$23	2.4409 (0.0047)	68.59 (0.19)	65.58 (0.21)	169.95 (0.27)	67.25 (0.24)	117.95 (0.24)	118.72 (0.12)	62.17 (0.13)	
	B07 -	B02_\$20	B11_\$23	B09_\$39	B13	B08_\$38	B07_\$10	Sc2_\$14	
B08 - Distance Angles									
B08_\$33	1.6644 (0.0086)								
B09	1.7451 (0.0053)	121.17 (0.22)							
B07_\$34	1.8136 (0.0057)	123.69 (0.39)	60.67 (0.26)						
B12_\$15	1.8405 (0.0062)	123.19 (0.29)	105.90 (0.30)	105.64 (0.29)					
B11	1.8508 (0.0059)	127.10 (0.29)	105.02 (0.30)	58.38 (0.22)	57.57 (0.26)				
B10	1.8678 (0.0054)	117.87 (0.39)	62.31 (0.25)	110.66 (0.29)	57.99 (0.25)	105.08 (0.32)			
	B08 -	B08_\$33	B09	B07_\$34	B12_\$15	B11			
B09 - Distance Angles									
B06	1.6287 (0.0078)								
B08	1.7451 (0.0053)	116.51 (0.24)							
B08_\$36	1.7451 (0.0053)	116.50 (0.24)	115.16 (0.42)						
B07_\$34	1.7984 (0.0062)	121.24 (0.32)	61.55 (0.22)	114.43 (0.33)					
B07_\$32	1.7984 (0.0062)	121.24 (0.32)	114.43 (0.33)	61.55 (0.22)	63.63 (0.31)				
B10	1.8721 (0.0077)	117.27 (0.39)	62.06 (0.22)	62.06 (0.22)	111.15 (0.31)	111.15 (0.31)			
	B09 -	B06	B08	B08_\$36	B07_\$34	B07_\$32			

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B10 -	Distance	Angles						
B04_22	1.7546 (0.0078)							
B12_15	1.7976 (0.0051)	125.30 (0.32)						
B12_46	1.7976 (0.0051)	125.30 (0.32)	64.20 (0.42)					
B08_36	1.8677 (0.0055)	120.45 (0.24)	109.99 (0.34)	60.25 (0.24)				
B08	1.8678 (0.0055)	120.45 (0.24)	60.24 (0.24)	109.99 (0.34)	104.13 (0.37)			
B09	1.8721 (0.0077)	122.18 (0.40)	102.50 (0.31)	102.50 (0.31)	55.63 (0.20)			
Sc1_14	2.4972 (0.0056)	68.58 (0.25)	68.56 (0.23)	68.56 (0.23)	120.61 (0.21)	120.61 (0.21)	169.24 (0.34)	
	B10 -	B04_22	B12_15	B12_46	B08_36	B08	B09	
B11 -	Distance	Angles						
B14_14	1.7452 (0.0059)							
B12_15	1.7774 (0.0078)	59.74 (0.42)						
B07_2	1.7874 (0.0044)	103.86 (0.24)	109.51 (0.21)					
B07_34	1.7875 (0.0044)	103.85 (0.24)	109.51 (0.21)	139.76 (0.42)				
B08	1.8508 (0.0059)	104.56 (0.36)	60.92 (0.24)	137.16 (0.35)	59.77 (0.19)			
B08_10	1.8509 (0.0059)	104.56 (0.36)	60.93 (0.24)	59.77 (0.19)	137.16 (0.34)	82.38 (0.34)		
B13_2	1.8678 (0.0070)	58.69 (0.39)	109.71 (0.37)	58.98 (0.35)	114.94 (0.40)	162.02 (0.43)	107.09 (0.33)	
B13_32	1.8679 (0.0070)	58.69 (0.39)	109.71 (0.37)	114.95 (0.40)	58.98 (0.35)	107.09 (0.33)	162.02 (0.42)	59.86 (0.64)
Sc2	2.3549 (0.0063)	118.06 (0.42)	177.80 (0.38)	70.70 (0.21)	70.70 (0.21)	120.51 (0.25)	120.51 (0.25)	68.43 (0.28)
	B11 -	B14_14	B12_15	B07_2	B07_34	B08	B08_10	B13_2
B12 -	Distance	Angles						
B14_47	1.7547 (0.0095)							
B11_35	1.7774 (0.0078)	59.22 (0.32)						
B10_40	1.7976 (0.0051)	103.36 (0.23)	111.30 (0.23)					
B10_35	1.7976 (0.0052)	103.36 (0.23)	111.30 (0.23)	136.92 (0.44)				
B08_35	1.8405 (0.0062)	104.61 (0.29)	61.51 (0.24)	139.37 (0.37)	61.76 (0.21)			
B08_37	1.8405 (0.0062)	104.61 (0.29)	61.51 (0.24)	61.76 (0.21)	139.37 (0.37)	82.95 (0.37)		
B12_43	1.9105 (0.0103)	57.02 (0.22)	107.46 (0.22)	113.50 (0.21)	57.90 (0.21)	106.34 (0.19)	160.68 (0.20)	
B12_45	1.9105 (0.0104)	57.02 (0.22)	107.46 (0.22)	57.90 (0.21)	113.50 (0.22)	160.68 (0.20)	106.34 (0.19)	60.00 (0.00)
Sc1_47	2.4871 (0.0058)	114.73 (0.35)	173.95 (0.37)	69.16 (0.22)	69.16 (0.22)	122.36 (0.22)	122.36 (0.22)	67.41 (0.11)
	B12 -	B14_47	B11_35	B10_40	B10_35	B08_35	B08_37	B12_43
B13 -	Distance	Angles						
B15	1.7338 (0.0094)							
B14_1	1.7738 (0.0120)	104.28 (0.56)						
B07_10	1.8008 (0.0094)	138.27 (0.37)	102.15 (0.43)					
B07	1.8009 (0.0094)	138.27 (0.37)	102.15 (0.43)	63.53 (0.43)				
B13_28	1.8640 (0.0176)	57.49 (0.25)	58.30 (0.30)	114.49 (0.24)	160.21 (0.29)			
B13_26	1.8640 (0.0177)	57.49 (0.25)	58.30 (0.30)	160.21 (0.29)	114.48 (0.24)	60.00 (0.00)		
B11_39	1.8678 (0.0070)	113.13 (0.38)	57.20 (0.29)	58.28 (0.23)	108.26 (0.48)	60.07 (0.32)	107.33 (0.32)	
B11_23	1.8679 (0.0070)	113.13 (0.38)	57.20 (0.29)	108.26 (0.48)	58.28 (0.23)	107.34 (0.32)	60.07 (0.32)	105.67 (0.54)
Sc2_14	2.0990 (0.0097)	79.22 (0.34)	176.49 (0.61)	74.90 (0.37)	74.90 (0.37)	124.51 (0.22)	124.51 (0.22)	121.62 (0.34)
Sc2_39	2.4085 (0.0051)	70.73 (0.23)	114.25 (0.25)	69.16 (0.19)	124.86 (0.47)	67.23 (0.24)	119.59 (0.25)	65.41 (0.19)
Sc2_23	2.4085 (0.0051)	70.73 (0.23)	114.25 (0.25)	124.86 (0.47)	69.16 (0.19)	119.59 (0.25)	67.23 (0.24)	170.90 (0.45)
	B13 -	B15	B14_1	B07_10	B07	B13_28	B13_26	B11_39
B14 -	Distance	Angles						
B11_14	1.7451 (0.0059)							
B11_15	1.7451 (0.0059)	117.06 (0.21)						
B11_24	1.7453 (0.0059)	117.06 (0.21)	117.06 (0.21)					
B12_44	1.7547 (0.0095)	116.39 (0.35)	61.04 (0.29)	116.38 (0.35)				
B12_42	1.7547 (0.0095)	116.38 (0.35)	116.38 (0.35)	61.04 (0.29)	65.96 (0.44)			
B12_22	1.7547 (0.0095)	61.04 (0.29)	116.39 (0.35)	116.38 (0.35)	65.96 (0.44)	65.96 (0.44)		
B13_3	1.7738 (0.0120)	64.11 (0.26)	117.37 (0.63)	64.11 (0.26)	178.41 (0.54)	115.31 (0.30)	115.31 (0.30)	
B13_5	1.7738 (0.0120)	64.11 (0.26)	64.11 (0.26)	117.37 (0.63)	115.31 (0.30)	178.41 (0.54)	115.31 (0.30)	63.40 (0.60)
B13_1	1.7738 (0.0120)	117.37 (0.63)	64.11 (0.26)	64.11 (0.26)	115.31 (0.30)	115.31 (0.30)	178.41 (0.55)	63.40 (0.60)
	B14 -	B11_14	B11_15	B11_24	B12_44	B12_42	B12_22	B13_3
B15 -	Distance	Angles						
B13	1.7338 (0.0095)							
B13_1	1.7339 (0.0095)	180.00 (0.36)						
B13_5	1.7339 (0.0094)	114.97 (0.51)	65.03 (0.50)					
B13_28	1.7339 (0.0094)	65.03 (0.50)	114.97 (0.50)	180.00 (0.36)				
B13_26	1.7339 (0.0095)	65.03 (0.51)	114.97 (0.51)	114.97 (0.51)	65.03 (0.50)			
B13_3	1.7339 (0.0095)	114.97 (0.51)	65.03 (0.51)	65.03 (0.50)	114.97 (0.51)	180.00 (0.00)		
Sc2_15	2.4598 (0.0034)	112.44 (0.13)	67.56 (0.13)	67.56 (0.13)	112.44 (0.13)	56.96 (0.32)	123.04 (0.32)	
Sc2_39	2.4598 (0.0034)	67.56 (0.13)	112.44 (0.13)	112.44 (0.13)	67.56 (0.13)	123.04 (0.32)	56.96 (0.32)	180.00 (0.15)
Sc2_49	2.4598 (0.0034)	123.04 (0.32)	56.96 (0.32)	112.44 (0.13)	67.56 (0.13)	67.56 (0.13)	112.44 (0.13)	60.85 (0.02)
Sc2_14	2.4598 (0.0034)	56.96 (0.32)	123.04 (0.32)	67.56 (0.13)	112.44 (0.13)	112.44 (0.13)	67.56 (0.13)	119.15 (0.02)
Sc2_24	2.4598 (0.0034)	112.44 (0.13)	67.56 (0.13)	123.04 (0.32)	56.96 (0.32)	112.44 (0.13)	67.56 (0.13)	119.15 (0.02)

A.6 Ausgewählte Bindungswinkel und -längen in $Sc_{10.37}B_{309.59}$

Sc2_\$23	2.4598 (0.0034)	67.56 (0.13)	112.44 (0.13)	56.96 (0.32)	123.04 (0.32)	67.56 (0.13)	112.44 (0.13)	60.85 (0.02)
	B15 -	B13	B13_\$1	B13_\$5	B13_\$28	B13_\$26	B13_\$3	Sc2_\$15
Sc1 -	Distance	Angles						
B01_\$9	2.4215 (0.0042)							
B01_\$1	2.4215 (0.0042)	46.06 (0.19)						
B01_\$5	2.4215 (0.0042)	47.01 (0.19)	86.35 (0.14)					
B01_\$3	2.4215 (0.0042)	104.39 (0.19)	86.35 (0.14)	86.35 (0.14)				
B01_\$11	2.4215 (0.0042)	86.35 (0.14)	104.39 (0.19)	46.06 (0.19)	47.01 (0.19)			
B01_\$6	2.4215 (0.0042)	86.35 (0.14)	47.01 (0.19)	104.39 (0.19)	46.06 (0.19)	86.35 (0.14)		
B04_\$24	2.4726 (0.0056)	44.99 (0.14)	44.99 (0.14)	89.04 (0.13)	131.33 (0.16)	131.33 (0.16)	89.04 (0.13)	
B04_\$14	2.4726 (0.0057)	131.33 (0.16)	89.04 (0.13)	131.33 (0.16)	44.99 (0.14)	89.04 (0.13)	44.99 (0.14)	119.88 (0.02)
B04_\$15	2.4726 (0.0056)	89.04 (0.13)	131.33 (0.16)	44.99 (0.14)	89.04 (0.13)	44.99 (0.14)	131.33 (0.16)	119.88 (0.02)
B12_\$22	2.4871 (0.0058)	148.63 (0.14)	148.63 (0.13)	123.19 (0.10)	104.30 (0.16)	104.30 (0.15)	123.19 (0.10)	118.31 (0.20)
B12_\$42	2.4871 (0.0058)	123.19 (0.10)	104.30 (0.15)	148.63 (0.14)	123.19 (0.10)	148.63 (0.14)	104.30 (0.15)	79.01 (0.14)
B12_\$44	2.4871 (0.0058)	104.30 (0.16)	123.19 (0.10)	104.30 (0.15)	148.63 (0.14)	123.19 (0.10)	148.63 (0.13)	79.01 (0.14)
Sc1 -	B01_\$9	B01_\$1	B01_\$5	B01_\$3	B01_\$11	B01_\$6	B04_\$24	
Sc2 -	Distance	Angles						
B13_\$14	2.0989 (0.0097)							
B11	2.3549 (0.0063)	121.07 (0.33)						
B07_\$33	2.3830 (0.0048)	46.85 (0.25)	151.26 (0.15)					
B07_\$14	2.3831 (0.0048)	46.85 (0.25)	151.26 (0.16)	46.89 (0.20)				
B13_\$2	2.4085 (0.0051)	80.57 (0.44)	46.16 (0.22)	106.80 (0.24)	126.65 (0.27)			
B13_\$32	2.4085 (0.0051)	80.57 (0.44)	46.16 (0.23)	126.65 (0.27)	106.80 (0.24)	45.53 (0.48)		
B02_\$18	2.4309 (0.0042)	117.98 (0.12)	81.55 (0.14)	84.51 (0.14)	126.97 (0.17)	80.71 (0.27)	121.11 (0.25)	
B02_\$12	2.4311 (0.0042)	117.98 (0.12)	81.55 (0.14)	126.97 (0.17)	84.51 (0.14)	121.11 (0.25)	80.71 (0.26)	122.35 (0.23)
B01_\$11	2.4323 (0.0052)	125.86 (0.28)	107.63 (0.20)	79.08 (0.15)	97.27 (0.17)	125.69 (0.27)	152.97 (0.26)	45.48 (0.13)
B01_\$3	2.4323 (0.0052)	125.86 (0.28)	107.63 (0.19)	97.27 (0.17)	79.08 (0.15)	152.97 (0.26)	125.69 (0.27)	89.69 (0.17)
B07_\$2	2.4409 (0.0047)	115.64 (0.23)	43.72 (0.10)	112.27 (0.12)	157.83 (0.18)	43.59 (0.25)	78.92 (0.25)	42.21 (0.13)
B07_\$34	2.4410 (0.0047)	115.64 (0.23)	43.72 (0.10)	157.83 (0.18)	112.27 (0.12)	78.92 (0.25)	43.59 (0.25)	117.66 (0.18)
Sc2 -	B13_\$14	B11	B07_\$33	B07_\$14	B13_\$2	B13_\$32	B02_\$18	

B Molybdän-, Wolfram- und Rheniumboride

B.1 Ausgewählte Bindungswinkel und -längen in Mo₂B₄ (Neutronendaten)

Winkel (Angles) in Grad, Abstände (Length) in Å.

Vector	Length	Optr Cell	Neighbor atom coordinates		
Mo_Mo	3.01193(4)	1-1-1 0	-1.00000	-1.00000	0.07508
Mo_Mo	3.01193(4)	1-1 0 0	-1.00000	0.00000	0.07508
Mo_Mo	3.01193(4)	1 0-1 0	0.00000	-1.00000	0.07508
Mo_Mo	3.01193(4)	1 0 1 0	0.00000	1.00000	0.07508
Mo_Mo	3.01193(4)	1 1 0 0	1.00000	0.00000	0.07508
Mo_Mo	3.01193(4)	1 1 1 0	1.00000	1.00000	0.07508
Mo_Mo	3.14286(8)	-1 0 0 0	0.00000	0.00000	-0.07508
Mo_B1	2.34807(3)	101-1-1-1	-0.66667	-0.33333	-0.00031
Mo_B1	2.34807(3)	101 0-1-1	0.33333	-0.33333	-0.00031
Mo_B1	2.34807(3)	101 0 0-1	0.33333	0.66667	-0.00031
Mo_B1	2.33950(3)	-201-1-1 0	-0.33333	-0.66667	0.00031
Mo_B1	2.33950(3)	-201-1 0 0	-0.33333	0.33333	0.00031
Mo_B1	2.33950(3)	-201 0 0 0	0.66667	0.33333	0.00031
Mo_B2	2.22932(6)	1 0 0 0	0.00000	0.00000	0.18159
Mo_B2	2.36621(3)	-201-1-1 0	-0.33333	-0.66667	0.15175
Mo_B2	2.36621(3)	-201-1 0 0	-0.33333	0.33333	0.15175
Mo_B2	2.36621(3)	-201 0 0 0	0.66667	0.33333	0.15175

Angle	Degrees	atom 1 loc	atom 3 loc
B1_Mo_B1	79.787(1)	101-1-1-1	101 0-1-1
B1_Mo_B1	79.787(1)	101-1-1-1	101 0 0-1
B1_Mo_B1	43.551(1)	101-1-1-1	-201-1-1 0
B1_Mo_B1	43.551(1)	101-1-1-1	-201-1 0 0
B1_Mo_B1	95.794(2)	101-1-1-1	-201 0 0 0
B1_Mo_B2	132.219(1)	101-1-1-1	1 0 0 0
B1_Mo_B2	100.578(1)	101-1-1-1	-201-1-1 0
B1_Mo_B2	100.578(1)	101-1-1-1	-201-1 0 0
B1_Mo_B2	179.518(0)	101-1-1-1	-201 0 0 0
B1_Mo_B1	79.787(1)	101 0-1-1	101 0 0-1
B1_Mo_B1	43.551(1)	101 0-1-1	-201-1-1 0
B1_Mo_B1	95.794(2)	101 0-1-1	-201-1 0 0
B1_Mo_B1	43.551(1)	101 0-1-1	-201 0 0 0
B1_Mo_B2	132.219(1)	101 0-1-1	1 0 0 0
B1_Mo_B2	100.578(1)	101 0-1-1	-201-1-1 0
B1_Mo_B2	179.518(0)	101 0-1-1	-201-1 0 0
B1_Mo_B2	100.578(1)	101 0-1-1	-201 0 0 0
B1_Mo_B1	95.794(2)	101 0 0-1	-201-1-1 0
B1_Mo_B1	43.551(1)	101 0 0-1	-201-1 0 0
B1_Mo_B1	43.551(1)	101 0 0-1	-201 0 0 0
B1_Mo_B2	132.219(1)	101 0 0-1	1 0 0 0
B1_Mo_B2	179.518(0)	101 0 0-1	-201-1-1 0
B1_Mo_B2	100.578(1)	101 0 0-1	-201-1 0 0
B1_Mo_B2	100.578(1)	101 0 0-1	-201 0 0 0
B1_Mo_B1	80.138(1)	-201-1-1 0	-201-1 0 0
B1_Mo_B1	80.138(1)	-201-1-1 0	-201 0 0 0
B1_Mo_B2	131.987(1)	-201-1-1 0	1 0 0 0
B1_Mo_B2	84.688(2)	-201-1-1 0	-201-1-1 0
B1_Mo_B2	136.619(1)	-201-1-1 0	-201-1 0 0
B1_Mo_B2	136.619(1)	-201-1-1 0	-201 0 0 0
B1_Mo_B1	80.138(1)	-201-1 0 0	-201 0 0 0

