Anhang A

Tabellen

A.1 Thioprolin

173 K							
2θ	ω	χ	ϕ	Scan	Δ	Frames	t
-35°	-35°	54.7°	0°	ω	-0.3°	600	10 s
-35°	-35°	54.7°	90°	ω	-0.3°	600	10 s
-35°	-35°	54.7°	180°	ω	-0.3°	600	10 s
-35°	-35°	54.7°	270°	ω	-0.3°	600	10 s
-60°	-60°	54.7°	45°	ω	-0.3°	600	60 s
-60°	-60°	54.7°	135°	ω	-0.3°	600	60 s
-60°	-60°	54.7°	225°	ω	-0.3°	600	60 s
120 K							
-32°	-32°	54.7°	0°	ω	-0.3°	600	15 s
-32°	-32°	54.7°	90°	ω	-0.3°	600	15 s
-32°	-32°	54.7°	180°	ω	-0.3°	600	15 s
-32°	-32°	54.7°	270°	ω	-0.3°	600	15 s
-32°	-32°	54.7°	0°	ϕ	-0.3°	1200	15 s
-90°	-90°	54.7°	20°	ω	-0.3°	600	120 s
-90°	-90°	54.7°	90°	ω	-0.3°	600	120 s
-90°	-90°	54.7°	160°	ω	-0.3°	600	120 s
-90°	-90°	54.7°	230°	ω	-0.3°	600	120 s
-90°	-90°	54.7°	300°	ω	-0.3°	600	120 s

Tabelle A.1: Meßstrategien der Thioprolinmessungen bei 173 K und 120 K.

S(1)–C(1)	1.8010(2)	S(1)–C(4)	1.8105(3)	O(1)–C(3)	1.2442(4)
O(2)–C(3)	1.2585(4)	N(1)–C(1)	1.4956(3)	N(1)–C(2)	1.5002(3)
C(2)–C(3)	1.5432(3)	C(2)–C(4)	1.5233(3)	N(1)–H(3)	1.0330
N(1)–H(4)	1.0331	C(1)–H(1)	1.0940	C(1)–H(2)	1.0941
C(2)–H(5)	1.0940	C(4)–H(6)	1.0939	C(4)–H(7)	1.0940

Tabelle A.2: Thioprolin, Bindungslängen aus der 15 K Messung in [Å].

S(1)–C(1)	1.8027(2)	S(1)–C(4)	1.8176(2)	O(1)–C(3)	1.2489(4)
O(2)–C(3)	1.2598(3)	N(1)–C(1)	1.5021(3)	N(1)–C(2)	1.5034(3)
C(2)–C(3)	1.5450(3)	C(2)–C(4)	1.5279(3)	N(1)–H(3)	1.0328
N(1)–H(4)	1.0330	C(1)–H(1)	1.0942	C(1)–H(2)	1.0937
C(2)–H(5)	1.0938	C(4)–H(6)	1.0938	C(4)–H(7)	1.0940

Tabelle A.3: Thioprolin, Bindungslängen aus der 120 K Messung in [Å].

C(1)–S(1)–C(4)	88.22(1)	C(1)–N(1)–C(2)	111.25(2)	S(1)–C(1)–N(1)	106.24(2)
N(1)–C(2)–C(3)	109.24(2)	N(1)–C(2)–C(4)	107.43(2)	C(3)–C(2)–C(4)	113.15(2)
O(1)–C(3)–O(2)	127.43(3)	O(1)–C(3)–C(2)	117.25(2)	O(2)–C(3)–C(2)	115.28(2)
S(1)–C(4)–C(2)	103.86(2)				
C(1)–N(1)–H(3)	107.99	C(1)–N(1)–H(4)	107.67	C(2)–N(1)–H(3)	109.35
C(2)–N(1)–H(4)	109.28	H(3)–N(1)–H(4)	111.29	S(1)–C(1)–H(1)	108.88
S(1)–C(1)–H(2)	108.42	N(1)–C(1)–H(1)	108.23	N(1)–C(1)–H(2)	110.46
H(1)–C(1)–H(2)	114.30	N(1)–C(2)–H(5)	107.30	C(3)–C(2)–H(5)	107.65
C(4)–C(2)–H(5)	111.91	S(1)–C(4)–H(6)	109.87	S(1)–C(4)–H(7)	110.69
C(2)–C(4)–H(6)	110.02	C(2)–C(4)–H(7)	111.30	H(6)–C(4)–H(7)	110.88

Tabelle A.4: Thioprolin, Bindungswinkel aus der 15 K Messung in [°].

C(1)–S(1)–C(4)	88.26(1)	C(1)–N(1)–C(2)	111.24(2)	S(1)–C(1)–N(1)	106.38(1)
N(1)–C(2)–C(3)	109.09(2)	N(1)–C(2)–C(4)	107.40(2)	C(3)–C(2)–C(4)	113.23(2)
O(1)–C(3)–O(2)	127.33(2)	O(1)–C(3)–C(2)	117.33(2)	O(2)–C(3)–C(2)	115.29(2)
S(1)–C(4)–C(2)	103.85(1)				
C(1)–N(1)–H(3)	109.80	C(1)–N(1)–H(4)	108.09	C(2)–N(1)–H(3)	107.51
C(2)–N(1)–H(4)	109.33	H(3)–N(1)–H(4)	110.90	S(1)–C(1)–H(1)	109.03
S(1)–C(1)–H(2)	111.08	N(1)–C(1)–H(1)	107.46	N(1)–C(1)–H(2)	108.76
H(1)–C(1)–H(2)	113.80	N(1)–C(2)–H(5)	107.89	C(3)–C(2)–H(5)	108.24
C(4)–C(2)–H(5)	110.85	S(1)–C(4)–H(6)	111.62	S(1)–C(4)–H(7)	111.53
C(2)–C(4)–H(6)	110.74	C(2)–C(4)–H(7)	111.79	H(6)–C(4)–H(7)	107.37

Tabelle A.5: Thioprolin, Bindungswinkel aus der 120 K Messung in [°].