B1_Mo_B2	131.987(1)	-201-1 0 0	1 0 0 0
B1_Mo_B2	136.619(1)	-201-1 0 0	-201-1-1 0
B1_Mo_B2	84.688(2)	-201-1 0 0	-201-1 0 0
B1_Mo_B2	136.619(1)	-201-1 0 0	-201 0 0 0
B1_Mo_B2	131.987(1)	-201 0 0 0	1 0 0 0
B1_Mo_B2	136.619(1)	-201 0 0 0	-201-1-1 0
B1_Mo_B2	136.619(1)	-201 0 0 0	-201-1 0 0
B1_Mo_B2	84.688(2)	-201 0 0 0	-201 0 0 0
B2_Mo_B2	47.299(1)	1 0 0 0	-201-1-1 0
B2_Mo_B2	47.299(1)	1 0 0 0	-201-1 0 0
B2_Mo_B2	47.299(1)	1 0 0 0	-201 0 0 0
B2_Mo_B2	79.055(1)	-201-1-1 0	-201-1 0 0
B2_Mo_B2	79.055(1)	-201-1-1 0	-201 0 0 0
B2_Mo_B2	79.055(1)	-201-1 0 0	-201 0 0 0
Vector	Length	Optr Cell	Neighbor atom coordinates
B1_Mo	2.34807(3)	201-1-1 0	-0.33333 -0.66667 0.40841
B1_Mo	2.34807(3)	201-1 0 0	-0.33333 0.33333 0.40841
B1_Mo	2.34807(3)	201 0 0 0	0.66667 0.33333 0.40841
B1_Mo	2.33950(3)	-201-1-1 0	-0.33333 -0.66667 0.25826
B1_Mo	2.33950(3)	-201-1 0 0	-0.33333 0.33333 0.25826
B1_Mo	2.33950(3)	-201 0 0 0	0.66667 0.33333 0.25826
B1_B1	1.73899(2)	-101-1-1 0	-0.66667 -0.33333 0.33364
B1_B1	1.73899(2)	-101 0-1 0	0.33333 -0.33333 0.33364
B1_B1	1.73899(2)	-101 0 0 0	0.33333 0.66667 0.33364
Angle	Degrees	atom 1 loc	atom 3 loc
Mo_B1_Mo	79.787(1)	201-1-1 0	201-1 0 0
Mo_B1_Mo	79.787(1)	201-1-1 0	201 0 0 0
Mo_B1_Mo	84.206(2)	201-1-1 0	-201-1-1 0
Mo_B1_Mo	136.449(1)	201-1-1 0	-201-1 0 0
Mo_B1_Mo	136.449(1)	201-1-1 0	-201 0 0 0
Mo_B1_B1	67.962(0)	201-1-1 0	-101-1-1 0
Mo_B1_B1	67.962(0)	201-1-1 0	-101 0-1 0
Mo_B1_B1	137.360(1)	201-1-1 0	-101 0 0 0
Mo_B1_Mo	79.787(1)	201-1 0 0	201 0 0 0
Mo_B1_Mo	136.449(1)	201-1 0 0	-201-1-1 0
Mo_B1_Mo	84.206(2)	201-1 0 0	-201-1 0 0
Mo_B1_Mo	136.449(1)	201-1 0 0	-201 0 0 0
Mo_B1_B1	67.962(0)	201-1 0 0	-101-1-1 0
Mo_B1_B1	137.360(1)	201-1 0 0	-101 0-1 0
Mo_B1_B1	67.962(0)	201-1 0 0	-101 0 0 0
Mo_B1_Mo	136.449(1)	201 0 0 0	-201-1-1 0
Mo_B1_Mo	136.449(1)	201 0 0 0	-201-1 0 0
Mo_B1_Mo	84.206(2)	201 0 0 0	-201 0 0 0
Mo_B1_B1	137.360(1)	201 0 0 0	-101-1-1 0
Mo_B1_B1	67.962(0)	201 0 0 0	-101 0-1 0
Mo_B1_B1	67.962(0)	201 0 0 0	-101 0 0 0
Mo_B1_Mo	80.138(1)	-201-1-1 0	-201-1 0 0
Mo_B1_Mo	80.138(1)	-201-1-1 0	-201 0 0 0
Mo_B1_B1	68.487(0)	-201-1-1 0	-101-1-1 0
Mo_B1_B1	68.486(0)	-201-1-1 0	-101 0-1 0
Mo_B1_B1	138.434(1)	-201-1-1 0	-101 0 0 0
Mo_B1_Mo	80.138(1)	-201-1 0 0	-201 0 0 0
Mo_B1_B1	68.486(0)	-201-1 0 0	-101-1-1 0
Mo_B1_B1	138.434(1)	-201-1 0 0	-101 0-1 0
Mo_B1_B1	68.486(0)	-201-1 0 0	-101 0 0 0
Mo_B1_B1	138.434(1)	-201 0 0 0	-101-1-1 0
Mo_B1_B1	68.486(0)	-201 0 0 0	-101 0-1 0
Mo_B1_B1	68.487(0)	-201 0 0 0	-101 0 0 0
B1_B1_B1	119.995(0)	-101-1-1 0	-101 0-1 0
B1_B1_B1	119.995(0)	-101-1-1 0	-101 0 0 0
B1_B1_B1	119.995(0)	-101 0-1 0	-101 0 0 0
Vector	Length	Optr Cell	Neighbor atom coordinates
B2_Mo	2.22932(6)	1 0 0 0	0.00000 0.00000 0.07508
B2_Mo	2.36621(3)	-201-1-1 0	-0.33333 -0.66667 0.25826
B2_Mo	2.36621(3)	-201-1 0 0	-0.33333 0.33333 0.25826
B2_Mo	2.36621(3)	-201 0 0 0	0.66667 0.33333 0.25826
B2_B2	1.84772(2)	-201-1-1 0	-0.33333 -0.66667 0.15175
B2_B2	1.84772(2)	-201-1 0 0	-0.33333 0.33333 0.15175
B2_B2	1.84772(2)	-201 0 0 0	0.66667 0.33333 0.15175

B.2 Ausgewählte Bindungswinkel und -längen in MoB_{2-x} (Röntgendaten)

Angle	Degrees	atom 1 loc	atom 3 loc
Mo_B2_Mo	132.701(1)	1 0 0 0	-201-1-1 0
Mo_B2_Mo	132.701(1)	1 0 0 0	-201-1 0 0
Mo_B2_Mo	132.701(1)	1 0 0 0	-201 0 0 0
Mo_B2_B2	70.242(1)	1 0 0 0	-201-1-1 0
Mo_B2_B2	70.242(1)	1 0 0 0	-201-1 0 0
Mo_B2_B2	70.242(1)	1 0 0 0	-201 0 0 0
Mo_B2_Mo	79.055(1)	-201-1-1 0	-201-1 0 0
Mo_B2_Mo	79.055(1)	-201-1-1 0	-201 0 0 0
Mo_B2_B2	62.459(1)	-201-1-1 0	-201-1-1 0
Mo_B2_B2	125.105(0)	-201-1-1 0	-201-1 0 0
Mo_B2_B2	125.105(0)	-201-1-1 0	-201 0 0 0
Mo_B2_Mo	79.055(1)	-201-1 0 0	-201 0 0 0
Mo_B2_B2	125.105(0)	-201-1 0 0	-201-1-1 0
Mo_B2_B2	62.459(1)	-201-1 0 0	-201-1 0 0
Mo_B2_B2	125.105(0)	-201-1 0 0	-201 0 0 0
Mo_B2_B2	125.105(0)	-201 0 0 0	-201-1-1 0
Mo_B2_B2	125.105(0)	-201 0 0 0	-201-1 0 0
Mo_B2_B2	62.459(1)	-201 0 0 0	-201 0 0 0
B2_B2_B2	109.183(1)	-201-1-1 0	-201-1 0 0
B2_B2_B2	109.183(1)	-201-1-1 0	-201 0 0 0
B2_B2_B2	109.183(1)	-201-1 0 0	-201 0 0 0

B.2 Ausgewählte Bindungswinkel und -längen in MoB_{2-x} (Röntgendaten)

Winkel (Angles) in Grad, Abstände (Length) in Å.

Vector	Length	Optr Cell	Neighbor atom coordinates		
Mo_Mo	3.04056(19)	1-1-1 0	-1.00000	-1.00000	0.00000
Mo_Mo	3.04056(19)	1-1 0 0	-1.00000	0.00000	0.00000
Mo_Mo	3.04056(19)	1 0-1 0	0.00000	-1.00000	0.00000
Mo_Mo	3.06573(20)	1 0 0-1	0.00000	0.00000	-1.00000
Mo_Mo	3.06573(20)	1 0 0 1	0.00000	0.00000	1.00000
Mo_Mo	3.04056(19)	1 0 1 0	0.00000	1.00000	0.00000
Mo_Mo	3.04056(19)	1 1 0 0	1.00000	0.00000	0.00000
Mo_Mo	3.04056(19)	1 1 1 0	1.00000	1.00000	0.00000
Mo_B	2.33059(11)	1-1-1-1	-0.66670	-0.33330	-0.50000
Mo_B	2.33059(11)	1-1-1 0	-0.66670	-0.33330	0.50000
Mo_B	2.33039(11)	1 0-1-1	0.33330	-0.33330	-0.50000
Mo_B	2.33039(11)	1 0-1 0	0.33330	-0.33330	0.50000
Mo_B	2.33059(11)	1 0 0-1	0.33330	0.66670	-0.50000
Mo_B	2.33059(11)	1 0 0 0	0.33330	0.66670	0.50000
Mo_B	2.33059(11)	2 0-1-1	-0.33340	-0.66670	-0.50000
Mo_B	2.33059(11)	2 0-1 0	-0.33340	-0.66670	0.50000
Mo_B	2.33059(11)	2 0 0-1	-0.33340	0.33330	-0.50000
Mo_B	2.33059(11)	2 0 0 0	-0.33340	0.33330	0.50000
Mo_B	2.33039(11)	2 1 0-1	0.66660	0.33330	-0.50000
Mo_B	2.33039(11)	2 1 0 0	0.66660	0.33330	0.50000

Angle	Degrees	atom 1 loc	atom 3 loc
B_Mo_B	82.252(5)	1-1-1-1	1-1-1 0
B_Mo_B	81.437(4)	1-1-1-1	1 0-1-1
B_Mo_B	135.754(2)	1-1-1-1	1 0-1 0
B_Mo_B	81.433(4)	1-1-1-1	1 0 0-1
B_Mo_B	135.742(2)	1-1-1-1	1 0 0 0
B_Mo_B	44.251(2)	1-1-1-1	2 0-1-1
B_Mo_B	98.562(4)	1-1-1-1	2 0-1 0
B_Mo_B	44.244(2)	1-1-1-1	2 0 0-1
B_Mo_B	98.557(4)	1-1-1-1	2 0 0 0
B_Mo_B	97.744(5)	1-1-1-1	2 1 0-1
B_Mo_B	180.000(0)	1-1-1-1	2 1 0 0
B_Mo_B	135.754(2)	1-1-1 0	1 0-1-1

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B_Mo_B	81.437(4)	1-1-1 0	1 0-1 0
B_Mo_B	135.742(2)	1-1-1 0	1 0 0-1
B_Mo_B	81.433(4)	1-1-1 0	1 0 0 0
B_Mo_B	98.562(4)	1-1-1 0	2 0-1-1
B_Mo_B	44.251(2)	1-1-1 0	2 0-1 0
B_Mo_B	98.567(4)	1-1-1 0	2 0 0-1
B_Mo_B	44.244(2)	1-1-1 0	2 0 0 0
B_Mo_B	180.000(0)	1-1-1 0	2 1 0-1
B_Mo_B	97.744(5)	1-1-1 0	2 1 0 0
B_Mo_B	82.260(5)	1 0-1-1	1 0-1 0
B_Mo_B	81.437(4)	1 0-1-1	1 0 0-1
B_Mo_B	135.754(2)	1 0-1-1	1 0 0 0
B_Mo_B	44.253(2)	1 0-1-1	2 0-1-1
B_Mo_B	98.568(4)	1 0-1-1	2 0-1 0
B_Mo_B	97.744(5)	1 0-1-1	2 0 0-1
B_Mo_B	180.000(0)	1 0-1-1	2 0 0 0
B_Mo_B	44.248(2)	1 0-1-1	2 1 0-1
B_Mo_B	98.569(4)	1 0-1-1	2 1 0 0
B_Mo_B	135.754(2)	1 0-1 0	1 0 0-1
B_Mo_B	81.437(4)	1 0-1 0	1 0 0 0
B_Mo_B	98.568(4)	1 0-1 0	2 0-1-1
B_Mo_B	44.253(2)	1 0-1 0	2 0-1 0
B_Mo_B	180.000(0)	1 0-1 0	2 0 0-1
B_Mo_B	97.744(5)	1 0-1 0	2 0 0 0
B_Mo_B	98.569(4)	1 0-1 0	2 1 0-1
B_Mo_B	44.248(2)	1 0-1 0	2 1 0 0
B_Mo_B	82.252(5)	1 0 0-1	1 0 0 0
B_Mo_B	97.748(5)	1 0 0-1	2 0-1-1
B_Mo_B	180.000(0)	1 0 0-1	2 0-1 0
B_Mo_B	44.251(2)	1 0 0-1	2 0 0-1
B_Mo_B	98.562(4)	1 0 0-1	2 0 0 0
B_Mo_B	44.253(2)	1 0 0-1	2 1 0-1
B_Mo_B	98.568(4)	1 0 0-1	2 1 0 0
B_Mo_B	180.000(0)	1 0 0 0	2 0-1-1
B_Mo_B	97.748(5)	1 0 0 0	2 0-1 0
B_Mo_B	98.562(4)	1 0 0 0	2 0 0-1
B_Mo_B	44.251(2)	1 0 0 0	2 0 0 0
B_Mo_B	98.568(4)	1 0 0 0	2 1 0-1
B_Mo_B	44.253(2)	1 0 0 0	2 1 0 0
B_Mo_B	82.252(5)	2 0-1-1	2 0-1 0
B_Mo_B	81.433(4)	2 0-1-1	2 0 0-1
B_Mo_B	135.742(2)	2 0-1-1	2 0 0 0
B_Mo_B	81.437(4)	2 0-1-1	2 1 0-1
B_Mo_B	135.754(2)	2 0-1-1	2 1 0 0
B_Mo_B	135.742(2)	2 0-1 0	2 0 0-1
B_Mo_B	81.433(4)	2 0-1 0	2 0 0 0
B_Mo_B	135.754(2)	2 0-1 0	2 1 0-1
B_Mo_B	81.437(4)	2 0-1 0	2 1 0 0
B_Mo_B	82.252(5)	2 0 0-1	2 0 0 0
B_Mo_B	81.437(4)	2 0 0-1	2 1 0-1
B_Mo_B	135.754(2)	2 0 0-1	2 1 0 0
B_Mo_B	135.754(2)	2 0 0 0	2 1 0-1
B_Mo_B	81.437(4)	2 0 0 0	2 1 0 0
B_Mo_B	82.260(5)	2 1 0-1	2 1 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
B_Mo	2.33059(11)	1 0 0 0	0.00000	0.00000	0.00000
B_Mo	2.33059(11)	1 0 0 1	0.00000	0.00000	1.00000
B_Mo	2.33039(11)	1 0 1 0	0.00000	1.00000	0.00000
B_Mo	2.33039(11)	1 0 1 1	0.00000	1.00000	1.00000
B_Mo	2.33059(11)	1 1 1 0	1.00000	1.00000	0.00000
B_Mo	2.33059(11)	1 1 1 1	1.00000	1.00000	1.00000
B_B	1.75556(11)	2 0 0 0	-0.33340	0.33330	0.50000
B_B	1.75556(11)	2 1 0 0	0.66660	0.33330	0.50000
B_B	1.75529(11)	2 1 1 0	0.66660	1.33330	0.50000

Angle	Degrees	atom 1 loc	atom 3 loc
Mo_B_Mo	82.252(5)	1 0 0 0	1 0 0 1
Mo_B_Mo	81.437(4)	1 0 0 0	1 0 1 0
Mo_B_Mo	135.754(2)	1 0 0 0	1 0 1 1
Mo_B_Mo	81.433(4)	1 0 0 0	1 1 1 0
Mo_B_Mo	135.742(2)	1 0 0 0	1 1 1 1

B.3 Ausgewählte Bindungswinkel und -längen in WB (Neutronendaten)

Mo_B_B	67.875(1)	1 0 0 0	2 0 0 0
Mo_B_B	67.868(1)	1 0 0 0	2 1 0 0
Mo_B_B	138.874(3)	1 0 0 0	2 1 1 0
Mo_B_Mo	135.754(2)	1 0 0 1	1 0 1 0
Mo_B_Mo	81.437(4)	1 0 0 1	1 0 1 1
Mo_B_Mo	135.742(2)	1 0 0 1	1 1 1 0
Mo_B_Mo	81.433(4)	1 0 0 1	1 1 1 1
Mo_B_B	67.875(1)	1 0 0 1	2 0 0 0
Mo_B_B	67.868(1)	1 0 0 1	2 1 0 0
Mo_B_B	138.874(3)	1 0 0 1	2 1 1 0
Mo_B_Mo	82.260(5)	1 0 1 0	1 0 1 1
Mo_B_Mo	81.437(4)	1 0 1 0	1 1 1 0
Mo_B_Mo	135.754(2)	1 0 1 0	1 1 1 1
Mo_B_B	67.880(1)	1 0 1 0	2 0 0 0
Mo_B_B	138.870(3)	1 0 1 0	2 1 0 0
Mo_B_B	67.876(1)	1 0 1 0	2 1 1 0
Mo_B_Mo	135.754(2)	1 0 1 1	1 1 1 0
Mo_B_Mo	81.437(4)	1 0 1 1	1 1 1 1
Mo_B_B	67.880(1)	1 0 1 1	2 0 0 0
Mo_B_B	138.870(3)	1 0 1 1	2 1 0 0
Mo_B_B	67.876(1)	1 0 1 1	2 1 1 0
Mo_B_Mo	82.252(5)	1 1 1 0	1 1 1 1
Mo_B_B	138.874(3)	1 1 1 0	2 0 0 0
Mo_B_B	67.875(1)	1 1 1 0	2 1 0 0
Mo_B_B	67.878(1)	1 1 1 0	2 1 1 0
Mo_B_B	138.874(3)	1 1 1 1	2 0 0 0
Mo_B_B	67.875(1)	1 1 1 1	2 1 0 0
Mo_B_B	67.878(1)	1 1 1 1	2 1 1 0
B_B_B	119.990(0)	2 0 0 0	2 1 0 0
B_B_B	120.005(0)	2 0 0 0	2 1 1 0
B_B_B	120.005(0)	2 1 0 0	2 1 1 0

B.3 Ausgewählte Bindungswinkel und -längen in WB (Neutronendaten)

Winkel (Angles) in Grad, Abstände (Length) in Å.

Vector	Length	Optr Cell	Neighbor atom coordinates		
W1_W1	3.10481(4)	1-1 0 0	-1.00000	0.75000	0.32273
W1_W1	3.10481(4)	1 0-1 0	0.00000	-0.25000	0.32273
W1_W1	3.10481(4)	1 0 1 0	0.00000	1.75000	0.32273
W1_W1	3.10481(4)	1 1 0 0	1.00000	0.75000	0.32273
W1_W1	2.8210(13)	-2-1 1 1	-0.50000	0.25000	0.42727
W1_W1	2.8210(13)	-2-1 2 1	-0.50000	1.25000	0.42727
W1_W1	2.8210(13)	-2 0 1 1	0.50000	0.25000	0.42727
W1_W1	2.8210(13)	-2 0 2 1	0.50000	1.25000	0.42727
W1_W1	2.9130(18)	-3 0 0 1	-0.50000	0.75000	0.17727
W1_W1	2.9130(18)	-3 1 0 1	0.50000	0.75000	0.17727
W1_B1	2.4806(12)	1 0 0 0	0.00000	0.75000	0.46912
W1_B1	2.3436(9)	4-1 0-1	0.00000	0.25000	0.21912
W1_B1	2.3436(9)	4-1 1-1	0.00000	1.25000	0.21912
W1_B1	2.3071(5)	-2-1 1 1	-0.50000	0.25000	0.28088
W1_B1	2.3071(5)	-2-1 2 1	-0.50000	1.25000	0.28088
W1_B1	2.3071(5)	-2 0 1 1	0.50000	0.25000	0.28088
W1_B1	2.3071(5)	-2 0 2 1	0.50000	1.25000	0.28088

Angle	Degrees	atom 1 loc	atom 3 loc
B1_W1_B1	82.97(4)	4-1 0-1	4-1 1-1
B1_W1_B1	47.469(31)	4-1 0-1	-2-1 1 1
B1_W1_B1	102.44(4)	4-1 0-1	-2-1 2 1
B1_W1_B1	47.469(31)	4-1 0-1	-2 0 1 1
B1_W1_B1	102.44(4)	4-1 0-1	-2 0 2 1
B1_W1_B1	102.44(4)	4-1 1-1	-2-1 1 1
B1_W1_B1	47.469(31)	4-1 1-1	-2-1 2 1
B1_W1_B1	102.44(4)	4-1 1-1	-2 0 1 1
B1_W1_B1	47.469(31)	4-1 1-1	-2 0 2 1

B1_W1_B1	84.578(23)	-2-1 1 1	-2-1 2 1
B1_W1_B1	84.578(23)	-2-1 1 1	-2 0 1 1
B1_W1_B1	144.20(8)	-2-1 1 1	-2 0 2 1
B1_W1_B1	144.20(8)	-2-1 2 1	-2 0 1 1
B1_W1_B1	84.578(23)	-2-1 2 1	-2 0 2 1
B1_W1_B1	84.578(23)	-2 0 1 1	-2 0 2 1

Vector	Length	Optr Cell	Neighbor atom coordinates		
B1_W1	2.4806(12)	1 0 0 0	0.00000	0.75000	0.32273
B1_W1	2.3436(9)	2 0 0 0	-0.50000	0.75000	0.57273
B1_W1	2.3436(9)	2 1 0 0	0.50000	0.75000	0.57273
B1_W1	2.3071(5)	-2-1 1 1	-0.50000	0.25000	0.42727
B1_W1	2.3071(5)	-2-1 2 1	-0.50000	1.25000	0.42727
B1_W1	2.3071(5)	-2 0 1 1	0.50000	0.25000	0.42727
B1_W1	2.3071(5)	-2 0 2 1	0.50000	1.25000	0.42727
B1_B1	1.8722(11)	-1 0 1 1	0.00000	0.25000	0.53088
B1_B1	1.8722(11)	-1 0 2 1	0.00000	1.25000	0.53088

Angle	Degrees	atom 1 loc	atom 3 loc
W1_B1_W1	82.97(4)	2 0 0 0	2 1 0 0
W1_B1_W1	77.56(4)	2 0 0 0	-2-1 1 1
W1_B1_W1	77.56(4)	2 0 0 0	-2-1 2 1
W1_B1_W1	132.531(31)	2 0 0 0	-2 0 1 1
W1_B1_W1	132.531(31)	2 0 0 0	-2 0 2 1
W1_B1_B1	65.24(4)	2 0 0 0	-1 0 1 1
W1_B1_B1	65.24(4)	2 0 0 0	-1 0 2 1
W1_B1_W1	132.531(31)	2 1 0 0	-2-1 1 1
W1_B1_W1	132.531(31)	2 1 0 0	-2-1 2 1
W1_B1_W1	77.56(4)	2 1 0 0	-2 0 1 1
W1_B1_W1	77.56(4)	2 1 0 0	-2 0 2 1
W1_B1_B1	65.24(4)	2 1 0 0	-1 0 1 1
W1_B1_B1	65.24(4)	2 1 0 0	-1 0 2 1
W1_B1_W1	84.578(23)	-2-1 1 1	-2-1 2 1
W1_B1_W1	84.578(23)	-2-1 1 1	-2 0 1 1
W1_B1_W1	144.20(8)	-2-1 1 1	-2 0 2 1
W1_B1_B1	67.287(21)	-2-1 1 1	-1 0 1 1
W1_B1_B1	136.866(28)	-2-1 1 1	-1 0 2 1
W1_B1_W1	144.20(8)	-2-1 2 1	-2 0 1 1
W1_B1_W1	84.578(23)	-2-1 2 1	-2 0 2 1
W1_B1_B1	136.866(28)	-2-1 2 1	-1 0 1 1
W1_B1_B1	67.287(21)	-2-1 2 1	-1 0 2 1
W1_B1_W1	84.578(23)	-2 0 1 1	-2 0 2 1
W1_B1_B1	67.287(21)	-2 0 1 1	-1 0 1 1
W1_B1_B1	136.866(28)	-2 0 1 1	-1 0 2 1
W1_B1_B1	136.866(28)	-2 0 2 1	-1 0 1 1
W1_B1_B1	67.287(21)	-2 0 2 1	-1 0 2 1
B1_B1_B1	112.03(10)	-1 0 1 1	-1 0 2 1

B.4 Ausgewählte Bindungswinkel und -längen in WB₄ (Neutronendaten)

Winkel (Angles) in Grad, Abstände (Length) in Å.

Vector	Length	Optr Cell	Neighbor atom coordinates		
W1_W2	3.00154(3)	1 0 0 0	0.00000	0.00000	0.25000
W1_W2	3.00109(3)	1 0 1 0	0.00000	1.00000	0.25000
W1_W2	3.00154(3)	1 1 1 0	1.00000	1.00000	0.25000
W1_B1	2.35199(3)	1 0 1 0	0.33080	1.00000	0.00000
W1_B1	2.35238(3)	2 0 0 0	0.33080	0.33080	0.50000
W1_B1	2.35219(3)	3 0 0 0	0.00000	0.33080	0.00000
W1_B1	2.35219(3)	4 1 1 0	0.66920	1.00000	0.50000
W1_B1	2.35238(3)	5 1 1 0	0.66920	0.66920	0.00000
W1_B1	2.35199(3)	6 0 1 0	0.00000	0.66920	0.50000
W1_B1	2.35219(3)	7 1 1 0	0.66920	1.00000	0.00000
W1_B1	2.35238(3)	8 1 1 0	0.66920	0.66920	0.50000
W1_B1	2.35199(3)	9 0 1 0	0.00000	0.66920	0.00000

B.4 Ausgewählte Bindungswinkel und -längen in WB₄ (Neutronendaten)

W1_B1	2.35199(3)	10 0 1 0	0.33080	1.00000	0.50000
W1_B1	2.35238(3)	11 0 0 0	0.33080	0.33080	0.00000
W1_B1	2.35219(3)	12 0 0 0	0.00000	0.33080	0.50000
W1_B2	2.60303(6)	1 0 0 0	0.33330	0.66670	0.66100
W1_B2	2.60303(6)	-2 0 1 1	0.33340	0.66670	-0.16100

Angle	Degrees	atom 1 loc	atom 3 loc
B1_W1_B1	179.451(0)	1 0 1 0	2 0 0 0
B1_W1_B1	79.653(1)	1 0 1 0	3 0 0 0
B1_W1_B1	100.720(1)	1 0 1 0	4 1 1 0
B1_W1_B1	79.649(1)	1 0 1 0	5 1 1 0
B1_W1_B1	100.002(1)	1 0 1 0	6 0 1 0
B1_W1_B1	43.921(1)	1 0 1 0	7 1 1 0
B1_W1_B1	136.599(1)	1 0 1 0	8 1 1 0
B1_W1_B1	42.887(1)	1 0 1 0	9 0 1 0
B1_W1_B1	84.628(1)	1 0 1 0	10 0 1 0
B1_W1_B1	95.377(1)	1 0 1 0	11 0 0 0
B1_W1_B1	136.610(1)	1 0 1 0	12 0 0 0
B1_W1_B1	99.985(1)	2 0 0 0	3 0 0 0
B1_W1_B1	79.645(1)	2 0 0 0	4 1 1 0
B1_W1_B1	100.703(1)	2 0 0 0	5 1 1 0
B1_W1_B1	79.649(1)	2 0 0 0	6 0 1 0
B1_W1_B1	136.587(1)	2 0 0 0	7 1 1 0
B1_W1_B1	43.915(1)	2 0 0 0	8 1 1 0
B1_W1_B1	136.599(1)	2 0 0 0	9 0 1 0
B1_W1_B1	95.377(1)	2 0 0 0	10 0 1 0
B1_W1_B1	84.611(1)	2 0 0 0	11 0 0 0
B1_W1_B1	42.881(1)	2 0 0 0	12 0 0 0
B1_W1_B1	179.429(0)	3 0 0 0	4 1 1 0
B1_W1_B1	79.645(1)	3 0 0 0	5 1 1 0
B1_W1_B1	100.720(1)	3 0 0 0	6 0 1 0
B1_W1_B1	95.377(1)	3 0 0 0	7 1 1 0
B1_W1_B1	136.587(1)	3 0 0 0	8 1 1 0
B1_W1_B1	43.921(1)	3 0 0 0	9 0 1 0
B1_W1_B1	136.610(1)	3 0 0 0	10 0 1 0
B1_W1_B1	42.881(1)	3 0 0 0	11 0 0 0
B1_W1_B1	84.620(1)	3 0 0 0	12 0 0 0
B1_W1_B1	99.985(1)	4 1 1 0	5 1 1 0
B1_W1_B1	79.653(1)	4 1 1 0	6 0 1 0
B1_W1_B1	84.620(1)	4 1 1 0	7 1 1 0
B1_W1_B1	42.881(1)	4 1 1 0	8 1 1 0
B1_W1_B1	136.610(1)	4 1 1 0	9 0 1 0
B1_W1_B1	43.921(1)	4 1 1 0	10 0 1 0
B1_W1_B1	136.587(1)	4 1 1 0	11 0 0 0
B1_W1_B1	95.377(1)	4 1 1 0	12 0 0 0
B1_W1_B1	179.451(0)	5 1 1 0	6 0 1 0
B1_W1_B1	42.881(1)	5 1 1 0	7 1 1 0
B1_W1_B1	84.611(1)	5 1 1 0	8 1 1 0
B1_W1_B1	95.377(1)	5 1 1 0	9 0 1 0
B1_W1_B1	136.599(1)	5 1 1 0	10 0 1 0
B1_W1_B1	43.915(1)	5 1 1 0	11 0 0 0
B1_W1_B1	136.587(1)	5 1 1 0	12 0 0 0
B1_W1_B1	136.610(1)	6 0 1 0	7 1 1 0
B1_W1_B1	95.377(1)	6 0 1 0	8 1 1 0
B1_W1_B1	84.628(1)	6 0 1 0	9 0 1 0
B1_W1_B1	42.887(1)	6 0 1 0	10 0 1 0
B1_W1_B1	136.599(1)	6 0 1 0	11 0 0 0
B1_W1_B1	43.921(1)	6 0 1 0	12 0 0 0
B1_W1_B1	99.985(1)	7 1 1 0	8 1 1 0
B1_W1_B1	79.653(1)	7 1 1 0	9 0 1 0
B1_W1_B1	100.720(1)	7 1 1 0	10 0 1 0
B1_W1_B1	79.645(1)	7 1 1 0	11 0 0 0
B1_W1_B1	179.431(0)	7 1 1 0	12 0 0 0
B1_W1_B1	179.452(0)	8 1 1 0	9 0 1 0
B1_W1_B1	79.649(1)	8 1 1 0	10 0 1 0
B1_W1_B1	100.703(1)	8 1 1 0	11 0 0 0
B1_W1_B1	79.645(1)	8 1 1 0	12 0 0 0
B1_W1_B1	100.002(1)	9 0 1 0	10 0 1 0
B1_W1_B1	79.649(1)	9 0 1 0	11 0 0 0
B1_W1_B1	100.720(1)	9 0 1 0	12 0 0 0
B1_W1_B1	179.452(0)	10 0 1 0	11 0 0 0
B1_W1_B1	79.653(1)	10 0 1 0	12 0 0 0

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Vector	Length	Optr Cell	Neighbor atom coordinates		
B1_W1_B1	99.985(1)	11 0 0 0	12 0 0 0		
W2_W1	3.00154(3)	1 -1 -1 0	-0.66670	-0.33330	0.25000
W2_W1	3.00109(3)	1 0 -1 0	0.33330	-0.33330	0.25000
W2_W1	3.00154(3)	1 0 0 0	0.33330	0.66670	0.25000
W2_W2	3.16671(7)	2 0 0 -1	0.00000	0.00000	-0.25000
W2_W2	3.16671(7)	2 0 0 0	0.00000	0.00000	0.75000
W2_B1	2.33759(3)	1 0 0 0	0.33080	0.00000	0.00000
W2_B1	2.33759(3)	2 0 0 0	0.33080	0.33080	0.50000
W2_B1	2.33759(3)	3 0 0 0	0.00000	0.33080	0.00000
W2_B1	2.33759(3)	4 0 0 0	-0.33080	0.00000	0.50000
W2_B1	2.33759(3)	5 0 0 0	-0.33080	-0.33080	0.00000
W2_B1	2.33759(3)	6 0 0 0	0.00000	-0.33080	0.50000
W2_B1	2.33759(3)	7 0 0 0	-0.33080	0.00000	0.00000
W2_B1	2.33759(3)	8 0 0 0	-0.33080	-0.33080	0.50000
W2_B1	2.33759(3)	9 0 0 0	0.00000	-0.33080	0.00000
W2_B1	2.33759(3)	10 0 0 0	0.33080	0.00000	0.50000
W2_B1	2.33759(3)	11 0 0 0	0.33080	0.33080	0.00000
W2_B1	2.33759(3)	12 0 0 0	0.00000	0.33080	0.50000

Angle	Degrees	atom 1 loc	atom 3 loc
B1_W2_B1	100.847(1)	1 0 0 0	2 0 0 0
B1_W2_B1	79.153(1)	1 0 0 0	3 0 0 0
B1_W2_B1	180.000(0)	1 0 0 0	4 0 0 0
B1_W2_B1	79.153(1)	1 0 0 0	5 0 0 0
B1_W2_B1	100.847(1)	1 0 0 0	6 0 0 0
B1_W2_B1	94.727(1)	1 0 0 0	7 0 0 0
B1_W2_B1	136.836(1)	1 0 0 0	8 0 0 0
B1_W2_B1	43.164(1)	1 0 0 0	9 0 0 0
B1_W2_B1	85.273(1)	1 0 0 0	10 0 0 0
B1_W2_B1	43.164(1)	1 0 0 0	11 0 0 0
B1_W2_B1	136.836(1)	1 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	2 0 0 0	3 0 0 0
B1_W2_B1	79.153(1)	2 0 0 0	4 0 0 0
B1_W2_B1	180.000(0)	2 0 0 0	5 0 0 0
B1_W2_B1	79.153(1)	2 0 0 0	6 0 0 0
B1_W2_B1	136.836(1)	2 0 0 0	7 0 0 0
B1_W2_B1	94.727(1)	2 0 0 0	8 0 0 0
B1_W2_B1	136.836(1)	2 0 0 0	9 0 0 0
B1_W2_B1	43.164(1)	2 0 0 0	10 0 0 0
B1_W2_B1	85.273(1)	2 0 0 0	11 0 0 0
B1_W2_B1	43.164(1)	2 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	3 0 0 0	4 0 0 0
B1_W2_B1	79.153(1)	3 0 0 0	5 0 0 0
B1_W2_B1	180.000(0)	3 0 0 0	6 0 0 0
B1_W2_B1	43.164(1)	3 0 0 0	7 0 0 0
B1_W2_B1	136.836(1)	3 0 0 0	8 0 0 0
B1_W2_B1	94.727(1)	3 0 0 0	9 0 0 0
B1_W2_B1	136.836(1)	3 0 0 0	10 0 0 0
B1_W2_B1	43.164(1)	3 0 0 0	11 0 0 0
B1_W2_B1	85.273(1)	3 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	4 0 0 0	5 0 0 0
B1_W2_B1	79.153(1)	4 0 0 0	6 0 0 0
B1_W2_B1	85.273(1)	4 0 0 0	7 0 0 0
B1_W2_B1	43.164(1)	4 0 0 0	8 0 0 0
B1_W2_B1	136.836(1)	4 0 0 0	9 0 0 0
B1_W2_B1	94.727(1)	4 0 0 0	10 0 0 0
B1_W2_B1	136.836(1)	4 0 0 0	11 0 0 0
B1_W2_B1	43.164(1)	4 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	5 0 0 0	6 0 0 0
B1_W2_B1	43.164(1)	5 0 0 0	7 0 0 0
B1_W2_B1	85.273(1)	5 0 0 0	8 0 0 0
B1_W2_B1	43.164(1)	5 0 0 0	9 0 0 0
B1_W2_B1	136.836(1)	5 0 0 0	10 0 0 0
B1_W2_B1	94.727(1)	5 0 0 0	11 0 0 0
B1_W2_B1	136.836(1)	5 0 0 0	12 0 0 0
B1_W2_B1	136.836(1)	6 0 0 0	7 0 0 0
B1_W2_B1	43.164(1)	6 0 0 0	8 0 0 0
B1_W2_B1	85.273(1)	6 0 0 0	9 0 0 0
B1_W2_B1	43.164(1)	6 0 0 0	10 0 0 0
B1_W2_B1	136.836(1)	6 0 0 0	11 0 0 0