C(4) S(1) C(1) N(1)	38.34(2)	C(1) S(1) C(4) C(2)	-44.37(2)	C(2) N(1) C(1) S(1)	-21.71(2)
C(1) N(1) C(2) C(3)	112.12(2)	C(1) N(1) C(2) C(4)	-10.96(2)	N(1) C(2) C(3) O(1)	13.67(3)
N(1) C(2) C(3) O(2)	-168.25(2)	C(4) C(2) C(3) O(1)	133.28(3)	C(4) C(2) C(3) O(2)	-48.64(3)
N(1) C(2) C(4) S(1)	38.45(2)	C(3) C(2) C(4) S(1)	-82.20(2)		
C(4) S(1) C(1) H(1)	-78.02	C(4) S(1) C(1) H(2)	157.07	C(1) S(1) C(4) H(6)	73.29
C(1) S(1) C(4) H(7)	-163.92	C(2) N(1) C(1) H(1)	95.09	C(2) N(1) C(1) H(2)	-139.09
H(3) N(1) C(1) S(1)	-141.71	H(3) N(1) C(1) H(1)	-24.92	H(3) N(1) C(1) H(2)	100.91
H(4) N(1) C(1) S(1)	98.01	H(4) N(1) C(1) H(1)	-145.20	H(4) N(1) C(1) H(2)	-19.37
C(1) N(1) C(2) H(5)	-131.45	H(3) N(1) C(2) C(3)	-128.68	H(3) N(1) C(2) C(4)	108.23
H(3) N(1) C(2) H(5)	-12.26	H(4) N(1) C(2) C(3)	-6.63	H(4) N(1) C(2) C(4)	-129.72
H(4) N(1) C(2) H(5)	109.79	H(5) C(2) C(3) O(1)	-102.54	H(5) C(2) C(3) O(2)	75.55
N(1) C(2) C(4) H(6)	-79.10	N(1) C(2) C(4) H(7)	157.58	C(3) C(2) C(4) H(6)	160.25
C(3) C(2) C(4) H(7)	36.93	H(5) C(2) C(4) S(1)	155.97	H(5) C(2) C(4) H(6)	38.42
H(5) C(2) C(4) H(7)	-84.90				

Tabelle A.6: Thioprolin, Torsionswinkel aus der 15 K Messung in [°].

C(4) S(1) C(1) N(1)	38.05(1)	C(1) S(1) C(4) C(2)	-44.30(1)	C(2) N(1) C(1) S(1)	-21.31(2)
C(1) N(1) C(2) C(3)	111.73(2)	C(1) N(1) C(2) C(4)	-11.36(2)	N(1) C(2) C(3) O(1)	14.14(3)
N(1) C(2) C(3) O(2)	-168.32(2)	C(4) C(2) C(3) O(1)	133.67(2)	C(4) C(2) C(3) O(2)	-48.78(3)
N(1) C(2) C(4) S(1)	38.57(2)	C(3) C(2) C(4) S(1)	-81.92(2)		
C(4) S(1) C(1) H(1)	-77.56	C(4) S(1) C(1) H(2)	156.25	C(1) S(1) C(4) H(6)	75.04
C(1) S(1) C(4) H(7)	-164.84	C(2) N(1) C(1) H(1)	95.35	C(2) N(1) C(1) H(2)	-141.03
H(3) N(1) C(1) S(1)	-140.19	H(3) N(1) C(1) H(1)	-23.53	H(3) N(1) C(1) H(2)	100.09
H(4) N(1) C(1) S(1)	98.72	H(4) N(1) C(1) H(1)	-144.62	H(4) N(1) C(1) H(2)	-21.00
C(1) N(1) C(2) H(5)	-130.91	H(3) N(1) C(2) C(3)	-128.03	H(3) N(1) C(2) C(4)	108.88
H(3) N(1) C(2) H(5)	-10.67	H(4) N(1) C(2) C(3)	-7.57	H(4) N(1) C(2) C(4)	-130.65
H(4) N(1) C(2) H(5)	109.80	H(5) C(2) C(3) O(1)	-103.01	H(5) C(2) C(3) O(2)	74.54
N(1) C(2) C(4) H(6)	-81.38	N(1) C(2) C(4) H(7)	158.94	C(3) C(2) C(4) H(6)	158.13
C(3) C(2) C(4) H(7)	38.45	H(5) C(2) C(4) S(1)	156.21	H(5) C(2) C(4) H(6)	36.26
H(5) C(2) C(4) H(7)	-83.42				

Tabelle A.7: Thioprolin, Torsionswinkel aus der 120 K Messung in [°].