B.5 Ausgewählte Bindungswinkel und -längen in ReB₂ (Neutronendaten)

B1_W2_B1	94.727(1)	6 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	7 0 0 0	8 0 0 0
B1_W2_B1	79.153(1)	7 0 0 0	9 0 0 0
B1_W2_B1	180.000(0)	7 0 0 0	10 0 0 0
B1_W2_B1	79.153(1)	7 0 0 0	11 0 0 0
B1_W2_B1	100.847(1)	7 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	8 0 0 0	9 0 0 0
B1_W2_B1	79.153(1)	8 0 0 0	10 0 0 0
B1_W2_B1	180.000(0)	8 0 0 0	11 0 0 0
B1_W2_B1	79.153(1)	8 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	9 0 0 0	10 0 0 0
B1_W2_B1	79.153(1)	9 0 0 0	11 0 0 0
B1_W2_B1	180.000(0)	9 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	10 0 0 0	11 0 0 0
B1_W2_B1	79.153(1)	10 0 0 0	12 0 0 0
B1_W2_B1	100.847(1)	11 0 0 0	12 0 0 0
Vector	Length	Optr Cell	Neighbor atom coordinates
B1_W1	2.35199(3)	1 0 -1 0	0.33330 -0.33330 0.25000
B1_W1	2.35199(3)	2 1 0 -1	0.66660 0.33330 -0.25000
B1_W2	2.33759(3)	1 0 0 0	0.00000 0.00000 0.25000
B1_W2	2.33759(3)	2 0 0 -1	0.00000 0.00000 -0.25000
B1_B1	1.75919(2)	7 1 0 0	0.66920 0.00000 0.00000
B1_B1	1.71968(2)	9 0 0 0	0.00000 -0.33080 0.00000
B1_B1	1.71968(2)	11 0 0 0	0.33080 0.33080 0.00000
B1_B2	2.01609(2)	2 1 0 -1	0.66660 0.33330 0.16100
B1_B2	2.01631(2)	-2 0 0 1	0.33340 -0.33330 -0.16100
Angle	Degrees	atom 1 loc	atom 3 loc
W1_B1_W1	136.091(1)	1 0 -1 0	2 1 0 -1
W1_B1_W2	79.575(1)	1 0 -1 0	1 0 0 0
W1_B1_W2	136.973(1)	1 0 -1 0	2 0 0 -1
W1_B1_B1	68.046(0)	1 0 -1 0	7 1 0 0
W1_B1_B1	68.557(0)	1 0 -1 0	9 0 0 0
W1_B1_B1	137.684(1)	1 0 -1 0	11 0 0 0
W1_B1_W2	136.973(1)	2 1 0 -1	1 0 0 0
W1_B1_W2	79.575(1)	2 1 0 -1	2 0 0 -1
W1_B1_B1	68.046(0)	2 1 0 -1	7 1 0 0
W1_B1_B1	137.684(1)	2 1 0 -1	9 0 0 0
W1_B1_B1	68.557(0)	2 1 0 -1	11 0 0 0
W2_B1_W2	85.273(1)	1 0 0 0	2 0 0 -1
W2_B1_B1	137.363(1)	1 0 0 0	7 1 0 0
W2_B1_B1	68.418(0)	1 0 0 0	9 0 0 0
W2_B1_B1	68.418(0)	1 0 0 0	11 0 0 0
W2_B1_B1	137.363(1)	2 0 0 -1	7 1 0 0
W2_B1_B1	68.418(0)	2 0 0 -1	9 0 0 0
W2_B1_B1	68.418(0)	2 0 0 -1	11 0 0 0
B1_B1_B1	120.000(0)	7 1 0 0	9 0 0 0
B1_B1_B1	120.000(0)	7 1 0 0	11 0 0 0
B1_B1_B1	120.000(0)	9 0 0 0	11 0 0 0
Vector	Length	Optr Cell	Neighbor atom coordinates
B2_W1	2.60303(6)	1 0 0 0	0.33330 0.66670 0.25000
B2_B1	2.01654(2)	2 0 0 0	0.33080 0.33080 0.50000
B2_B1	2.01631(2)	4 1 1 0	0.66920 1.00000 0.50000
B2_B1	2.01609(2)	6 0 1 0	0.00000 0.66920 0.50000
B2_B1	2.01654(2)	8 1 1 0	0.66920 0.66920 0.50000
B2_B1	2.01609(2)	10 0 1 0	0.33080 1.00000 0.50000
B2_B1	2.01631(2)	12 0 0 0	0.00000 0.33080 0.50000
B2_B2	1.12735(2)	-2 0 1 2	0.33340 0.66670 0.83900

B.5 Ausgewählte Bindungswinkel und -längen in ReB₂ (Neutronendaten)

Winkel (Angles) in Grad, Abstände (Length) in Å.

Vector	Length	Optr Cell	Neighbor atom coordinates		
Re1_Re1	2.90038(2)	1 -1 -1 0	-0.66667	-0.33333	0.25000
Re1_Re1	2.90038(2)	1 -1 0 0	-0.66667	0.66667	0.25000
Re1_Re1	2.90038(2)	1 0 -1 0	0.33333	-0.33333	0.25000
Re1_Re1	2.90038(2)	1 0 1 0	0.33333	1.66667	0.25000
Re1_Re1	2.90038(2)	1 1 0 0	1.33333	0.66667	0.25000
Re1_Re1	2.90038(2)	1 1 1 0	1.33333	1.66667	0.25000
Re1_B1	2.2422(15)	1 0 0 0	0.33333	0.66667	0.54989
Re1_B1	2.2456(10)	2 0 0 -1	-0.33334	0.33333	0.04989
Re1_B1	2.2456(10)	2 1 0 -1	0.66666	0.33333	0.04989
Re1_B1	2.2456(10)	2 1 1 -1	0.66666	1.33333	0.04989
Re1_B1	2.2456(10)	-1 0 1 1	-0.33333	0.33333	0.45011
Re1_B1	2.2456(10)	-1 1 1 1	0.66667	0.33333	0.45011
Re1_B1	2.2456(10)	-1 1 2 1	0.66667	1.33333	0.45011
Re1_B1	2.2422(15)	-2 0 1 1	0.33334	0.66667	-0.04989
Re1_B2	2.50959(2)	1 0 0 0	0.00000	0.00000	0.00000
Re1_B2	2.50957(2)	1 0 1 0	0.00000	1.00000	0.00000
Re1_B2	2.50959(2)	1 1 1 0	1.00000	1.00000	0.00000
Re1_B2	2.50959(2)	2 0 0 0	0.00000	0.00000	0.50000
Re1_B2	2.50957(2)	2 0 1 0	0.00000	1.00000	0.50000
Re1_B2	2.50959(2)	2 1 1 0	1.00000	1.00000	0.50000

Angle	Degrees	atom 1 loc	atom 3 loc
B1_Re1_B1	131.781(28)	1 0 0 0	2 0 0 -1
B1_Re1_B1	131.781(28)	1 0 0 0	2 1 0 -1
B1_Re1_B1	131.782(28)	1 0 0 0	2 1 1 -1
B1_Re1_B1	48.218(28)	1 0 0 0	-1 0 1 1
B1_Re1_B1	48.219(28)	1 0 0 0	-1 1 1 1
B1_Re1_B1	48.218(28)	1 0 0 0	-1 1 2 1
B1_Re1_B1	180.000(0)	1 0 0 0	-2 0 1 1
B1_Re1_B1	80.45(4)	2 0 0 -1	2 1 0 -1
B1_Re1_B1	80.45(4)	2 0 0 -1	2 1 1 -1
B1_Re1_B1	83.56(6)	2 0 0 -1	-1 0 1 1
B1_Re1_B1	136.217(20)	2 0 0 -1	-1 1 1 1
B1_Re1_B1	136.218(20)	2 0 0 -1	-1 1 2 1
B1_Re1_B1	48.220(28)	2 0 0 -1	-2 0 1 1
B1_Re1_B1	80.45(4)	2 1 0 -1	2 1 1 -1
B1_Re1_B1	136.216(20)	2 1 0 -1	-1 0 1 1
B1_Re1_B1	83.56(6)	2 1 0 -1	-1 1 1 1
B1_Re1_B1	136.217(20)	2 1 0 -1	-1 1 2 1
B1_Re1_B1	48.218(28)	2 1 0 -1	-2 0 1 1
B1_Re1_B1	136.218(20)	2 1 1 -1	-1 0 1 1
B1_Re1_B1	136.217(20)	2 1 1 -1	-1 1 1 1
B1_Re1_B1	83.56(6)	2 1 1 -1	-1 1 2 1
B1_Re1_B1	48.218(28)	2 1 1 -1	-2 0 1 1
B1_Re1_B1	80.45(4)	-1 0 1 1	-1 1 1 1
B1_Re1_B1	80.45(4)	-1 0 1 1	-1 1 2 1
B1_Re1_B1	131.782(28)	-1 0 1 1	-2 0 1 1
B1_Re1_B1	80.45(4)	-1 1 1 1	-1 1 2 1
B1_Re1_B1	131.780(28)	-1 1 1 1	-2 0 1 1
B1_Re1_B1	131.782(28)	-1 1 2 1	-2 0 1 1

Vector	Length	Optr Cell	Neighbor atom coordinates		
B1_Re1	2.2422(15)	1 0 0 0	0.33333	0.66667	0.25000
B1_Re1	2.2456(10)	2 0 0 0	-0.33334	0.33333	0.75000
B1_Re1	2.2456(10)	2 1 0 0	0.66666	0.33333	0.75000
B1_Re1	2.2456(10)	2 1 1 0	0.66666	1.33333	0.75000
B1_B1	1.8332(12)	-1 0 1 1	-0.33333	0.33333	0.45011
B1_B1	1.8332(12)	-1 1 1 1	0.66667	0.33333	0.45011
B1_B1	1.8332(12)	-1 1 2 1	0.66667	1.33333	0.45011
B1_B2	1.71558(32)	2 0 0 0	0.00000	0.00000	0.50000
B1_B2	1.71556(32)	2 0 1 0	0.00000	1.00000	0.50000
B1_B2	1.71558(32)	2 1 1 0	1.00000	1.00000	0.50000

Angle	Degrees	atom 1 loc	atom 3 loc
Re1_B1_Re1	131.781(28)	1 0 0 0	2 0 0 0
Re1_B1_Re1	131.781(28)	1 0 0 0	2 1 0 0
Re1_B1_Re1	131.782(28)	1 0 0 0	2 1 1 0
Re1_B1_B1	65.99(9)	1 0 0 0	-1 0 1 1
Re1_B1_B1	65.99(9)	1 0 0 0	-1 1 1 1
Re1_B1_B1	65.99(9)	1 0 0 0	-1 1 2 1
Re1_B1_B2	77.44(5)	1 0 0 0	2 0 0 0

B.5 Ausgewählte Bindungswinkel und -längen in ReB₂ (Neutronendaten)

Re1_B1_B2	77.44(5)	1 0 0 0	2 0 1 0
Re1_B1_B2	77.44(5)	1 0 0 0	2 1 1 0
Re1_B1_Re1	80.45(4)	2 0 0 0	2 1 0 0
Re1_B1_Re1	80.45(4)	2 0 0 0	2 1 1 0
Re1_B1_B1	65.79(6)	2 0 0 0	-1 0 1 1
Re1_B1_B1	127.71(5)	2 0 0 0	-1 1 1 1
Re1_B1_B1	127.71(5)	2 0 0 0	-1 1 2 1
Re1_B1_B2	77.346(22)	2 0 0 0	2 0 0 0
Re1_B1_B2	77.346(22)	2 0 0 0	2 0 1 0
Re1_B1_B2	150.78(8)	2 0 0 0	2 1 1 0
Re1_B1_Re1	80.45(4)	2 1 0 0	2 1 1 0
Re1_B1_B1	127.71(5)	2 1 0 0	-1 0 1 1
Re1_B1_B1	65.79(6)	2 1 0 0	-1 1 1 1
Re1_B1_B1	127.71(5)	2 1 0 0	-1 1 2 1
Re1_B1_B2	77.345(22)	2 1 0 0	2 0 0 0
Re1_B1_B2	150.78(8)	2 1 0 0	2 0 1 0
Re1_B1_B2	77.346(22)	2 1 0 0	2 1 1 0
Re1_B1_B1	127.71(5)	2 1 1 0	-1 0 1 1
Re1_B1_B1	127.71(5)	2 1 1 0	-1 1 1 1
Re1_B1_B1	65.79(6)	2 1 1 0	-1 1 2 1
Re1_B1_B2	150.78(8)	2 1 1 0	2 0 0 0
Re1_B1_B2	77.346(22)	2 1 1 0	2 0 1 0
Re1_B1_B2	77.346(22)	2 1 1 0	2 1 1 0
B1_B1_B1	104.57(10)	-1 0 1 1	-1 1 1 1
B1_B1_B1	104.57(10)	-1 0 1 1	-1 1 2 1
B1_B1_B2	57.705(17)	-1 0 1 1	2 0 0 0
B1_B1_B2	57.706(17)	-1 0 1 1	2 0 1 0
B1_B1_B2	143.43(13)	-1 0 1 1	2 1 1 0
B1_B1_B1	104.57(10)	-1 1 1 1	-1 1 2 1
B1_B1_B2	57.705(17)	-1 1 1 1	2 0 0 0
B1_B1_B2	143.43(13)	-1 1 1 1	2 0 1 0
B1_B1_B2	57.705(17)	-1 1 1 1	2 1 1 0
B1_B1_B2	143.43(13)	-1 1 2 1	2 0 0 0
B1_B1_B2	57.706(17)	-1 1 2 1	2 0 1 0
B1_B1_B2	57.705(17)	-1 1 2 1	2 1 1 0
B2_B1_B2	115.411(34)	2 0 0 0	2 0 1 0
B2_B1_B2	115.409(34)	2 0 0 0	2 1 1 0
B2_B1_B2	115.411(34)	2 0 1 0	2 1 1 0
Vector	Length	Optr Cell	Neighbor atom coordinates
B2_Re1	2.50959(2)	1-1-1 0	-0.66667 -0.33333 0.25000
B2_Re1	2.50957(2)	1 0-1 0	0.33333 -0.33333 0.25000
B2_Re1	2.50959(2)	1 0 0 0	0.33333 0.66667 0.25000
B2_Re1	2.50959(2)	2 0-1-1	-0.33334 -0.66667 -0.25000
B2_Re1	2.50959(2)	2 0 0-1	-0.33334 0.33333 -0.25000
B2_Re1	2.50957(2)	2 1 0-1	0.66666 0.33333 -0.25000
B2_B1	1.71558(32)	2 0-1-1	-0.33334 -0.66667 0.04989
B2_B1	1.71558(32)	2 0 0-1	-0.33334 0.33333 0.04989
B2_B1	1.71556(32)	2 1 0-1	0.66666 0.33333 0.04989
B2_B1	1.71556(32)	-2-1 0 1	-0.66666 -0.33333 -0.04989
B2_B1	1.71558(32)	-2 0 0 1	0.33334 -0.33333 -0.04989
B2_B1	1.71558(32)	-2 0 1 1	0.33334 0.66667 -0.04989
Angle	Degrees	atom 1 loc	atom 3 loc
B1_B2_B1	115.409(34)	2 0-1-1	2 0 0-1
B1_B2_B1	115.411(34)	2 0-1-1	2 1 0-1
B1_B2_B1	64.589(34)	2 0-1-1	-2-1 0 1
B1_B2_B1	64.591(34)	2 0-1-1	-2 0 0 1
B1_B2_B1	179.966(0)	2 0-1-1	-2 0 1 1
B1_B2_B1	115.411(34)	2 0 0-1	2 1 0-1
B1_B2_B1	64.589(34)	2 0 0-1	-2-1 0 1
B1_B2_B1	179.972(0)	2 0 0-1	-2 0 0 1
B1_B2_B1	64.591(34)	2 0 0-1	-2 0 1 1
B1_B2_B1	179.972(0)	2 1 0-1	-2-1 0 1
B1_B2_B1	64.589(34)	2 1 0-1	-2 0 0 1
B1_B2_B1	64.589(34)	2 1 0-1	-2 0 1 1
B1_B2_B1	115.411(34)	-2-1 0 1	-2 0 0 1
B1_B2_B1	115.411(34)	-2-1 0 1	-2 0 1 1
B1_B2_B1	115.409(34)	-2 0 0 1	-2 0 1 1