	S(1)	O(1)	O(2)	N(1)	C(1)	C(2)	C(3)	C(4)
P_v	6.19(1)	6.33(1)	6.33(1)	5.35(2)	4.38(1)	4.15(1)	3.90(1)	4.40(1)
P_{11}	-0.06(1)	-0.08(1)	-0.08(1)	-0.05(1)	-0.06(1)	-0.03(1)	–	-0.11(1)
P_{1-1}	–	-0.03(1)	-0.03(1)	–	-0.13(1)	-0.27(1)	–	-0.10(1)
P_{10}	–	–	–	–	–	-0.06(1)	-0.11(1)	–
P_{20}	0.17(1)	-0.05(1)	-0.05(1)	0.09(1)	0.22(1)	0.28(1)	0.03(1)	0.16(1)
P_{21}	–	–	–	–	–	0.03(1)	–	–
P_{2-1}	–	–	–	–	–	0.05(1)	–	–
P_{22}	-0.04(1)	-0.06(1)	-0.06(1)	-0.03(1)	0.06(1)	0.22(1)	0.22(1)	-0.07(1)
P_{2-2}	–	–	–	0.04(1)	0.09(1)	0.12(1)	–	0.08(1)
P_{30}	–	–	–	–	–	-0.06(1)	0.26(1)	–
P_{31}	-0.11(1)	–	–	-0.15(1)	-0.20(1)	-0.23(1)	–	-0.20(1)
P_{3-1}	-0.12(1)	–	–	-0.21(1)	-0.24(1)	-0.30(1)	–	-0.26(1)
P_{32}	0.03(1)	–	–	–	–	–	-0.21(1)	–
P_{3-2}	0.03(1)	–	–	–	–	-0.04(1)	–	–
P_{33}	0.13(1)	–	–	0.14(1)	0.16(1)	0.23(1)	–	0.15(1)
P_{3-3}	-0.16(1)	–	–	-0.03(1)	-0.06(1)	-0.07(1)	–	-0.09(1)
P_{40}	0.05(1)	–	–	–	0.03(1)	0.06(1)	0.07(1)	–
P_{41}	–	–	–	–	–	–	–	–
P_{4-1}	–	–	–	–	–	0.03(1)	–	–
P_{42}	–	–	–	-0.03(1)	–	0.06(1)	-0.05(1)	–
P_{4-2}	-0.03(1)	–	–	0.09(1)	0.10(1)	0.14(1)	–	0.12(1)
P_{43}	–	–	–	–	–	–	–	–
P_{4-3}	–	–	–	–	–	–	–	–
P_{44}	0.16(1)	–	–	0.03(1)	0.04(1)	0.06(1)	0.07(1)	0.05(1)
P_{4-4}	-0.03(1)	–	–	–	0.03(1)	0.04(1)	–	–

Tabelle A.8: Multipolparameter ($P > 2\sigma(P)$) der DFT-Verfeinerung von Thioprolin

	S(1)	O(1)	O(2)	N(1)	C(1)	C(2)	C(3)	C(4)
P_v	6.50(2)	6.40(1)	6.48(1)	5.07(2)	3.84(2)	4.01(2)	3.75(2)	4.11(2)
P_{11}	0.06(1)	–	–	–	–	-0.04(1)	–	–
P_{1-1}	–	–	–	–	-0.05(1)	-0.06(1)	–	-0.05(1)
P_{10}	-0.04(1)	-0.11(1)	-0.11(1)	–	–	–	–	-0.03(1)
P_{20}	-0.10(1)	-0.07(1)	-0.09(1)	-0.04(1)	-0.03(1)	–	-0.29(1)	–
P_{21}	–	–	–	–	–	–	–	–
P_{2-1}	0.08(1)	–	–	–	0.08(1)	0.08(1)	–	0.04(1)
P_{22}	0.17(1)	-0.09(1)	-0.09(1)	0.05(1)	0.11(1)	0.10(1)	-0.09(1)	0.07(1)
P_{2-2}	0.03(1)	–	–	–	–	–	–	-0.04(1)
P_{30}	0.15(1)	0.03(1)	0.04(1)	0.17(1)	0.26(1)	0.25(1)	0.04(1)	0.25(1)
P_{31}	-0.04(1)	–	–	–	–	0.04(1)	-0.04(1)	–
P_{3-1}	-0.12(1)	–	–	0.03(1)	-0.04(1)	–	–	–
P_{32}	0.04(1)	–	–	–	-0.03(1)	–	–	-0.03(1)
P_{3-2}	–	–	–	–	–	–	–	-0.04(1)
P_{33}	–	–	–	–	–	–	0.38(1)	–
P_{3-3}	-0.05(1)	–	–	-0.15(1)	-0.23(1)	-0.22(1)	–	-0.21(1)
P_{40}	0.05(1)	–	–	0.03(1)	0.05(1)	0.07(1)	0.03(1)	0.08(1)
P_{41}	–	–	–	–	–	–	–	–
P_{4-1}	–	–	–	–	–	–	–	–
P_{42}	0.04(1)	–	–	–	0.04(1)	–	-0.05(1)	–
P_{4-2}	–	–	–	–	–	–	–	–
P_{43}	–	–	–	–	–	–	–	–
P_{4-3}	–	–	–	0.07(1)	0.09(1)	0.08(1)	–	0.09(1)
P_{44}	0.03(1)	–	–	–	0.05(1)	–	–	–
P_{4-4}	–	–	–	–	0.03(1)	–	–	–

Tabelle A.9: Multipolparameter ($P > 2\sigma(P)$) der PHF-Verfeinerung von Thioprolin