C Aluminiumboride und -boridcarbide

C.1 Ausgewählte Bindungswinkel und -längen in $Al_{12.47}B_{176}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 -	Distance	Angles							
B10	1.7200 (0.0056)								
B04	1.7376 (0.0055)	111.99 (0.30)							
B05	1.7605 (0.0058)	115.85 (0.31)	60.61 (0.23)						
B07_#4	1.8239 (0.0055)	119.07 (0.31)	61.59 (0.22)	110.51 (0.28)					
B06	1.8399 (0.0056)	127.76 (0.31)	109.27 (0.28)	61.52 (0.22)	108.05 (0.27)				
B03_#10	1.8547 (0.0057)	130.06 (0.31)	107.56 (0.27)	109.55 (0.27)	58.05 (0.21)	60.34 (0.21)			
Al1A_#22	2.2784 (0.0043)	70.87 (0.21)	173.91 (0.28)	113.37 (0.24)	122.28 (0.24)	65.50 (0.18)	72.99 (0.19)		
Al3_#5	2.4212 (0.0081)	68.19 (0.27)	118.43 (0.30)	65.37 (0.25)	172.56 (0.32)	64.64 (0.25)	116.62 (0.29)	57.04 (0.20)	
	B01 -	B10	B04	B05	B07_#4	B06	B03_#10	Al1A_#22	
B02 -	Distance	Angles							
B05_#5	1.7013 (0.0056)								
B06_#10	1.8075 (0.0056)	119.12 (0.30)							
B12	1.8153 (0.0058)	125.88 (0.30)	110.56 (0.28)						
B03_#7	1.8186 (0.0054)	128.44 (0.30)	61.60 (0.23)	60.74 (0.22)					
B11_#5	1.8350 (0.0061)	115.30 (0.29)	59.74 (0.21)	107.07 (0.27)	107.60 (0.27)				
B10	1.8539 (0.0058)	119.21 (0.30)	107.57 (0.27)	58.87 (0.22)	106.65 (0.27)	58.89 (0.22)			
Al3	2.3029 (0.0083)	69.15 (0.25)	112.32 (0.29)	73.49 (0.27)	65.35 (0.25)	171.91 (0.30)	125.85 (0.31)		
	B02 -	B05_#5	B06_#10	B12	B03_#7	B11_#5	B10		
B03 -	Distance	Angles							
B14	1.7515 (0.0057)								
B07_#14	1.7850 (0.0056)	116.17 (0.29)							
B02_#6	1.8186 (0.0054)	130.48 (0.30)	108.81 (0.28)						
B12_#6	1.8373 (0.0059)	128.36 (0.30)	61.46 (0.22)	59.54 (0.22)					
B01_#3	1.8547 (0.0057)	113.75 (0.29)	60.11 (0.22)	105.72 (0.27)	107.53 (0.26)				
B06_#3	1.8568 (0.0056)	119.59 (0.29)	108.99 (0.29)	58.90 (0.21)	107.43 (0.26)	59.43 (0.21)			
Al3_#6	2.2622 (0.0084)	69.56 (0.27)	126.26 (0.32)	67.70 (0.26)	74.15 (0.26)	171.57 (0.32)	112.14 (0.28)		
Al2_#20	2.3578 (0.0046)	67.01 (0.20)	70.17 (0.20)	113.05 (0.24)	64.56 (0.18)	124.24 (0.23)	171.57 (0.26)	64.09 (0.23)	
Al1A_#20	2.4816 (0.0043)	65.26 (0.20)	114.06 (0.23)	113.81 (0.22)	166.36 (0.25)	61.39 (0.17)	60.72 (0.17)	115.58 (0.26)	
	B03 -	B14	B07_#14	B02_#6	B12_#6	B01_#3	B06_#3	Al3_#6	
B04 -	Distance	Angles							
B04_#5	1.6261 (0.0075)								
B01	1.7376 (0.0055)	124.99 (0.31)							
B09	1.7612 (0.0057)	112.47 (0.18)	111.29 (0.26)						
B05	1.7652 (0.0057)	125.40 (0.28)	60.34 (0.23)	112.75 (0.29)					
B08	1.7820 (0.0060)	119.52 (0.37)	109.27 (0.27)	62.82 (0.23)	60.74 (0.22)				
B07_#4	1.8249 (0.0056)	118.03 (0.37)	61.53 (0.22)	60.04 (0.22)	110.26 (0.28)	109.52 (0.27)			
	B04 -	B04_#5	B01	B09	B05	B08			
B05 -	Distance	Angles							
B02_#5	1.7014 (0.0056)								
B01	1.7605 (0.0058)	120.82 (0.31)							
B04	1.7652 (0.0057)	114.09 (0.29)	59.05 (0.23)						
B11_#18	1.7835 (0.0058)	126.91 (0.33)	108.53 (0.29)	106.92 (0.29)					
B08	1.7933 (0.0056)	116.87 (0.30)	107.73 (0.29)	60.10 (0.24)	58.94 (0.22)				
B06	1.8427 (0.0057)	129.52 (0.31)	61.36 (0.22)	107.94 (0.28)	60.02 (0.23)	107.58 (0.28)			
Al3_#5	2.3256 (0.0082)	67.72 (0.26)	71.15 (0.26)	122.10 (0.32)	115.77 (0.31)	174.26 (0.33)	66.83 (0.26)		
	B05 -	B02_#5	B01	B04	B11_#18	B08	B06		
B06 -	Distance	Angles							
B02_#3	1.8075 (0.0056)								

C Aluminiumboride und -boridcarbide

B11_\$18	1.8143 (0.0058)	60.88 (0.23)							
B01	1.8399 (0.0056)	106.81 (0.28)	103.86 (0.27)						
B05	1.8427 (0.0057)	107.20 (0.27)	58.37 (0.21)	57.12 (0.21)					
B03_\$10	1.8569 (0.0056)	59.49 (0.21)	106.86 (0.27)	60.23 (0.21)	105.96 (0.27)				
B13_\$23	1.8865 (0.0057)	114.86 (0.28)	119.28 (0.29)	130.29 (0.29)	127.53 (0.28)	121.64 (0.27)			
Al1A_\$22	2.2582 (0.0043)	125.52 (0.23)	169.23 (0.26)	66.65 (0.18)	110.97 (0.23)	73.45 (0.18)	67.52 (0.18)		
Al3_\$5	2.3305 (0.0082)	173.74 (0.31)	114.24 (0.28)	69.85 (0.25)	66.55 (0.25)	120.92 (0.29)	70.64 (0.25)	58.62 (0.21)	
	B06 -	B02_\$3	B11_\$18	B01	B05	B03_\$10	B13_\$23	Al1A_\$22	
B07 - Distance Angles									
B16	1.7228 (0.0059)								
B03_\$8	1.7850 (0.0056)	121.41 (0.31)							
B09_\$4	1.7951 (0.0057)	121.06 (0.31)	110.40 (0.29)						
B01_\$4	1.8239 (0.0055)	121.59 (0.31)	61.84 (0.23)	105.90 (0.28)					
B04_\$4	1.8249 (0.0056)	122.61 (0.30)	106.83 (0.29)	58.22 (0.22)	56.87 (0.22)				
B12_\$19	1.8516 (0.0058)	123.30 (0.30)	60.66 (0.22)	61.47 (0.23)	108.24 (0.28)	105.93 (0.28)			
Al2	2.3804 (0.0047)	65.67 (0.21)	110.22 (0.24)	71.92 (0.20)	170.92 (0.28)	125.44 (0.24)	62.83 (0.19)		
Al2_\$15	2.4268 (0.0050)	68.47 (0.20)	66.06 (0.19)	114.49 (0.24)	122.10 (0.24)	168.43 (0.27)	62.82 (0.18)	53.53 (0.14)	
	B07 -	B16	B03_\$8	B09_\$4	B01_\$4	B04_\$4	B12_\$19	Al2	
B08 - Distance Angles									
B17	1.7448 (0.0057)								
B11_\$18	1.7598 (0.0056)	120.89 (0.33)							
B10_\$3	1.7625 (0.0056)	115.79 (0.31)	61.98 (0.24)						
B04	1.7820 (0.0060)	125.76 (0.29)	107.22 (0.28)	107.66 (0.30)					
B05	1.7933 (0.0056)	126.04 (0.30)	60.25 (0.23)	109.97 (0.29)	59.17 (0.23)				
B09	1.8467 (0.0061)	118.18 (0.29)	110.66 (0.28)	61.93 (0.23)	58.04 (0.22)	107.54 (0.29)			
Al1A_\$20	2.3147 (0.0044)	59.98 (0.18)	124.25 (0.25)	69.31 (0.19)	112.08 (0.23)	170.95 (0.30)	63.88 (0.18)		
	B08 -	B17	B11_\$18	B10_\$3	B04	B05	B09		
B09 - Distance Angles									
B04	1.7612 (0.0057)								
B07_\$4	1.7951 (0.0057)	61.74 (0.23)							
B08	1.8467 (0.0061)	59.14 (0.23)	107.97 (0.28)						
B10_\$3	1.8585 (0.0059)	104.44 (0.29)	106.45 (0.28)	56.81 (0.21)					
B12_\$3	1.8643 (0.0057)	108.06 (0.27)	60.76 (0.22)	104.29 (0.27)	57.95 (0.21)				
B23_\$25	1.8820 (0.0055)	105.38 (0.27)	114.33 (0.26)	117.75 (0.25)	137.34 (0.28)	135.60 (0.30)			
Al3_\$18	2.2359 (0.0087)	174.89 (0.33)	121.00 (0.30)	115.88 (0.30)	70.85 (0.26)	71.38 (0.27)	77.71 (0.28)		
Al1A_\$20	2.2372 (0.0045)	116.60 (0.24)	175.64 (0.28)	68.28 (0.19)	69.75 (0.19)	117.40 (0.24)	69.87 (0.15)	60.32 (0.22)	
Al2_\$4	2.4974 (0.0047)	122.26 (0.24)	64.97 (0.19)	164.36 (0.25)	110.40 (0.23)	60.09 (0.18)	77.59 (0.17)	62.13 (0.22)	
	B09 -	B04	B07_\$4	B08	B10_\$3	B12_\$3	B23_\$25	Al3_\$18	
B10 - Distance Angles									
B01	1.7200 (0.0056)								
B08_\$10	1.7625 (0.0056)	116.55 (0.31)							
B12	1.8035 (0.0056)	125.76 (0.32)	110.50 (0.29)						
B11_\$5	1.8136 (0.0060)	117.89 (0.30)	58.93 (0.23)	108.51 (0.29)					
B02	1.8539 (0.0058)	124.00 (0.31)	107.64 (0.29)	59.50 (0.22)	60.03 (0.23)				
B09_\$10	1.8584 (0.0059)	122.71 (0.31)	61.26 (0.24)	61.19 (0.22)	107.77 (0.29)	107.69 (0.28)			
Al1A_\$22	2.3625 (0.0045)	65.67 (0.20)	66.43 (0.19)	114.14 (0.24)	119.11 (0.25)	170.10 (0.26)	62.68 (0.17)		
Al3_\$5	2.3930 (0.0088)	69.95 (0.27)	112.15 (0.30)	68.48 (0.26)	169.66 (0.32)	122.50 (0.29)	61.96 (0.25)	56.40 (0.20)	
	B10 -	B01	B08_\$10	B12	B11_\$5	B02	B09_\$10	Al1A_\$22	
B11 - Distance Angles									
B20	1.6701 (0.0060)								
B08_\$11	1.7597 (0.0056)	116.05 (0.32)							
B05_\$11	1.7835 (0.0058)	117.53 (0.34)	60.81 (0.22)						
B10_\$5	1.8136 (0.0060)	121.78 (0.32)	59.08 (0.23)	108.11 (0.29)					
B06_\$11	1.8143 (0.0058)	123.32 (0.32)	110.34 (0.30)	61.61 (0.23)	109.04 (0.30)				
B02_\$5	1.8350 (0.0061)	126.79 (0.30)	108.60 (0.30)	108.57 (0.29)	61.07 (0.23)	59.38 (0.22)			
	B11 -	B20	B08_\$11	B05_\$11	B10_\$5	B06_\$11			
B12 - Distance Angles									
B10	1.8035 (0.0056)								
B12_\$5	1.8150 (0.0078)	117.76 (0.25)							
B02	1.8153 (0.0058)	61.63 (0.23)	113.33 (0.26)						
B03_\$7	1.8373 (0.0059)	108.00 (0.28)	121.21 (0.34)	59.72 (0.21)					
B07_\$13	1.8516 (0.0058)	106.39 (0.27)	130.66 (0.19)	106.09 (0.27)	57.88 (0.22)				
B09_\$10	1.8643 (0.0057)	60.86 (0.22)	128.19 (0.37)	109.09 (0.27)	105.16 (0.27)	57.77 (0.21)			
Al2_\$13	2.2516 (0.0047)	124.54 (0.25)	67.33 (0.17)	173.19 (0.28)	113.85 (0.24)	70.14 (0.20)	74.04 (0.20)		
Al2_\$9	2.2832 (0.0047)	176.60 (0.28)	65.50 (0.15)	116.64 (0.24)	68.83 (0.19)	71.01 (0.20)	118.29 (0.24)	57.03 (0.16)	
Al3_\$5	2.4111 (0.0087)	67.42 (0.26)	70.76 (0.30)	123.42 (0.30)	166.62 (0.30)	110.41 (0.28)	61.50 (0.25)	63.37 (0.21)	

C.1 Ausgewählte Bindungswinkel und -längen in $Al_{12.47}B_{176}$

A13	2.4946 (0.0082)	118.30 (0.29)	65.86 (0.28)	62.26 (0.25)	60.73 (0.24)	111.79 (0.28)	165.56 (0.31)	113.33 (0.24)
	B12 -	B10	B12_5\$	B02	B03_57	B07_13	B09_10	A12_13
B13 -	Distance	Angles						
B18_1	1.7876 (0.0059)							
B22_4	1.8376 (0.0059)	61.74 (0.23)						
B15_16	1.8432 (0.0059)	57.23 (0.23)	107.41 (0.29)					
B20_27	1.8537 (0.0060)	102.76 (0.28)	104.88 (0.28)	58.45 (0.22)				
B06_12	1.8865 (0.0057)	122.39 (0.29)	130.26 (0.29)	114.06 (0.27)	119.54 (0.29)			
B21_27	1.9164 (0.0060)	106.13 (0.27)	58.89 (0.21)	105.74 (0.26)	58.21 (0.21)	128.46 (0.28)		
A11A_37	2.3240 (0.0043)	107.74 (0.24)	68.16 (0.19)	162.19 (0.27)	138.99 (0.26)	63.88 (0.18)	86.98 (0.21)	
A13_48	2.4648 (0.0085)	66.66 (0.26)	79.85 (0.25)	106.74 (0.28)	165.13 (0.31)	63.13 (0.24)	133.34 (0.28)	55.88 (0.20)
A11_37	2.5213 (0.0063)	112.89 (0.25)	55.44 (0.20)	160.39 (0.28)	113.29 (0.25)	85.55 (0.22)	58.59 (0.21)	28.39 (0.13)
	B13 -	B18_1	B22_4	B15_16	B20_27	B06_12	B21_27	A11A_37
B14 -	Distance	Angles						
B03	1.7515 (0.0057)							
B18_5	1.7604 (0.0056)	124.87 (0.32)						
B21	1.8266 (0.0061)	124.22 (0.29)	108.83 (0.29)					
B22_5	1.8346 (0.0057)	133.83 (0.32)	61.14 (0.23)	60.58 (0.23)				
B17	1.8737 (0.0057)	115.10 (0.28)	104.96 (0.28)	57.01 (0.23)	104.37 (0.29)			
A11_20	2.2865 (0.0063)	96.74 (0.26)	73.69 (0.24)	112.77 (0.28)	125.10 (0.27)	57.88 (0.23)		
A12_20	2.3239 (0.0048)	69.06 (0.20)	117.70 (0.25)	73.98 (0.21)	69.77 (0.20)	123.05 (0.26)	165.10 (0.24)	
A13_6	2.3277 (0.0084)	65.60 (0.27)	70.49 (0.27)	128.72 (0.31)	78.02 (0.27)	173.28 (0.33)	115.55 (0.30)	63.64 (0.22)
A11A_20	2.3639 (0.0044)	72.45 (0.20)	101.93 (0.24)	112.56 (0.25)	153.25 (0.27)	57.67 (0.19)	29.94 (0.14)	135.70 (0.19)
	B14 -	B03	B18_5	B21	B22_5	B17	A11_20	A12_20
B15 -	Distance	Angles						
B21_37	1.7197 (0.0056)							
B18_31	1.7395 (0.0057)	124.36 (0.31)						
B20_36	1.8051 (0.0061)	121.57 (0.31)	106.76 (0.28)					
B16_25	1.8275 (0.0059)	120.28 (0.30)	106.87 (0.28)	59.10 (0.23)				
B13_25	1.8432 (0.0059)	121.66 (0.31)	59.78 (0.23)	61.06 (0.24)	109.00 (0.28)			
B19_25	1.8581 (0.0044)	124.40 (0.33)	60.18 (0.25)	103.61 (0.24)	57.23 (0.20)	107.26 (0.30)		
A11_24	2.3527 (0.0064)	64.38 (0.23)	72.25 (0.23)	170.40 (0.30)	111.70 (0.29)	123.75 (0.25)	67.40 (0.19)	
A12_47	2.5080 (0.0050)	70.69 (0.21)	108.51 (0.25)	120.21 (0.24)	65.23 (0.20)	165.94 (0.26)	58.69 (0.21)	52.82 (0.16)
	B15 -	B21_37	B18_31	B20_36	B16_25	B13_25	B19_25	A11_24
B16 -	Distance	Angles						
B07	1.7228 (0.0059)							
B19	1.7652 (0.0046)	127.18 (0.34)						
B20_27	1.7917 (0.0062)	117.15 (0.31)	108.08 (0.31)					
B17_27	1.8022 (0.0056)	119.77 (0.30)	106.42 (0.28)	57.96 (0.24)				
B15_16	1.8274 (0.0059)	120.33 (0.30)	62.26 (0.21)	59.82 (0.24)	106.79 (0.31)			
A11_43	2.1526 (0.0062)	105.93 (0.29)	73.78 (0.19)	117.10 (0.28)	61.52 (0.22)	129.12 (0.28)		
A12	2.2925 (0.0051)	71.11 (0.21)	64.60 (0.22)	171.74 (0.29)	119.11 (0.25)	116.77 (0.26)	58.24 (0.18)	
A12_15	2.4061 (0.0050)	69.76 (0.20)	61.86 (0.21)	126.30 (0.26)	167.95 (0.27)	71.17 (0.21)	110.02 (0.23)	54.81 (0.15)
	B16 -	B07	B19	B20_27	B17_27	B15_16	A11_43	A12
B17 -	Distance	Angles						
B20	1.7413 (0.0058)							
B08	1.7448 (0.0057)	115.52 (0.28)						
B21	1.7664 (0.0058)	63.06 (0.24)	122.80 (0.31)					
B16_24	1.8021 (0.0056)	60.72 (0.23)	113.84 (0.30)	112.11 (0.29)				
B14	1.8737 (0.0057)	109.93 (0.29)	128.20 (0.30)	60.15 (0.24)	109.15 (0.27)			
A11_20	2.0451 (0.0063)	125.58 (0.30)	99.72 (0.27)	128.47 (0.28)	67.71 (0.25)	71.24 (0.24)		
A11A_20	2.0884 (0.0045)	158.56 (0.29)	73.68 (0.21)	130.13 (0.26)	97.98 (0.25)	73.03 (0.20)	33.83 (0.16)	
	B17 -	B20	B08	B21	B16_24	B14	A11_20	
B18 -	Distance	Angles						
B15_29	1.7395 (0.0057)							
B14_5	1.7604 (0.0056)	124.70 (0.31)						
B13_22	1.7876 (0.0059)	62.99 (0.24)	134.22 (0.32)					
B19_22	1.8065 (0.0064)	63.16 (0.22)	109.74 (0.27)	112.04 (0.26)				
B22	1.8294 (0.0059)	170.14 (0.34)	61.43 (0.24)	119.52 (0.31)	108.17 (0.28)			
B22_33	1.8606 (0.0057)	110.94 (0.29)	122.53 (0.31)	60.45 (0.22)	106.83 (0.25)	65.87 (0.30)		
B18_33	1.8868 (0.0084)	110.14 (0.26)	108.90 (0.36)	108.30 (0.34)	58.52 (0.17)	60.06 (0.22)	58.44 (0.20)	
A13_49	2.4041 (0.0088)	113.12 (0.30)	65.87 (0.26)	70.28 (0.26)	171.96 (0.30)	76.09 (0.28)	81.09 (0.27)	128.77 (0.21)
A11_42	2.4628 (0.0061)	65.48 (0.22)	63.00 (0.22)	120.66 (0.27)	65.42 (0.19)	116.39 (0.27)	172.20 (0.28)	115.48 (0.22)
	B18 -	B15_29	B14_5	B13_22	B19_22	B22	B22_33	B18_33
B19 -	Distance	Angles						