	S(1)	O(1)	O(2)	N(1)	C(1)	C(2)	C(3)	C(4)
P_v	6.12(3)	6.34(2)	6.37(2)	5.51(6)	3.99(6)	4.30(6)	3.97(4)	4.25(6)
P_{11}	–	0.10(1)	-0.06(1)	0.03(1)	–	–	-0.06(1)	–
P_{1-1}	–	-0.03(1)	–	-0.06(1)	-0.09(1)	-0.05(1)	0.04(1)	-0.06(1)
P_{10}	-0.05(1)	–	-0.04(1)	–	-0.04(1)	0.03(1)	-0.03(1)	–
P_{20}	-0.06(1)	–	–	-0.04(1)	–	-0.03(1)	-0.32(1)	-0.07(1)
P_{21}	–	-0.04(1)	–	–	–	–	-0.08(1)	–
P_{2-1}	0.05(1)	–	–	–	0.13(1)	0.08(1)	0.05(1)	0.03(1)
P_{22}	0.07(1)	-0.06(1)	-0.05(1)	0.07(1)	0.07(1)	0.09(1)	-0.10(1)	0.04(1)
P_{2-2}	0.05(1)	–	–	–	–	0.05(1)	–	-0.03(1)
P_{30}	0.23(2)	–	–	0.24(1)	0.25(1)	0.31(2)	–	0.25(1)
P_{31}	–	-0.06(1)	–	–	–	0.09(1)	–	–
P_{3-1}	-0.27(2)	–	–	–	–	–	–	-0.05(1)
P_{32}	0.06(2)	0.06(1)	–	0.03(1)	–	–	–	-0.04(1)
P_{3-2}	0.09(2)	–	–	0.03(1)	–	–	–	–
P_{33}	–	0.05(1)	–	–	–	–	0.36(1)	–
P_{3-3}	-0.10(2)	–	-0.03(1)	-0.16(1)	-0.16(1)	-0.29(1)	–	-0.22(1)
P_{40}	0.18(2)	–	–	0.04(1)	–	0.10(2)	-0.05(2)	0.04(1)
P_{41}	–	–	–	–	0.04(2)	0.07(2)	0.05(2)	–
P_{4-1}	-0.07(2)	–	–	-0.04(1)	-0.03(1)	0.08(2)	–	–
P_{42}	–	–	–	–	–	–	–	0.05(1)
P_{4-2}	-0.06(2)	–	–	-0.03(1)	0.05(1)	–	–	–
P_{43}	–	–	–	–	–	–	–	0.06(1)
P_{4-3}	–	–	–	0.04(1)	–	0.09(2)	–	0.07(1)
P_{44}	0.09(2)	–	–	–	-0.03(1)	–	–	0.09(1)
P_{4-4}	-0.12(2)	0.03(1)	–	–	–	–	-0.05(2)	–

Tabelle A.10: Multipolparameter ($P > 2\sigma(P)$) der X120-Verfeinerung von Thioprolin

	S(1)	O(1)	O(2)	N(1)	C(1)	C(2)	C(3)	C(4)
P_v	6.01(5)	6.33(4)	6.32(5)	5.30(12)	4.26(9)	4.45(12)	3.99(9)	4.31(10)
P_{11}	–	–	–	–	0.05(2)	-0.11(3)	-0.12(3)	–
P_{1-1}	–	–	–	-0.06(2)	-0.11(2)	-0.13(3)	–	-0.09(3)
P_{10}	–	-0.07(1)	-0.08(1)	–	–	–	–	-0.05(2)
P_{20}	-0.17(3)	–	-0.04(1)	–	-0.07(2)	–	-0.29(2)	–
P_{21}	-0.21(2)	–	–	–	–	–	0.06(2)	–
P_{2-1}	0.07(3)	–	0.03(1)	0.07(2)	0.05(2)	0.17(3)	–	0.07(2)
P_{22}	–	–	-0.03(1)	0.06(2)	0.12(2)	0.12(2)	-0.13(2)	–
P_{2-2}	0.05(2)	-0.03(1)	–	-0.06(2)	–	0.06(2)	-0.08(2)	–
P_{30}	0.27(4)	–	0.04(1)	0.22(2)	0.25(2)	0.37(3)	–	0.21(3)
P_{31}	–	–	–	–	–	–	–	–
P_{3-1}	-0.28(6)	–	–	–	–	–	–	–
P_{32}	–	–	–	–	–	–	–	–
P_{3-2}	–	–	–	–	–	–	–	–
P_{33}	–	–	–	–	-0.06(2)	–	0.47(3)	–
P_{3-3}	-0.15(4)	–	–	-0.19(2)	-0.19(2)	-0.29(3)	-0.08(3)	-0.26(2)
P_{40}	0.14(5)	–	0.04(1)	–	–	–	–	–
P_{41}	-0.21(4)	–	–	–	-0.10(3)	–	–	–
P_{4-1}	–	–	–	–	–	–	–	–
P_{42}	–	–	–	–	–	–	–	–
P_{4-2}	–	–	–	–	–	–	–	–
P_{43}	–	–	–	–	–	–	–	–
P_{4-3}	–	–	–	0.05(2)	–	0.23(4)	–	0.09(3)
P_{44}	–	–	–	–	–	–	–	–
P_{4-4}	–	–	–	–	–	–	-0.09(4)	–

Tabelle A.11: Multipolparameter ($P > 2\sigma(P)$) der X15-Verfeinerung von Thioprolin

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S(1)–C(1)	0.8890	0.9147	-6.57	-5.59	6.23	-5.9(1)	1.24(1)	0.17
S(1)–C(4)	0.9626	0.8552	-6.55	-5.71	7.48	-4.8(1)	1.20(1)	0.15
C(1)–N(1)	0.6417	0.8604	-11.46	-11.25	12.81	-9.9(1)	1.63(1)	0.02
N(1)–C(2)	0.9020	0.6026	-9.69	-9.08	12.36	-6.4(1)	1.41(1)	0.07
C(2)–C(3)	0.8336	0.7117	-12.52	-10.49	10.40	-12.6(1)	1.69(1)	0.19
C(3)–O(1)	0.4429	0.8068	-20.35	-19.76	19.70	-20.4(1)	2.54(1)	0.03
C(3)–O(2)	0.4521	0.8088	-19.93	-19.21	16.80	-22.3(1)	2.50(1)	0.04
C(2)–C(4)	0.7791	0.7500	-12.44	-10.88	11.04	-12.3(1)	1.72(1)	0.14
C(1)–H(1)	0.6369	0.3371	-26.95	-26.28	20.51	-32.7(1)	2.47(1)	0.03
C(1)–H(2)	0.5866	0.3317	-29.82	-28.92	17.57	-41.2(1)	2.69(1)	0.03
N(1)–H(3)	0.6567	0.2116	-56.09	-55.49	38.21	-73.4(3)	3.33(3)	0.01
N(1)–H(4)	0.6647	0.2185	-53.31	-52.74	37.72	-68.3(1)	3.24(1)	0.01
C(2)–H(5)	0.6170	0.3197	-29.26	-26.89	17.74	-38.4(1)	2.65(1)	0.09
C(4)–H(6)	0.6160	0.3490	-25.87	-25.58	17.74	-33.7(1)	2.47(1)	0.01
C(4)–H(7)	0.5957	0.3480	-26.76	-26.47	16.46	-36.8(1)	2.55(1)	0.01

Tabelle A.12: Bindungstopologische Parameter der DFT-Verfeinerung von Thioprolin

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S(1)–C(1)	0.9468	0.8567	-7.50	-6.40	9.10	-4.8(1)	1.26(1)	0.17
S(1)–C(4)	0.9676	0.8507	-7.07	-6.31	8.91	-4.5(1)	1.23(1)	0.12
C(1)–N(1)	0.6481	0.8546	-13.25	-13.02	12.91	-13.4(1)	1.68(1)	0.02
N(1)–C(2)	0.8647	0.6392	-12.93	-11.83	11.73	-13.0(1)	1.67(1)	0.09
C(2)–C(3)	0.7688	0.7764	-14.00	-12.87	10.80	-16.1(1)	1.78(1)	0.09
C(3)–O(1)	0.4621	0.7873	-28.86	-24.33	12.85	-40.4(1)	2.71(1)	0.19
C(3)–O(2)	0.4665	0.7939	-27.01	-22.93	12.36	-37.6(1)	2.63(2)	0.18
C(2)–C(4)	0.7749	0.7532	-12.99	-12.49	10.46	-15.0(1)	1.75(1)	0.04
C(1)–H(1)	0.7114	0.3696	-20.05	-19.29	16.84	-22.5(1)	1.97(1)	0.04
C(1)–H(2)	0.7124	0.3671	-19.36	-18.78	17.41	-20.7(1)	1.95(1)	0.03
N(1)–H(3)	0.7613	0.2417	-31.60	-31.34	29.72	-33.2(1)	2.26(2)	0.01
N(1)–H(4)	0.7877	0.2704	-25.60	-25.22	25.76	-25.1(1)	1.99(1)	0.02
C(2)–H(5)	0.7065	0.3747	-19.16	-18.30	17.38	-20.1(1)	1.97(1)	0.05
C(4)–H(6)	0.7052	0.3782	-18.91	-18.64	15.60	-22.0(1)	1.96(1)	0.01
C(4)–H(7)	0.7091	0.3701	-19.20	-18.72	16.56	-21.4(1)	1.98(1)	0.03

Tabelle A.13: Bindungstopologische Parameter der PHF-Verfeinerung von Thioprolin

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S(1)–C(1)	0.9421	0.8646	-7.05	-5.99	7.69	-5.4(1)	1.26(1)	0.18
S(1)–C(4)	0.9454	0.8725	-7.60	-7.39	8.13	-6.9(1)	1.34(1)	0.03
C(1)–N(1)	0.6219	0.8806	-10.58	-9.48	11.92	-8.2(1)	1.59(2)	0.12
N(1)–C(2)	0.8512	0.6522	-12.45	-11.60	13.37	-10.7(1)	1.74(1)	0.07
C(2)–C(3)	0.7813	0.7640	-10.97	-10.27	10.52	-10.7(1)	1.64(1)	0.07
C(3)–O(1)	0.4422	0.8072	-22.16	-20.61	19.43	-23.3(1)	2.67(2)	0.08
C(3)–O(2)	0.4381	0.8219	-24.08	-20.72	20.61	-24.2(1)	2.60(2)	0.16
C(2)–C(4)	0.7821	0.7460	-11.62	-10.83	10.12	-12.3(1)	1.70(1)	0.07
C(1)–H(1)	0.6581	0.4377	-17.39	-16.46	17.69	-16.2(1)	1.89(6)	0.06
C(1)–H(2)	0.6571	0.4370	-18.68	-17.41	17.19	-18.9(1)	1.97(2)	0.07
N(1)–H(3)	0.7675	0.2654	-25.99	-25.38	30.89	-20.5(6)	1.98(11)	0.02
N(1)–H(4)	0.7771	0.2560	-28.19	-27.39	30.49	-25.1(5)	2.07(8)	0.03
C(2)–H(5)	0.7000	0.3943	-17.05	-16.38	17.42	-16.0(1)	1.89(3)	0.04
C(4)–H(6)	0.6517	0.4435	-17.33	-16.84	16.28	-17.9(1)	1.93(2)	0.03
C(4)–H(7)	0.6643	0.4299	-19.28	-18.09	17.61	-19.8(1)	2.04(2)	0.07

Tabelle A.14: Bindungstopologische Parameter der X120-Verfeinerung von Thioprolin