C Aluminiumboride und -boridcarbide

B16	1.7652 (0.0046)								
B16_\$15	1.7653 (0.0046)	137.10 (0.45)							
B18_\$1	1.8065 (0.0063)	106.68 (0.23)	109.68 (0.23)						
B18_\$4	1.8065 (0.0063)	109.68 (0.23)	106.68 (0.23)	62.96 (0.34)					
B15_\$16	1.8580 (0.0044)	60.51 (0.19)	126.29 (0.21)	56.66 (0.20)	108.50 (0.32)				
B15_\$17	1.8581 (0.0044)	126.29 (0.21)	60.51 (0.19)	108.50 (0.32)	56.66 (0.20)	164.34 (0.44)			
A12_\$15	2.2134 (0.0056)	73.45 (0.22)	69.32 (0.22)	119.37 (0.15)	175.74 (0.18)	75.48 (0.18)	119.23 (0.25)		
A12	2.2135 (0.0056)	69.32 (0.22)	73.45 (0.22)	175.74 (0.18)	119.37 (0.15)	119.23 (0.25)	75.48 (0.18)	58.56 (0.19)	
A11_\$41	2.3722 (0.0049)	113.28 (0.20)	60.61 (0.18)	70.75 (0.18)	123.51 (0.27)	66.29 (0.17)	115.95 (0.17)	56.26 (0.15)	
A11_\$43	2.3722 (0.0049)	60.61 (0.18)	113.28 (0.20)	123.51 (0.27)	70.75 (0.18)	115.95 (0.17)	66.29 (0.17)	109.14 (0.24)	
	B19 -	B16	B16_\$15	B18_\$1	B18_\$4	B15_\$16	B15_\$17	A12_\$15	
B20 -	Distance	Angles							
B11	1.6701 (0.0060)								
B17	1.7413 (0.0058)	118.45 (0.31)							
B16_\$24	1.7917 (0.0062)	121.72 (0.33)	61.32 (0.24)						
B15_\$28	1.8050 (0.0061)	123.23 (0.30)	110.48 (0.30)	61.07 (0.24)					
B21	1.8346 (0.0058)	117.78 (0.32)	59.13 (0.22)	109.44 (0.29)	110.89 (0.29)				
B13_\$24	1.8537 (0.0060)	120.69 (0.32)	110.17 (0.29)	110.12 (0.30)	60.49 (0.22)	62.61 (0.23)			
	B20 -	B11	B17	B16_\$24	B15_\$28	B21			
B21 -	Distance	Angles							
B15_\$21	1.7198 (0.0056)								
B17	1.7664 (0.0058)	114.39 (0.29)							
B14	1.8266 (0.0061)	116.72 (0.30)	62.84 (0.23)						
B20	1.8346 (0.0058)	122.34 (0.31)	57.80 (0.23)	107.95 (0.30)					
B22_\$5	1.8466 (0.0057)	127.68 (0.33)	108.34 (0.28)	59.92 (0.22)	105.28 (0.28)				
B13_\$24	1.9164 (0.0060)	129.58 (0.29)	106.32 (0.28)	107.53 (0.27)	59.19 (0.22)	58.42 (0.21)			
A11_\$40	2.2346 (0.0066)	71.68 (0.24)	168.21 (0.29)	105.54 (0.26)	128.73 (0.28)	61.59 (0.21)	74.36 (0.22)		
A12_\$20	2.5287 (0.0049)	69.39 (0.21)	117.66 (0.24)	62.05 (0.19)	168.14 (0.27)	64.73 (0.19)	115.97 (0.23)	53.68 (0.17)	
	B21 -	B15_\$21	B17	B14	B20	B22_\$5	B13_\$24	A11_\$40	
B22 -	Distance	Angles							
B23_\$22	1.8035 (0.0062)								
B18	1.8294 (0.0059)	105.15 (0.28)							
B14_\$5	1.8345 (0.0057)	127.01 (0.28)	57.43 (0.23)						
B13_\$4	1.8376 (0.0059)	122.22 (0.26)	108.65 (0.30)	110.63 (0.29)					
B21_\$5	1.8467 (0.0057)	144.86 (0.29)	105.05 (0.28)	59.50 (0.22)	62.69 (0.24)				
B18_\$33	1.8605 (0.0057)	103.88 (0.25)	61.50 (0.29)	106.89 (0.29)	57.81 (0.22)	106.05 (0.29)			
B22_\$33	2.0064 (0.0081)	56.20 (0.16)	57.81 (0.22)	111.45 (0.31)	108.69 (0.30)	158.93 (0.19)	56.32 (0.20)		
A11_\$45	2.1160 (0.0060)	78.41 (0.21)	166.85 (0.32)	110.15 (0.27)	78.90 (0.26)	68.27 (0.23)	130.56 (0.29)	131.05 (0.21)	
A11A_\$45	2.3664 (0.0044)	67.95 (0.15)	162.50 (0.27)	139.81 (0.25)	65.73 (0.19)	87.35 (0.21)	103.58 (0.22)	107.08 (0.22)	
A12_\$42	2.4121 (0.0047)	81.33 (0.18)	110.83 (0.25)	64.69 (0.19)	125.25 (0.25)	71.45 (0.20)	171.46 (0.26)	124.07 (0.25)	
	B22 -	B23_\$22	B18	B14_\$5	B13_\$4	B21_\$5	B18_\$33	B22_\$33	
B23 -	Distance	Angles							
B22_\$4	1.8034 (0.0062)								
B22_\$1	1.8034 (0.0062)	67.60 (0.33)							
B09_\$16	1.8820 (0.0055)	116.24 (0.19)	125.28 (0.19)						
B09_\$17	1.8820 (0.0055)	125.28 (0.19)	116.24 (0.19)	104.30 (0.38)					
A11A_\$37	2.3766 (0.0016)	67.35 (0.15)	114.20 (0.25)	116.71 (0.20)	62.10 (0.14)				
A11A_\$44	2.3766 (0.0016)	114.20 (0.25)	67.35 (0.15)	62.11 (0.14)	116.72 (0.20)	178.29 (0.30)			
A11_\$44	2.4892 (0.0045)	121.05 (0.29)	56.38 (0.17)	85.22 (0.19)	96.39 (0.19)	151.56 (0.13)	28.52 (0.13)		
A11_\$37	2.4892 (0.0045)	56.38 (0.17)	121.05 (0.29)	96.39 (0.19)	85.22 (0.19)	28.52 (0.13)	151.56 (0.13)	177.39 (0.36)	
A13_\$2	2.5981 (0.0076)	71.39 (0.24)	76.76 (0.24)	57.23 (0.21)	161.10 (0.34)	127.22 (0.19)	53.49 (0.16)	79.16 (0.20)	
	B23 -	B22_\$4	B22_\$1	B09_\$16	B09_\$17	A11A_\$37	A11A_\$44	A11_\$44	
A11 -	Distance	Angles							
A11A	1.2034 (0.0054)								
B17_\$9	2.0451 (0.0063)	75.06 (0.28)							
B22_\$39	2.1160 (0.0060)	86.33 (0.27)	149.81 (0.29)						
B16_\$30	2.1526 (0.0062)	119.76 (0.35)	50.77 (0.19)	126.91 (0.29)					
A12_\$30	2.1665 (0.0056)	143.65 (0.34)	114.30 (0.26)	68.55 (0.19)	64.12 (0.19)				
B21_\$38	2.2347 (0.0065)	113.71 (0.33)	159.95 (0.28)	50.14 (0.18)	126.24 (0.28)	70.12 (0.19)			
B14_\$9	2.2865 (0.0063)	78.59 (0.27)	50.89 (0.19)	148.11 (0.30)	84.82 (0.22)	135.66 (0.25)	111.46 (0.25)		
B15_\$27	2.3528 (0.0064)	141.93 (0.37)	117.94 (0.25)	91.37 (0.23)	91.59 (0.23)	67.27 (0.19)	43.94 (0.16)	83.85 (0.21)	
B19_\$35	2.3723 (0.0049)	153.03 (0.34)	80.23 (0.20)	120.64 (0.27)	45.60 (0.15)	58.16 (0.19)	86.75 (0.19)	77.52 (0.22)	
B18_\$32	2.4629 (0.0061)	119.20 (0.32)	78.93 (0.21)	131.25 (0.26)	78.18 (0.21)	97.14 (0.22)	81.12 (0.20)	43.32 (0.16)	
B23_\$21	2.4892 (0.0045)	70.54 (0.22)	105.28 (0.26)	45.21 (0.19)	97.52 (0.24)	73.13 (0.16)	94.74 (0.23)	145.69 (0.27)	
B13_\$21	2.5213 (0.0063)	66.66 (0.25)	137.59 (0.29)	45.66 (0.17)	171.47 (0.28)	107.36 (0.22)	47.05 (0.17)	102.46 (0.23)	
	A11 -	A11A	B17_\$9	B22_\$39	B16_\$30	A12_\$30	B21_\$38	B14_\$9	

C.2 Ausgewählte Bindungswinkel und -längen in $Al_{10.72}B_{192}C_8$

Al1A -	Distance	Angles							
Al1	1.2034 (0.0054)								
B17_\$9	2.0885 (0.0045)	71.11 (0.26)							
B09_\$9	2.2372 (0.0045)	117.71 (0.28)	90.81 (0.17)						
Al3_\$46	2.2473 (0.0075)	137.94 (0.32)	144.67 (0.23)	59.81 (0.23)					
B06_\$1	2.2582 (0.0043)	118.94 (0.27)	129.32 (0.17)	118.20 (0.16)	62.30 (0.22)				
B01_\$1	2.2784 (0.0043)	151.21 (0.27)	97.81 (0.17)	88.15 (0.16)	64.68 (0.21)	47.85 (0.15)			
B08_\$9	2.3148 (0.0044)	106.95 (0.27)	46.34 (0.15)	47.83 (0.16)	98.87 (0.22)	128.16 (0.17)	80.31 (0.15)		
B13_\$21	2.3241 (0.0043)	84.95 (0.27)	149.80 (0.17)	117.12 (0.17)	65.23 (0.22)	48.60 (0.15)	94.55 (0.16)	163.83 (0.17)	
B10_\$1	2.3625 (0.0045)	151.21 (0.28)	83.51 (0.16)	47.56 (0.15)	62.49 (0.22)	87.52 (0.15)	43.46 (0.14)	44.26 (0.14)	
B14_\$9	2.3639 (0.0044)	71.47 (0.25)	49.30 (0.15)	135.96 (0.17)	143.09 (0.23)	84.84 (0.15)	81.16 (0.15)	88.18 (0.16)	
B22_\$39	2.3664 (0.0044)	63.17 (0.25)	128.69 (0.17)	90.60 (0.15)	74.77 (0.22)	93.85 (0.16)	133.50 (0.16)	129.41 (0.17)	
B23_\$21	2.3767 (0.0016)	80.94 (0.23)	107.90 (0.19)	48.03 (0.15)	68.31 (0.20)	122.53 (0.18)	127.78 (0.12)	85.74 (0.18)	
Al1A -	Al1	B17_\$9	B09_\$9	Al3_\$46	B06_\$1	B01_\$1	B08_\$9		

Al2 -	Distance	Angles							
Al2_\$15	2.1652 (0.0048)								
Al1_\$43	2.1665 (0.0056)	119.28 (0.15)							
B19	2.2135 (0.0056)	60.72 (0.10)	65.58 (0.15)						
B12_\$19	2.2517 (0.0047)	62.22 (0.13)	129.56 (0.20)	117.33 (0.17)					
B12_\$20	2.2832 (0.0047)	60.75 (0.13)	176.65 (0.21)	116.01 (0.16)	47.18 (0.20)				
B16	2.2925 (0.0051)	65.26 (0.14)	57.65 (0.16)	46.09 (0.12)	87.63 (0.17)	120.98 (0.17)			
B14_\$9	2.3239 (0.0048)	140.19 (0.20)	92.41 (0.19)	122.93 (0.16)	116.90 (0.18)	89.05 (0.17)	149.96 (0.18)		
B03_\$9	2.3579 (0.0046)	98.69 (0.16)	135.42 (0.20)	124.49 (0.15)	87.28 (0.16)	46.61 (0.15)	163.65 (0.18)	43.93 (0.15)	
B07	2.3804 (0.0047)	64.33 (0.15)	85.99 (0.18)	85.61 (0.13)	47.02 (0.15)	91.17 (0.17)	43.22 (0.15)	147.67 (0.18)	
B16_\$15	2.4062 (0.0050)	59.92 (0.14)	98.66 (0.19)	44.69 (0.11)	117.47 (0.18)	84.23 (0.16)	88.71 (0.20)	94.13 (0.16)	
B22_\$32	2.4121 (0.0047)	173.74 (0.18)	54.74 (0.17)	114.94 (0.16)	119.29 (0.18)	125.10 (0.17)	108.50 (0.17)	45.53 (0.14)	
B07_\$15	2.4269 (0.0050)	62.14 (0.15)	137.12 (0.20)	84.50 (0.14)	90.75 (0.16)	46.17 (0.15)	120.80 (0.18)	78.35 (0.16)	
Al2 -	Al2_\$15	Al1_\$43	B19	B12_\$19	B12_\$20	B16	B14_\$9		

Al3 -	Distance	Angles							
B09_\$11	2.2358 (0.0087)								
Al1A_\$46	2.2473 (0.0075)	59.87 (0.22)							
B03_\$7	2.2622 (0.0083)	121.36 (0.36)	175.10 (0.39)						
B02	2.3029 (0.0083)	126.63 (0.37)	136.96 (0.35)	46.94 (0.21)					
B05_\$5	2.3256 (0.0082)	124.52 (0.36)	95.57 (0.29)	87.40 (0.30)	43.13 (0.19)				
B14_\$7	2.3277 (0.0084)	113.53 (0.34)	130.33 (0.35)	44.84 (0.19)	88.87 (0.29)	119.20 (0.35)			
B06_\$5	2.3305 (0.0082)	115.27 (0.34)	59.08 (0.21)	121.37 (0.36)	87.57 (0.29)	46.62 (0.20)	120.97 (0.35)		
B10_\$5	2.3929 (0.0087)	47.19 (0.21)	61.12 (0.21)	123.50 (0.35)	92.16 (0.29)	77.35 (0.27)	153.86 (0.38)	85.17 (0.27)	
B18_\$34	2.4042 (0.0087)	115.34 (0.34)	91.58 (0.28)	83.64 (0.28)	113.84 (0.33)	114.08 (0.34)	43.64 (0.19)	85.68 (0.28)	
B12_\$5	2.4111 (0.0087)	47.12 (0.21)	97.72 (0.30)	85.77 (0.29)	80.06 (0.27)	96.90 (0.31)	110.73 (0.32)	126.44 (0.34)	
B01_\$5	2.4212 (0.0081)	84.73 (0.29)	58.28 (0.21)	125.96 (0.35)	79.13 (0.26)	43.48 (0.19)	161.73 (0.39)	45.51 (0.19)	
Al2_\$9	2.4527 (0.0075)	64.18 (0.22)	119.50 (0.32)	59.85 (0.21)	94.60 (0.29)	135.75 (0.35)	58.10 (0.21)	177.59 (0.37)	
Al3 -	B09_\$11	Al1A_\$46	B03_\$7	B02	B05_\$5	B14_\$7	B06_\$5		

C.2 Ausgewählte Bindungswinkel und -längen in $Al_{10.72}B_{192}C_8$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

B01 -	Distance	Angles					
C1_\$20	1.6306 (0.0095)						
B07	1.7778 (0.0069)	118.39 (0.35)					
B02_\$5	1.8100 (0.0077)	122.74 (0.38)	110.34 (0.39)				
B04	1.8292 (0.0070)	120.78 (0.36)	111.40 (0.40)	59.67 (0.27)			
B12_\$18	1.8393 (0.0089)	123.63 (0.46)	61.61 (0.28)	104.62 (0.35)	58.45 (0.27)		
B08_\$5	1.8508 (0.0080)	122.49 (0.37)	59.66 (0.29)	61.30 (0.34)	109.05 (0.38)	105.49 (0.36)	
Al1B_\$5	2.3416 (0.0097)	70.88 (0.34)	114.81 (0.33)	62.41 (0.29)	114.66 (0.32)	165.41 (0.46)	63.22 (0.30)
B01 -	C1_\$20	B07	B02_\$5	B04	B12_\$18	B08_\$5	

B02 -	Distance	Angles							
B14	1.7209 (0.0074)								
B01_\$1	1.8100 (0.0077)	128.14 (0.37)							
B04_\$1	1.8107 (0.0074)	117.80 (0.36)	60.69 (0.28)						
B06_\$11	1.8285 (0.0072)	111.70 (0.39)	111.72 (0.37)	64.60 (0.25)					
B10_\$11	1.8326 (0.0075)	118.18 (0.38)	106.96 (0.34)	111.89 (0.35)	60.97 (0.30)				
B08	1.8666 (0.0084)	128.32 (0.32)	60.43 (0.26)	109.17 (0.29)	106.81 (0.32)	56.22 (0.24)			
Al1B	2.1984 (0.0097)	70.99 (0.29)	70.74 (0.28)	122.63 (0.34)	170.78 (0.39)	109.86 (0.33)	66.19 (0.23)		
Al1A	2.2851 (0.0058)	65.50 (0.24)	82.90 (0.26)	136.29 (0.31)	158.73 (0.35)	100.76 (0.30)	66.03 (0.19)	13.71 (0.12)	

C Aluminiumboride und -boridcarbide

	B02 -	B14	B01_\$1	B04_\$1	B06_\$11	B10_\$11	B08	A11B
B03 -	Distance	Angles						
B19	1.7198 (0.0085)							
B09_\$14	1.7454 (0.0086)	129.84 (0.41)						
B05_\$14	1.8030 (0.0082)	119.71 (0.42)	59.11 (0.31)					
B12_\$17	1.8234 (0.0083)	117.61 (0.44)	105.86 (0.39)	111.18 (0.40)				
B11	1.8491 (0.0099)	131.03 (0.37)	58.57 (0.31)	104.94 (0.31)	55.54 (0.27)			
B07_\$10	1.8656 (0.0072)	110.13 (0.41)	112.54 (0.40)	66.68 (0.27)	60.30 (0.30)	104.97 (0.32)		
A11B	2.1332 (0.0104)	74.26 (0.33)	69.34 (0.31)	121.35 (0.35)	107.96 (0.37)	65.56 (0.26)	168.26 (0.39)	
A11A	2.3027 (0.0068)	66.80 (0.28)	82.00 (0.30)	134.43 (0.34)	101.03 (0.34)	67.88 (0.22)	158.25 (0.37)	13.34 (0.11)
	B03 -	B19	B09_\$14	B05_\$14	B12_\$17	B11	B07_\$10	A11B
B04 -	Distance	Angles						
B24	1.7656 (0.0073)							
B11_\$8	1.7792 (0.0073)	136.95 (0.41)						
B12_\$18	1.7912 (0.0070)	111.43 (0.36)	57.28 (0.33)					
B02_\$5	1.8107 (0.0074)	119.29 (0.34)	103.29 (0.35)	106.60 (0.35)				
B01	1.8292 (0.0070)	101.72 (0.34)	105.13 (0.41)	61.06 (0.32)	59.64 (0.30)			
B06_\$12	1.9447 (0.0036)	142.24 (0.49)	57.68 (0.29)	104.37 (0.40)	58.15 (0.24)	105.84 (0.43)		
	B04 -	B24	B11_\$8	B12_\$18	B02_\$5	B01		
B05 -	Distance	Angles						
B10	1.6792 (0.0063)							
B09	1.7511 (0.0072)	66.08 (0.33)						
B08_\$4	1.7776 (0.0073)	60.49 (0.30)	110.78 (0.39)					
B03_\$7	1.8030 (0.0081)	111.42 (0.37)	58.80 (0.34)	105.09 (0.37)				
B16	1.8861 (0.0077)	117.84 (0.39)	106.44 (0.37)	135.72 (0.39)	114.39 (0.35)			
B07_\$9	2.0171 (0.0036)	106.31 (0.37)	105.51 (0.41)	56.42 (0.26)	58.14 (0.25)	132.96 (0.40)		
A12B	2.0356 (0.0058)	152.57 (0.59)	139.04 (0.52)	94.35 (0.61)	84.21 (0.33)	71.37 (0.42)	61.85 (0.39)	
A12A	2.1073 (0.0053)	144.48 (0.36)	144.55 (0.38)	86.05 (0.33)	87.22 (0.29)	76.95 (0.28)	57.18 (0.24)	8.35 (0.45)
	B05 -	B10	B09	B08_\$4	B03_\$7	B16	B07_\$9	A12B
B06 -	Distance	Angles						
B17	1.7536 (0.0083)							
B11_\$7	1.8022 (0.0089)	119.01 (0.39)						
B09	1.8112 (0.0076)	101.37 (0.39)	58.32 (0.34)					
B02_\$4	1.8285 (0.0072)	138.51 (0.44)	101.67 (0.36)	106.94 (0.42)				
B10	1.8573 (0.0073)	112.52 (0.41)	105.02 (0.38)	61.33 (0.33)	59.63 (0.30)			
B04_\$9	1.9447 (0.0036)	141.22 (0.51)	56.54 (0.26)	104.66 (0.45)	57.25 (0.26)	105.09 (0.41)		
	B06 -	B17	B11_\$7	B09	B02_\$4	B10		
B07 -	Distance	Angles						
B01	1.7778 (0.0069)							
B08_\$5	1.8061 (0.0076)	62.18 (0.32)						
B23_\$16	1.8294 (0.0075)	104.55 (0.34)	121.70 (0.35)					
B12_\$18	1.8532 (0.0068)	60.83 (0.32)	106.76 (0.36)	113.95 (0.36)				
B03_\$8	1.8656 (0.0072)	106.92 (0.38)	101.44 (0.34)	134.91 (0.38)	58.72 (0.30)			
A12A_\$12	1.9752 (0.0052)	149.06 (0.37)	89.37 (0.28)	79.23 (0.28)	146.27 (0.36)	89.54 (0.34)		
B05_\$12	2.0171 (0.0036)	104.12 (0.40)	55.08 (0.25)	142.35 (0.41)	101.16 (0.36)	55.17 (0.26)	63.71 (0.25)	
A12B_\$12	2.0827 (0.0093)	153.69 (0.42)	91.92 (0.30)	84.49 (0.40)	138.20 (0.54)	81.38 (0.55)	8.22 (0.39)	59.51 (0.32)
	B07 -	B01	B08_\$5	B23_\$16	B12_\$18	B03_\$8	A12A_\$12	B05_\$12
B08 -	Distance	Angles						
B10_\$11	1.7431 (0.0077)							
B05_\$11	1.7775 (0.0073)	56.96 (0.29)						
B13	1.7889 (0.0077)	120.18 (0.40)	114.40 (0.39)					
B07_\$1	1.8061 (0.0076)	113.30 (0.39)	68.50 (0.27)	115.24 (0.38)				
B01_\$1	1.8509 (0.0080)	109.05 (0.36)	111.33 (0.37)	125.36 (0.37)	58.16 (0.27)			
B02	1.8666 (0.0084)	60.91 (0.27)	106.01 (0.32)	129.60 (0.33)	106.62 (0.29)	58.27 (0.26)		
A11B	2.2368 (0.0103)	111.73 (0.36)	168.56 (0.39)	71.75 (0.28)	118.63 (0.34)	69.16 (0.28)	64.05 (0.21)	
A11A	2.2892 (0.0063)	103.51 (0.33)	158.62 (0.36)	65.58 (0.25)	132.10 (0.32)	81.92 (0.27)	65.80 (0.19)	13.70 (0.11)
	B08 -	B10_\$11	B05_\$11	B13	B07_\$1	B01_\$1	B02	A11B
B09 -	Distance	Angles						
C1_\$6	1.6929 (0.0099)							
B03_\$7	1.7453 (0.0086)	121.96 (0.38)						
B05	1.7511 (0.0072)	116.00 (0.37)	62.08 (0.33)					
B11_\$7	1.7607 (0.0089)	127.46 (0.40)	63.66 (0.41)	111.14 (0.43)				
B06	1.8112 (0.0076)	120.63 (0.38)	112.80 (0.44)	108.21 (0.43)	60.58 (0.33)			
B10	1.8713 (0.0087)	119.04 (0.46)	105.39 (0.37)	55.11 (0.26)	106.13 (0.37)	60.55 (0.29)		
A11B_\$7	2.2292 (0.0103)	73.10 (0.35)	63.56 (0.32)	118.85 (0.35)	64.63 (0.33)	116.96 (0.36)	167.59 (0.47)	

C.2 Ausgewählte Bindungswinkel und -längen in Al_{10.72}B₁₉₂C₈

	B09 -	C1_\$6	B03_\$7	B05	B11_\$7	B06	B10	
B10 -	Distance	Angles						
B12	1.6730 (0.0040)							
B05	1.6792 (0.0063)	119.99 (0.28)						
B08_\$4	1.7432 (0.0077)	113.80 (0.29)	62.55 (0.29)					
B02_\$4	1.8326 (0.0075)	117.26 (0.28)	111.90 (0.40)	62.87 (0.36)				
B06	1.8573 (0.0073)	124.21 (0.27)	109.28 (0.44)	110.93 (0.41)	59.41 (0.27)			
B09	1.8713 (0.0087)	131.31 (0.32)	58.80 (0.28)	106.88 (0.40)	104.30 (0.37)	58.12 (0.28)		
	B10 -	B12	B05	B08_\$4	B02_\$4	B06		
B11 -	Distance	Angles						
B12_\$17	1.7112 (0.0083)							
B09_\$14	1.7606 (0.0089)	110.22 (0.42)						
B15	1.7777 (0.0087)	117.72 (0.46)	124.73 (0.40)					
B04_\$10	1.7792 (0.0073)	61.71 (0.33)	114.32 (0.42)	111.63 (0.43)				
B06_\$14	1.8021 (0.0089)	114.36 (0.42)	61.09 (0.33)	116.30 (0.42)	65.78 (0.28)			
B03	1.8491 (0.0099)	61.47 (0.31)	57.77 (0.29)	127.22 (0.36)	111.25 (0.35)	108.46 (0.34)		
A11B	2.1693 (0.0108)	110.83 (0.40)	68.20 (0.30)	70.30 (0.31)	172.49 (0.43)	120.40 (0.36)	63.54 (0.24)	
A11A	2.3485 (0.0068)	102.87 (0.38)	80.35 (0.29)	64.07 (0.27)	161.07 (0.40)	133.12 (0.35)	65.28 (0.21)	13.02 (0.12)
	B11 -	B12_\$17	B09_\$14	B15	B04_\$10	B06_\$14	B03	A11B
B12 -	Distance	Angles						
B10	1.6730 (0.0040)							
B11_\$6	1.7112 (0.0083)	118.14 (0.33)						
B04_\$2	1.7911 (0.0070)	124.39 (0.28)	61.01 (0.32)					
B03_\$6	1.8234 (0.0083)	114.33 (0.30)	62.99 (0.41)	111.91 (0.43)				
B01_\$2	1.8392 (0.0089)	128.67 (0.33)	107.56 (0.43)	60.49 (0.29)	106.14 (0.41)			
B07_\$2	1.8532 (0.0068)	118.78 (0.28)	111.46 (0.44)	109.70 (0.43)	60.98 (0.28)	57.56 (0.27)		
	B12 -	B10	B11_\$6	B04_\$2	B03_\$6	B01_\$2		
B13 -	Distance	Angles						
B20	1.7671 (0.0065)							
B24_\$3	1.7677 (0.0068)	62.72 (0.28)						
B18_\$26	1.7847 (0.0064)	107.36 (0.32)	114.24 (0.32)					
B08	1.7889 (0.0077)	123.98 (0.37)	115.17 (0.35)	120.25 (0.35)				
B23_\$26	1.8056 (0.0083)	112.15 (0.32)	63.81 (0.29)	62.83 (0.29)	114.74 (0.36)			
B19	1.8926 (0.0035)	59.35 (0.32)	111.97 (0.41)	58.00 (0.33)	125.16 (0.49)	110.07 (0.44)		
A11A	2.2483 (0.0056)	67.52 (0.20)	118.78 (0.30)	112.80 (0.29)	67.99 (0.27)	175.51 (0.32)	65.74 (0.32)	
A11B	2.3869 (0.0074)	78.97 (0.25)	131.62 (0.33)	104.25 (0.31)	62.87 (0.32)	164.51 (0.34)	65.40 (0.36)	12.99 (0.10)
	B13 -	B20	B24_\$3	B18_\$26	B08	B23_\$26	B19	A11A
B14 -	Distance	Angles						
B02	1.7209 (0.0074)							
B21	1.7750 (0.0067)	119.38 (0.36)						
B23_\$25	1.7911 (0.0070)	118.02 (0.37)	113.35 (0.34)					
B24_\$16	1.8049 (0.0085)	114.73 (0.37)	64.00 (0.30)	63.37 (0.30)				
B22	1.8570 (0.0064)	125.68 (0.38)	105.81 (0.32)	61.35 (0.26)	111.15 (0.32)			
B15	1.8719 (0.0034)	126.76 (0.51)	57.89 (0.34)	107.50 (0.43)	109.29 (0.47)	56.64 (0.31)		
A11A	2.2186 (0.0060)	69.60 (0.27)	112.19 (0.30)	117.21 (0.30)	175.11 (0.33)	66.34 (0.20)	65.82 (0.34)	
A11B	2.3086 (0.0075)	64.20 (0.33)	103.23 (0.33)	130.73 (0.34)	165.48 (0.35)	78.07 (0.25)	65.62 (0.38)	13.57 (0.10)
	B14 -	B02	B21	B23_\$25	B24_\$16	B22	B15	A11A
B15 -	Distance	Angles						
B21	1.7671 (0.0072)							
B22	1.7689 (0.0067)	110.05 (0.36)						
B11	1.7777 (0.0086)	117.74 (0.41)	124.54 (0.42)					
B16_\$17	1.7776 (0.0078)	113.21 (0.38)	59.42 (0.29)	118.74 (0.41)				
B17_\$24	1.7862 (0.0094)	59.99 (0.32)	114.69 (0.39)	112.67 (0.41)	67.52 (0.35)			
B14	1.8719 (0.0034)	58.30 (0.34)	61.26 (0.33)	125.64 (0.53)	108.88 (0.44)	108.45 (0.48)		
A11A	2.2415 (0.0067)	111.48 (0.32)	67.07 (0.23)	70.43 (0.30)	118.61 (0.33)	171.47 (0.37)	64.55 (0.34)	
A11B	2.2949 (0.0078)	104.03 (0.33)	80.14 (0.29)	62.87 (0.36)	131.85 (0.36)	160.52 (0.39)	66.39 (0.38)	13.66 (0.11)
	B15 -	B21	B22	B11	B16_\$17	B17_\$24	B14	A11A
B16 -	Distance	Angles						
B22_\$6	1.7577 (0.0073)							
B18_\$22	1.7685 (0.0085)	61.91 (0.25)						
B19_\$28	1.7752 (0.0093)	109.70 (0.36)	60.50 (0.27)					
B15_\$6	1.7777 (0.0078)	60.04 (0.27)	107.40 (0.37)	104.67 (0.38)				
B05	1.8861 (0.0077)	95.48 (0.34)	113.10 (0.35)	142.43 (0.41)	112.08 (0.37)			
B17_\$25	1.9804 (0.0098)	106.24 (0.32)	106.78 (0.33)	59.05 (0.31)	56.45 (0.32)	139.97 (0.36)		
A12B	2.2908 (0.0127)	133.28 (0.40)	92.45 (0.46)	85.26 (0.33)	160.14 (0.52)	57.35 (0.26)	118.87 (0.36)	

C Aluminiumboride und -boridcarbide

A12A	2.4906 (0.0076)	136.99 (0.32)	98.11 (0.30)	87.63 (0.29)	154.49 (0.38)	55.51 (0.22)	116.25 (0.31)	5.69 (0.32)
	B16 -	B22_§6	B18_§22	B19_§28	B15_§6	B05	B17_§25	A12B
B17 -	Distance	Angles						
B06	1.7536 (0.0083)							
B21_§22	1.7764 (0.0085)	113.51 (0.37)						
B15_§22	1.7862 (0.0094)	140.24 (0.43)	59.47 (0.27)					
B20_§6	1.7964 (0.0078)	103.13 (0.37)	61.18 (0.25)	104.92 (0.34)				
B19_§6	1.8594 (0.0078)	117.51 (0.40)	107.24 (0.36)	100.95 (0.37)	59.50 (0.26)			
B16_§21	1.9804 (0.0098)	141.73 (0.38)	103.82 (0.32)	56.04 (0.30)	101.89 (0.31)	54.96 (0.31)		
	B17 -	B06	B21_§22	B15_§22	B20_§6	B19_§6		
B18 -	Distance	Angles						
B18_§27	1.6732 (0.0047)							
B16_§24	1.7686 (0.0085)	122.53 (0.24)						
B13_§19	1.7848 (0.0064)	115.39 (0.24)	110.52 (0.29)					
B19_§19	1.7853 (0.0071)	113.82 (0.26)	59.93 (0.34)	64.03 (0.14)				
B22_§21	1.8137 (0.0033)	131.01 (0.23)	58.75 (0.29)	106.24 (0.29)	106.77 (0.31)			
B23	1.8714 (0.0081)	122.12 (0.22)	110.20 (0.17)	59.13 (0.31)	111.95 (0.29)	60.67 (0.28)		
	B18 -	B18_§27	B16_§24	B13_§19	B19_§19	B22_§21		
B19 -	Distance	Angles						
B03	1.7198 (0.0085)							
B16_§23	1.7752 (0.0093)	118.88 (0.42)						
B18_§26	1.7852 (0.0071)	119.97 (0.40)	59.57 (0.32)					
B20	1.8150 (0.0068)	125.20 (0.42)	109.67 (0.37)	105.28 (0.34)				
B17_§17	1.8594 (0.0078)	121.21 (0.41)	65.98 (0.34)	111.45 (0.35)	58.52 (0.29)			
B13	1.8926 (0.0035)	125.10 (0.52)	105.47 (0.46)	57.97 (0.32)	56.88 (0.32)	104.95 (0.41)		
A11A	2.2671 (0.0064)	68.99 (0.30)	170.14 (0.36)	111.93 (0.32)	66.40 (0.22)	116.16 (0.33)	64.70 (0.31)	
A11B	2.3490 (0.0075)	60.94 (0.36)	164.00 (0.39)	105.74 (0.33)	79.15 (0.28)	129.04 (0.35)	67.50 (0.37)	13.34 (0.11)
	B19 -	B03	B16_§23	B18_§26	B20	B17_§17	B13	A11A
B20 -	Distance	Angles						
C1	1.7144 (0.0031)							
B13	1.7671 (0.0065)	120.03 (0.35)						
B17_§17	1.7965 (0.0078)	119.37 (0.48)	113.24 (0.28)					
B19	1.8150 (0.0068)	120.17 (0.35)	63.77 (0.14)	61.97 (0.33)				
B21_§25	1.8183 (0.0033)	123.45 (0.19)	106.98 (0.31)	58.87 (0.33)	107.37 (0.34)			
B24_§3	1.8395 (0.0073)	117.73 (0.47)	58.66 (0.30)	113.32 (0.16)	112.29 (0.29)	62.48 (0.31)		
A11A	2.2670 (0.0029)	64.33 (0.12)	66.40 (0.20)	118.99 (0.34)	66.41 (0.22)	172.22 (0.17)	114.69 (0.31)	
	B20 -	C1	B13	B17_§17	B19	B21_§25	B24_§3	
B21 -	Distance	Angles						
B21_§29	1.6869 (0.0048)							
B15	1.7671 (0.0072)	115.68 (0.27)						
B14	1.7750 (0.0067)	113.89 (0.25)	63.81 (0.14)					
B17_§24	1.7765 (0.0085)	121.19 (0.23)	60.54 (0.34)	113.40 (0.29)				
B20_§21	1.8183 (0.0033)	132.64 (0.24)	104.80 (0.31)	105.19 (0.31)	59.95 (0.31)			
B24_§16	1.8972 (0.0080)	122.03 (0.21)	109.81 (0.28)	58.77 (0.31)	111.52 (0.17)	59.31 (0.29)		
	B21 -	B21_§29	B15	B14	B17_§24	B20_§21		
B22 -	Distance	Angles						
C1	1.6909 (0.0031)							
B16_§17	1.7577 (0.0074)	123.93 (0.47)						
B15	1.7689 (0.0067)	122.34 (0.34)	60.54 (0.32)					
B18_§25	1.8138 (0.0033)	125.53 (0.19)	59.34 (0.32)	105.82 (0.32)				
B14	1.8570 (0.0064)	118.36 (0.34)	110.43 (0.27)	62.11 (0.14)	105.16 (0.30)			
B23_§25	1.8619 (0.0069)	117.29 (0.45)	111.13 (0.16)	108.90 (0.29)	61.20 (0.31)	57.58 (0.28)		
A11A	2.2503 (0.0029)	65.03 (0.13)	119.10 (0.31)	66.55 (0.23)	169.01 (0.19)	64.56 (0.21)	112.69 (0.29)	
	B22 -	C1	B16_§17	B15	B18_§25	B14	B23_§25	
B23 -	Distance	Angles						
B14_§21	1.7912 (0.0070)							
B13_§19	1.8056 (0.0083)	102.24 (0.33)						
B07_§16	1.8294 (0.0075)	117.88 (0.35)	139.80 (0.36)					
B22_§21	1.8619 (0.0069)	61.07 (0.24)	103.41 (0.30)	98.24 (0.31)				
B18	1.8714 (0.0081)	105.49 (0.34)	58.04 (0.23)	109.57 (0.32)	58.13 (0.21)			
B24_§33	1.8888 (0.0086)	58.67 (0.30)	57.12 (0.27)	144.34 (0.32)	107.29 (0.28)	105.01 (0.29)		
A12A_§34	2.4284 (0.0069)	159.22 (0.35)	88.27 (0.26)	53.04 (0.20)	134.26 (0.28)	95.29 (0.27)	115.85 (0.28)	
	B23 -	B14_§21	B13_§19	B07_§16	B22_§21	B18	B24_§33	
B24 -	Distance	Angles						