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S(1)–C(1)	0.9494	0.8545	-7.05	-5.48	8.89	-3.6(1)	1.19(3)	0.29
S(1)–C(4)	0.9637	0.8488	-7.61	-6.89	9.33	-5.2(1)	1.34(2)	0.11
C(1)–N(1)	0.6293	0.8669	-12.01	-11.59	11.87	-11.7(1)	1.70(4)	0.04
N(1)–C(2)	0.8714	0.6289	-12.44	-11.71	10.16	-14.0(1)	1.68(3)	0.06
C(2)–C(3)	0.7728	0.7714	-13.07	-10.83	9.53	-14.4(1)	1.71(3)	0.21
C(3)–O(1)	0.4403	0.8040	-26.56	-23.32	18.21	-31.7(2)	2.86(4)	0.14
C(3)–O(2)	0.4293	0.8295	-26.13	-23.05	23.88	-25.3(2)	2.66(4)	0.13
C(2)–C(4)	0.7822	0.7417	-11.98	-11.24	10.00	-13.2(1)	1.77(3)	0.07
C(1)–H(1)	0.6788	0.4160	-19.66	-17.60	17.57	-19.7(2)	1.94(10)	0.12
C(1)–H(2)	0.6967	0.3975	-19.03	-17.37	20.37	-16.0(1)	1.98(4)	0.10
N(1)–H(3)	0.7466	0.2865	-26.94	-26.67	30.80	-22.8(9)	2.13(28)	0.01
N(1)–H(4)	0.7687	0.2643	-27.15	-25.79	33.11	-19.8(9)	2.04(19)	0.05
C(2)–H(5)	0.7473	0.3474	-18.18	-16.95	19.17	-16.0(2)	1.85(6)	0.07
C(4)–H(6)	0.6836	0.4107	-18.73	-17.66	18.37	-18.0(1)	1.96(4)	0.06
C(4)–H(7)	0.6717	0.4226	-17.98	-16.15	17.17	-17.0(1)	1.89(4)	0.11

Tabelle A.15: Bindungstopologische Parameter der X15-Verfeinerung von Thioprolin

A.2 Penicilline

2θ	ω	χ	ϕ	Scan	Δ	Frames	t
0°	70°	-54°	30°	ω	-0.1°	700	1.5 s
0°	70°	-54°	120°	ω	-0.1°	700	1.5 s
0°	70°	0°	0°	ϕ	-0.1°	450	1.5 s
-30°	70°	-54°	0°	ω	-0.1°	1000	1 s
-30°	70°	-54°	90°	ω	-0.1°	1000	1 s
-30°	70°	-54°	180°	ω	-0.1°	1000	1 s
-30°	70°	-54°	270°	ω	-0.1°	1000	1 s
-30°	0°	0°	0°	ϕ	-0.1°	1800	1 s
-55°	15°	-54°	0°	ω	-0.1°	700	6 s
-55°	15°	-54°	90°	ω	-0.1°	700	6 s
-55°	15°	-54°	180°	ω	-0.1°	700	6 s
-55°	40°	-90°	30°	ω	-0.1°	990	6 s
-55°	40°	-90°	120°	ω	-0.1°	900	6 s
-55°	0°	-54°	180°	ϕ	-0.1°	900	6 s
-55°	-30°	-90°	180°	ϕ	-0.1°	900	6 s
-55°	0°	0°	180°	ϕ	-0.1°	450	6 s

Tabelle A.16: Penamecillin, Meßstrategie. Detektorabstand für $2\theta = 0°$ Stellung 6.5 cm, sonst 4 cm.

2θ	ω	χ	ϕ	Scan	Δ	Frames	t
0°	70°	-54°	30°	ω	-0.1°	734	1 s
0°	70°	-54°	120°	ω	-0.1°	700	1 s
0°	70°	-54°	0°	ϕ	-0.1°	400	1 s
0°	70°	0°	-40°	ϕ	-0.1°	1199	1 s
30°	30°	54°	0°	ω	-0.1°	900	1 s
30°	30°	54°	90°	ω	-0.1°	900	1 s
30°	30°	54°	180°	ω	-0.1°	900	1 s
30°	30°	54°	270°	ω	-0.1°	900	1 s
30°	0°	54°	0°	ϕ	-0.1°	1120	1 s
-30°	0°	0°	180°	ϕ	-0.1°	885	2 s
-30°	70°	-54°	180°	ω	-0.1°	900	2 s
-30°	70°	-54°	0°	ω	-0.1°	900	2 s
55°	61°	54°	0°	ω	-0.15°	786	10 s
55°	61°	54°	90°	ω	-0.15°	786	10 s
55°	61°	54°	180°	ω	-0.15°	786	10 s
55°	61°	54°	270°	ω	-0.15°	786	10 s
55°	0°	0°	180°	ϕ	-0.15°	626	10 s
-55°	15°	-54°	0°	ω	-0.15°	466	10 s
-55°	0°	0°	0°	ϕ	-0.15°	1200	10 s

Tabelle A.17: Penamecillin-1β-sulfoxid, Meßstrategie. Detektorabstand für $2\theta = 0°$ Stellung 6 cm, sonst 4 cm.

Schale $\sin\theta/\lambda_{max}$ [Å^{-1}]	Schale d_{min} [Å]	gemessene Reflexe	fehlende Reflexe	Vollständigkeit [%]
0.4550	1.099	835	20	97.5
0.5733	0.872	829	0	100.0
0.6562	0.762	812	0	100.0
0.7223	0.692	814	1	99.9
0.7781	0.643	799	0	100.0
0.8268	0.605	798	1	99.9
0.8704	0.574	815	3	99.6
0.9100	0.549	805	4	99.5
0.9465	0.528	755	32	95.9
0.9803	0.510	698	109	86.5
1.0119	0.494	655	128	83.7
1.0417	0.480	688	137	83.4
1.0699	0.467	637	142	81.8
1.0967	0.456	647	149	81.3
1.1222	0.446	649	167	79.5
1.1466	0.436	622	173	78.2
1.1700	0.427	620	164	79.1
1.1925	0.419	622	194	76.2
1.2142	0.412	579	202	74.1
1.2351	0.405	247	549	31.0

Tabelle A.18: Penamecillin, Vollständigkeit des Datensatzes in Schalen unterschiedlicher Auflösung (nach Mittelung).

Schale $\sin\theta/\lambda_{max}$ [Å^{-1}]	Schale d_{min} [Å]	gemessene Reflexe	fehlende Reflexe	Vollständigkeit [%]
0.4573	1.093	881	3	99.5
0.5762	0.868	865	0	100.0
0.6596	0.758	836	1	99.9
0.7260	0.689	829	1	99.9
0.7820	0.639	842	1	99.9
0.8310	0.602	839	4	99.5
0.8748	0.572	823	2	99.8
0.9147	0.547	811	1	99.9
0.9513	0.526	851	10	98.8
0.9853	0.507	796	19	97.7
1.0171	0.492	824	20	97.6
1.0470	0.478	793	17	97.9
1.0753	0.465	803	20	97.6
1.1022	0.454	832	17	98.0
1.1279	0.443	796	27	96.7
1.1524	0.434	780	22	97.3
1.1759	0.425	792	35	95.8
1.1985	0.417	777	48	94.2
1.2203	0.410	780	59	93.0
1.2414	0.403	583	211	73.4

Tabelle A.19: Penamecillin-1β-sulfoxid, Vollständigkeit des Datensatzes in Schalen unterschiedlicher Auflösung (nach Mittelung).

	S(1)	O(8)	O(14)	N(4)	N(20)	C(2)	C(3)	C(5)	C(6)	C(7)	C(10)	C(12)	C(21)	C(24)	C(25)
P_v	6.17(8)	6.23(4)	6.25(4)	5.17(8)	5.20(9)	3.78(6)	4.05(9)	4.30(9)	3.80(10)	4.02(9)	4.68(8)	3.90(7)	4.47(9)	3.98(8)	4.21(3)
P_{11}	-0.07(1)	–	–	–	–	-0.05(1)	-0.11(2)	-0.08(2)	-0.06(2)	-0.08(3)	–	–	-0.10(2)	–	–
P_{1-1}	–	–	-0.03(1)	–	-0.05(2)	–	–	–	–	0.11(2)	–	–	-0.10(2)	–	–
P_{10}	0.09(2)	–	-0.03(1)	–	–	–	–	–	0.13(2)	0.12(2)	-0.04(1)	–	–	-0.06(2)	0.03(1)
P_{20}	0.15(2)	-0.09(1)	–	–	–	0.04(1)	0.06(2)	–	0.05(2)	-0.24(2)	-0.06(1)	-0.28(2)	-0.22(2)	0.10(2)	0.13(1)
P_{21}	-0.12(3)	–	–	–	–	–	–	–	–	–	–	–	–	–	–
P_{2-1}	0.07(2)	–	–	–	–	–	–	-0.16(2)	0.10(2)	–	–	–	–	–	–
P_{22}	–	-0.03(1)	-0.04(1)	–	–	–	–	–	–	–	–	0.05(1)	-0.08(2)	-0.10(2)	-0.16(1)
P_{2-2}	0.07(2)	–	0.05(1)	–	–	0.06(1)	0.06(2)	–	–	0.09(2)	–	0.08(1)	–	–	–
P_{30}	0.12(5)	–	–	–	–	–	–	-0.09(3)	0.06(2)	–	0.25(2)	–	–	-0.18(2)	-0.28(1)
P_{31}	–	–	0.04(1)	–	–	-0.08(1)	-0.15(2)	-0.18(2)	-0.10(2)	–	–	–	-0.11(2)	–	–
P_{3-1}	–	–	-0.03(1)	-0.13(2)	–	-0.14(1)	-0.23(2)	-0.17(2)	-0.22(2)	–	–	–	–	–	–
P_{32}	0.22(5)	–	–	-0.08(2)	–	–	–	-0.08(2)	–	0.05(2)	–	–	–	-0.13(2)	-0.16(1)
P_{3-2}	–	–	–	–	–	–	-0.05(2)	–	-0.10(2)	–	–	–	–	–	–
P_{33}	0.08(3)	0.03(1)	0.09(1)	0.12(2)	0.20(2)	0.18(1)	0.17(2)	0.18(2)	0.21(2)	0.20(3)	-0.04(1)	0.30(2)	0.23(2)	–	–
P_{3-3}	-0.11(3)	–	–	–	–	-0.05(1)	-0.10(2)	–	–	-0.18(2)	-0.10(2)	–	-0.10(2)	–	–
P_{40}	-0.11(5)	–	–	0.07(2)	–	–	–	–	–	–	-0.05(2)	0.05(2)	0.07(3)	0.07(3)	0.04(1)
P_{41}	–	–	–	–	–	–	–	–	-0.10(3)	–	–	–	–	–	–
P_{4-1}	–	–	–	–	–	–	–	–	-0.07(3)	-0.10(3)	–	–	–	–	–
P_{42}	–	–	–	–	-0.07(2)	–	-0.13(3)	–	-0.10(3)	–	–	–	–	–	–
P_{4-2}	-0.21(4)	–	–	–	–	–	0.11(3)	–	0.13(3)	–	–	–	0.08(3)	–	–
P_{43}	–	–	–	–	–	–	0.08(3)	–	–	–	-0.10(2)	–	–	–	–
P_{4-3}	–	–	–	0.05(2)	–	–	–	–	–	–	–	–	–	–	–
P_{44}	0.13(3)	0.04(1)	-0.03(1)	–	-0.08(2)	0.05(2)	–	0.07(2)	–	–	–	–	–	–	0.04(1)
P_{4-4}	-0.22(3)	–	-0.03(1)	–	–	–	-0.05(2)	0.09(2)	–	-0.09(3)	–	0.05(2)	–	–	–

Tabelle A.20: Multipolparameter ($P > 2\sigma(P)$) der Verfeinerung von Penamecillin