C.2 Ausgewählte Bindungswinkel und -längen in $Al_{10.72}B_{192}C_8$

B04	1.7656 (0.0073)								
B13_\$20	1.7677 (0.0068)	120.51 (0.35)							
B14_\$16	1.8049 (0.0085)	136.22 (0.37)	103.20 (0.32)						
B20_\$20	1.8395 (0.0073)	101.58 (0.32)	58.62 (0.24)	103.12 (0.30)					
B23_\$32	1.8888 (0.0086)	144.42 (0.32)	59.07 (0.29)	57.96 (0.27)	105.33 (0.27)				
B21_\$16	1.8972 (0.0080)	110.03 (0.32)	103.64 (0.33)	57.24 (0.23)	58.21 (0.21)	103.82 (0.28)			
	B24 -	B04	B13_\$20	B14_\$16	B20_\$20	B23_\$32			
C1 - Distance Angles									
B01_\$3	1.6306 (0.0095)								
B22	1.6909 (0.0031)	100.68 (0.41)							
B09_\$17	1.6929 (0.0099)	132.52 (0.23)	97.87 (0.42)						
B20	1.7144 (0.0031)	97.51 (0.42)	140.16 (0.22)	95.35 (0.41)					
A11A	2.1704 (0.0035)	112.68 (0.42)	70.04 (0.12)	114.70 (0.43)	70.28 (0.12)				
A11B_\$20	2.3750 (0.0060)	68.68 (0.34)	110.55 (0.17)	63.90 (0.34)	109.04 (0.16)	178.48 (0.42)			
	C1 -	B01_\$3	B22	B09_\$17	B20	A11A			
A11A - Distance Angles									
A11B	0.5421 (0.0041)								
C1	2.1704 (0.0035)	173.56 (1.16)							
B14	2.2186 (0.0060)	92.71 (0.58)	87.97 (0.18)						
B15	2.2415 (0.0067)	88.78 (0.64)	86.78 (0.20)	49.63 (0.09)					
B13	2.2483 (0.0057)	98.22 (0.62)	86.05 (0.17)	131.70 (0.25)	172.63 (0.20)				
B22	2.2503 (0.0029)	132.49 (0.46)	44.93 (0.09)	49.10 (0.17)	46.38 (0.18)	127.49 (0.19)			
B19	2.2671 (0.0064)	91.96 (0.60)	87.15 (0.19)	174.83 (0.20)	128.31 (0.28)	49.56 (0.09)	125.76 (0.21)		
B20	2.2670 (0.0029)	136.17 (0.43)	45.39 (0.09)	128.95 (0.20)	126.67 (0.21)	46.08 (0.17)	90.27 (0.12)	47.19 (0.18)	
B02	2.2851 (0.0058)	74.01 (1.00)	110.66 (0.26)	44.90 (0.19)	90.42 (0.20)	93.71 (0.21)	89.18 (0.20)	139.04 (0.22)	
B08	2.2892 (0.0063)	77.65 (1.03)	108.74 (0.26)	91.50 (0.21)	138.45 (0.22)	46.43 (0.20)	122.62 (0.24)	91.66 (0.21)	
B03	2.3027 (0.0068)	65.24 (0.98)	110.18 (0.27)	136.82 (0.22)	91.28 (0.23)	89.59 (0.20)	120.20 (0.25)	44.21 (0.21)	
B11	2.3485 (0.0068)	64.32 (1.03)	109.28 (0.28)	90.58 (0.21)	45.50 (0.22)	136.31 (0.22)	86.07 (0.23)	89.44 (0.22)	
	A11A -	A11B	C1	B14	B15	B13	B22	B19	
A11B - Distance Angles									
A11A	0.5421 (0.0041)								
B03	2.1332 (0.0104)	101.42 (1.01)							
B11	2.1693 (0.0108)	102.67 (1.07)	50.90 (0.33)						
B02	2.1984 (0.0097)	92.28 (1.07)	166.03 (0.32)	128.77 (0.18)					
B09_\$14	2.2292 (0.0104)	144.45 (1.31)	47.11 (0.29)	47.17 (0.30)	120.54 (0.31)				
B08	2.2368 (0.0103)	88.65 (1.08)	127.05 (0.18)	168.68 (0.32)	49.77 (0.29)	122.11 (0.32)			
B15	2.2949 (0.0078)	77.56 (0.61)	94.33 (0.38)	46.83 (0.25)	91.26 (0.24)	87.71 (0.33)	138.38 (0.38)		
B14	2.3086 (0.0075)	73.72 (0.59)	142.32 (0.39)	92.90 (0.26)	44.81 (0.22)	118.89 (0.26)	90.53 (0.36)	47.99 (0.11)	
B01_\$1	2.3417 (0.0097)	131.98 (1.32)	119.68 (0.32)	121.86 (0.33)	46.86 (0.26)	83.42 (0.20)	47.62 (0.27)	119.42 (0.25)	
B19	2.3490 (0.0075)	74.71 (0.55)	44.81 (0.24)	91.85 (0.36)	139.35 (0.38)	86.51 (0.32)	90.87 (0.25)	121.79 (0.40)	
C1_\$3	2.3750 (0.0060)	171.52 (1.23)	83.48 (0.33)	85.80 (0.34)	82.59 (0.31)	43.00 (0.28)	82.88 (0.32)	109.18 (0.27)	
B13	2.3869 (0.0074)	68.79 (0.60)	90.20 (0.24)	138.90 (0.37)	92.25 (0.35)	118.66 (0.25)	45.38 (0.22)	146.27 (0.29)	
	A11B -	A11A	B03	B11	B02	B09_\$14	B08	B15	
A12A - Distance Angles									
B07_\$15	1.9752 (0.0052)								
B07_\$9	1.9752 (0.0052)	147.71 (0.48)							
B05_\$13	2.1073 (0.0053)	59.11 (0.10)	132.90 (0.10)						
B05	2.1073 (0.0053)	132.90 (0.10)	59.11 (0.10)	144.96 (0.46)					
B23_\$31	2.4284 (0.0069)	108.53 (0.31)	47.74 (0.21)	95.66 (0.21)	106.58 (0.21)				
B23_\$30	2.4284 (0.0069)	47.74 (0.21)	108.53 (0.31)	106.58 (0.21)	95.66 (0.21)	100.74 (0.36)			
B16_\$13	2.4905 (0.0076)	105.98 (0.23)	95.93 (0.22)	47.54 (0.21)	105.37 (0.31)	88.41 (0.09)	153.68 (0.09)		
B16	2.4906 (0.0076)	95.94 (0.22)	105.98 (0.23)	105.37 (0.31)	47.54 (0.21)	153.68 (0.09)	88.41 (0.09)	94.17 (0.36)	
	A12A -	B07_\$15	B07_\$9	B05_\$13	B05	B23_\$31	B23_\$30	B16_\$13	
A12B - Distance Angles									
B05_\$13	2.0356 (0.0058)								
B05	2.0356 (0.0059)	161.66 (1.10)							
B07_\$15	2.0827 (0.0092)	58.64 (0.13)	130.69 (0.32)						
B07_\$9	2.0827 (0.0092)	130.69 (0.32)	58.64 (0.13)	131.28 (0.99)					
B16_\$13	2.2908 (0.0127)	51.28 (0.30)	115.64 (0.66)	109.76 (0.26)	99.26 (0.24)				
B16	2.2908 (0.0127)	115.64 (0.66)	51.28 (0.30)	99.26 (0.24)	109.76 (0.26)	105.54 (0.81)			
	A12B -	B05_\$13	B05	B07_\$15	B07_\$9	B16_\$13			

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D.1 Ausgewählte Bindungswinkel und -längen in $\text{Si}_{3,22}\text{B}_{27,48}$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

Si1 -	Distance	Angles				
B2_\$7	2.0197 (0.0037)					
B2_\$8	2.0197 (0.0037)	112.15 (0.09)				
B2_\$10	2.0198 (0.0037)	112.15 (0.09)	112.15 (0.09)			
Si1_\$2	2.4220 (0.0028)	106.64 (0.10)	106.64 (0.10)	106.64 (0.10)		
	Si1 -	B2_\$7	B2_\$8	B2_\$10		
B1 -	Distance	Angles				
B1_\$3	1.6965 (0.0041)					
B2_\$9	1.9407 (0.0039)	119.47 (0.21)				
B2_\$5	1.9487 (0.0032)	124.21 (0.13)	57.00 (0.10)			
B2	1.9487 (0.0032)	124.21 (0.13)	57.00 (0.10)	100.27 (0.22)		
B1_\$5	2.1227 (0.0037)	128.19 (0.10)	102.93 (0.10)	57.00 (0.08)	102.88 (0.10)	
B1_\$4	2.1227 (0.0037)	128.19 (0.10)	102.93 (0.10)	102.88 (0.10)	57.00 (0.08)	60.00
	B1 -	B1_\$3	B2_\$9	B2_\$5	B2	B1_\$5
B2 -	Distance	Angles				
B2_\$6	1.8559 (0.0042)					
B2_\$9	1.8559 (0.0042)	107.40 (0.21)				
B1_\$6	1.9407 (0.0039)	61.72 (0.18)	61.72 (0.18)			
B1	1.9487 (0.0032)	113.42 (0.15)	61.28 (0.14)	116.41 (0.17)		
B1_\$4	1.9487 (0.0032)	61.28 (0.14)	113.42 (0.15)	116.41 (0.17)	66.00 (0.16)	
Si1_\$1	2.0197 (0.0037)	123.41 (0.01)	123.41 (0.01)	121.62 (0.18)	111.85 (0.15)	111.85 (0.15)
	B2 -	B2_\$6	B2_\$9	B1_\$6	B1	B1_\$4

D.2 Ausgewählte Bindungswinkel und -längen in $\text{Ca}_x\text{Ba}_{1-x}\text{B}_6$

Winkel (Angles) in Grad, Abstände (Distance) in Å.

Ca1 -	Distance	Angles						
B1_\$26	3.0630 (0.0010)							
B1_\$25	3.0630 (0.0010)	180.00 (0.12)						
B1_\$17	3.0630 (0.0010)	33.31 (0.10)	146.69 (0.10)					
B1_\$16	3.0630 (0.0010)	146.69 (0.10)	33.31 (0.10)	180.00 (0.12)				
B1_\$9	3.0630 (0.0010)	33.31 (0.10)	146.69 (0.10)	33.31 (0.10)	146.69 (0.10)			
B1_\$29	3.0630 (0.0010)	148.13 (0.12)	31.87 (0.12)	117.54 (0.02)	62.46 (0.02)	117.54 (0.02)		
B1_\$22	3.0630 (0.0010)	31.87 (0.12)	148.13 (0.12)	62.46 (0.02)	117.54 (0.02)	62.46 (0.02)	180.00	
B1_\$20	3.0630 (0.0010)	117.54 (0.02)	62.46 (0.02)	148.13 (0.12)	31.87 (0.12)	117.54 (0.02)	84.90 (0.09)	95.10 (0.09)
B1_\$13	3.0630 (0.0010)	62.46 (0.02)	117.54 (0.02)	31.87 (0.12)	148.13 (0.12)	62.46 (0.02)	95.10 (0.09)	84.90 (0.09)
B1_\$12	3.0630 (0.0010)	117.54 (0.02)	62.46 (0.02)	117.54 (0.02)	62.46 (0.02)	148.13 (0.12)	84.90 (0.09)	95.10 (0.09)
B1_\$8	3.0630 (0.0010)	62.46 (0.02)	117.54 (0.02)	62.46 (0.02)	117.54 (0.02)	31.87 (0.12)	95.10 (0.09)	84.90 (0.09)
B1_\$28	3.0630 (0.0010)	85.68 (0.03)	94.32 (0.03)	95.10 (0.09)	84.90 (0.09)	62.46 (0.02)	85.68 (0.03)	94.32 (0.03)
	Ca1 -	B1_\$26	B1_\$25	B1_\$17	B1_\$16	B1_\$9	B1_\$29	B1_\$22
B1 -	Distance	Angles						
B1_\$12	1.6821 (0.0065)							
B1_\$30	1.7558 (0.0046)	135.00						
B1_\$21	1.7558 (0.0046)	135.00 (0.00)	60.00					
B1_\$25	1.7558 (0.0046)	135.00	90.00	60.00				

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B1_\$16	1.7558 (0.0046)	135.00	60.00	90.00	60.00					
Ca1	3.0630 (0.0010)	74.06 (0.06)	132.45 (0.04)	132.45 (0.04)	73.34 (0.05)	73.34 (0.05)				
Ca1_\$6	3.0630 (0.0010)	74.06 (0.06)	73.34 (0.05)	73.34 (0.05)	132.45 (0.04)	132.45 (0.04)	148.12 (0.12)			
Ba1_\$6	3.0630 (0.0010)	74.06 (0.06)	73.34 (0.05)	73.34 (0.05)	132.45 (0.04)	132.45 (0.04)	148.12 (0.12)	0.00		
Ba1_\$4	3.0630 (0.0010)	74.06 (0.06)	132.45 (0.04)	73.34 (0.05)	73.34 (0.05)	132.45 (0.04)	85.68 (0.03)	85.68 (0.03)		
Ba1_\$5	3.0630 (0.0010)	74.06 (0.06)	73.34 (0.05)	132.45 (0.04)	132.45 (0.04)	73.34 (0.05)	85.68 (0.03)	85.68 (0.03)		
Ca1_\$4	3.0630 (0.0010)	74.06 (0.06)	132.45 (0.04)	73.34 (0.05)	73.34 (0.05)	132.45 (0.04)	85.68 (0.03)	85.68 (0.03)		
	B1 -	B1_\$12	B1_\$30	B1_\$21	B1_\$25	B1_\$16	Ca1	Ca1_\$6		

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Eidesstattliche Erklärung

Hiermit versichere ich an Eides Statt, daß ich meine Dissertation selbständig und nur mit den angegebenen Hilfsmittel angefertigt habe.

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Erklärung

Ich erkläre hiermit, noch keinen Promotionsversuch unternommen zu haben.

Lebenslauf

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Schulbildung

- 08/1978–06/1992 Grundschule, Gymnasium (Abschluß Abitur).
- 06/1988–06/1989 North Charleston High School, South Carolina, USA.
- 10/1992–06/2003 Rheinische Friedrich-Wilhelms-Universität Bonn, Studiengang Diplom Chemie.
- 07/2003–03/2004 Anfertigung einer Diplomarbeit an der Universität Hamburg mit dem Thema „Untersuchungen im System Kupfer-Bor“.
- 04/2004–09/2005 Beginn der Promotion zum Doktor der Naturwissenschaften an der Universität Hamburg im Arbeitskreis von Frau Prof. Albert.
- 10/2005–heute Abschluß der Promotion an der Technischen Universität Darmstadt mit dem Thema der Dissertation „Struktur und Charakterisierung von borreichen Boriden und Übergangsmetallboriden“, hierbei Aufbau und Betrieb von Hochtemperatur-Syntheseapparaturen mit Schutzgastechnik und Analytik mittels Diffraktometrie an Einkristallen und Pulvern mit Röntgen-, Synchrotron- und Neutronenstrahlung, Röntgenabsorptionsspektrometrie und Elektronenmikroskopie.
- 03/2006–04/2006 Forschungsaufenthalt an der Université de Rennes, Frankreich, Schwerpunkt Hochtemperaturchemie, Kristallographie und Elektronenmikroskopie an Boriden.

Berufserfahrung

- 01/1994–06/2003 Selbständiger Aufbau, Wartung und Systempflege der EDV-Infrastruktur des Dialysezentrums Bad Godesberg, Bonn.
- 07/1996–09/1996 Praktikum im Analytiklabor des Zentralen Technikum Organisch der Bayer AG in Leverkusen, Aufbau und Betrieb einer Analytikapparatur zur Bestimmung verschiedener organischer Lösemittel in Technikumsabwässern mittels eines Gas-Strip-Verfahrens für die Gaschromatographie.

- 07/1997–09/1997 Werksstudent im Analytiklabor des Zentralen Technikum Organisch der Bayer AG in Leverkusen, eigenverantwortliche Erarbeitung und Validierung von Verfahren für die Reinheitsüberprüfung von Technikumsprodukten sowie die Durchführung von Routineanalysen im laufenden Betrieb mittels Gaschromatographie und Titrationsmethoden.
- 01/2001–07/2002 Geschäftsleitung der Studentenbar im Studentenwohnheim Tannenbusch 2 in Bonn.
- 04/2004–heute Wissenschaftlicher Mitarbeiter an der Universität Hamburg und der Technischen Universität Darmstadt im Arbeitskreis von Frau Prof. Albert, Organisation und Durchführung von Studentenpraktika und Seminaren, Abnahme von Zwischenprüfungen, Aufbau und Betrieb von labortechnischen Anlagen, Verantwortlicher für die EDV-Infrastruktur der Arbeitsgruppe.
- 08/2005 Leitung der Technik bei der internationalen Konferenz „15th International Symposium on Boron, Borides and Related Materials“ in Hamburg.

Berufliche Weiterbildung

- 07/2003–heute Teilnahme an diversen Fortbildungen, Tagungen und Kolloquien mit anorganisch-chemischer, kristallographischer, computertheoretischer und meßapparativer Thematik.
- 04/2004–heute Diverse Meßzeiten an Großforschungseinrichtungen für Synchrotron (Hasylab/DESY, Hamburg) und Neutronenstrahlung (Forschungsneutronenquelle Heinz Maier-Leibnitz, Garching).

EDV

- Betriebssysteme UNIX (Linux), Microsoft Windows (alle Versionen).
- Anwendungen Systemadministration, Shellscrippte, LabVIEW-Programmierung, L^AT_EX, wissenschaftliche Software, allgemeine Standardanwendungen.

Fremdsprachen

Englisch (fließend), Latein.

Interessen

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Motorradfahren

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