	S(1)	O(8)	O(9)	O(14)	N(4)	N(20)	C(2)	C(3)	C(5)	C(6)	C(7)	C(10)	C(12)	C(15)	C(21)	C(24)	C(25)
P_v	5.99(9)	6.23(3)	6.24(7)	6.22(4)	5.14(8)	5.00(9)	4.13(7)	3.92(9)	4.32(9)	3.90(9)	3.75(8)	4.71(10)	3.85(6)	4.13(7)	4.05(7)	4.13(5)	4.13(3)
P_{11}	–	-0.04(1)	–	–	0.08(2)	–	–	-0.05(2)	–	–	–	–	–	–	–	–	–
P_{1-1}	–	–	–	-0.08(1)	–	–	-0.03(1)	–	-0.05(2)	–	–	–	-0.08(2)	-0.03(1)	-0.07(2)	–	–
P_{10}	0.05(2)	–	-0.12(2)	–	–	–	–	0.05(2)	–	–	0.05(2)	-0,05(2)	–	–	–	–	-0.04(1)
P_{20}	0.32(3)	-0.05(1)	-0.09(2)	0.04(1)	–	0.10(2)	0.11(1)	–	0.05(2)	0.06(2)	-0.29(2)	-0.08(2)	-0.25(2)	0.11(1)	-0.24(2)	–	0.11(1)
P_{21}	-0.10(3)	–	-0.16(2)	–	–	–	–	-0.05(2)	–	-0.07(2)	0.08(2)	–	–	–	–	–	–
P_{2-1}	0.10(3)	–	-0.10(2)	–	–	–	–	–	-0.17(2)	-0.06(2)	–	–	–	–	–	–	–
P_{22}	–	–	–	–	–	-0.06(2)	-0.07(1)	–	–	-0.07(2)	-0.05(2)	–	–	-0.07(1)	–	-0.23(2)	-0.19(1)
P_{2-2}	–	-0.03(1)	0.09(2)	0.09(1)	-0.07(2)	–	–	–	–	–	0.24(2)	–	0.05(2)	–	0.08(2)	–	–
P_{30}	0.57(6)	–	–	–	–	–	–	–	–	–	–	0.29(2)	–	–	–	-0.14(3)	-0.24(1)
P_{31}	-0.36(5)	0.03(1)	–	–	–	–	-0.14(2)	-0.08(3)	-0.10(3)	-0.16(3)	0.08(3)	–	–	-0.14(2)	-0.11(3)	–	–
P_{3-1}	-0.35(4)	–	–	-0.04(1)	–	–	-0.15(2)	-0.27(3)	-0.15(3)	-0.17(3)	–	–	-0.10(2)	-0.15(2)	–	–	–
P_{32}	–	–	–	–	–	–	–	–	-0.09(3)	–	–	–	–	–	–	-0.19(3)	-0.13(1)
P_{3-2}	–	–	-0.05(2)	–	–	–	–	–	–	–	–	–	–	–	–	–	–
P_{33}	–	0.03(1)	-0.11(2)	0.04(1)	0.07(2)	0.16(2)	0.14(2)	0.14(3)	0.20(3)	–	0.19(3)	0.12(2)	0.19(2)	0.14(2)	0.31(3)	–	–
P_{3-3}	-0.16(4)	–	–	–	-0.10(2)	–	-0.06(1)	-0.11(3)	-0.08(3)	-0.09(3)	-0.16(3)	–	-0.05(2)	-0.06(1)	-0.07(3)	–	–
P_{40}	0.42(6)	-0.05(1)	–	-0.07(2)	–	–	–	–	–	–	–	–	0.08(3)	–	0.08(3)	–	–
P_{41}	-0.24(6)	–	–	–	–	–	–	-0.08(3)	0.07(3)	–	–	–	–	–	–	–	–
P_{4-1}	-0.25(5)	–	–	–	–	–	–	–	–	0.08(3)	–	–	–	–	–	–	–
P_{42}	–	0.03(1)	–	–	–	–	–	–	–	–	–	–	–	–	–	-0.15(3)	–
P_{4-2}	-0.12(5)	-0.04(1)	-0.07(3)	–	–	–	0.06(2)	–	–	–	–	–	–	0.06(2)	–	–	–
P_{43}	-0.11(3)	–	–	–	–	–	–	0.08(3)	–	–	–	-0.05(2)	–	–	–	–	–
P_{4-3}	–	–	–	–	–	–	–	–	-0.19(3)	–	–	–	–	–	–	–	–
P_{44}	0.22(5)	–	0.06(2)	–	0.10(3)	-0.06(2)	0.05(2)	–	–	–	–	–	–	0.05(2)	–	-0.08(3)	–
P_{4-4}	0.11(5)	–	–	–	–	–	–	–	–	-0.08(3)	–	–	–	–	–	–	–

Tabelle A.21: Multipolparameter ($P > 2\sigma(P)$) der Verfeinerung von Penamecillin-1β-sulfoxid

S(1)–C(2)	1.8526(6)	S(1)–C(5)	1.8181(5)	O(8)–C(7)	1.2064(9)
O(13)–C(12)	1.2028(7)	O(14)–C(12)	1.3550(6)	O(14)–C(15)	1.4198(8)
O(16)–C(15)	1.4174(8)	O(16)–C(17)	1.3567(7)	O(18)–C(17)	1.2072(8)
O(22)–C(21)	1.2239(7)	N(4)–C(3)	1.4422(8)	N(4)–C(5)	1.4655(7)
N(4)–C(7)	1.3829(9)	N(20)–C(6)	1.4254(9)	N(20)–C(21)	1.3543(8)
C(2)–C(3)	1.5706(8)	C(2)–C(10)	1.5303(10)	C(2)–C(11)	1.5308(8)
C(3)–C(12)	1.5181(8)	C(5)–C(6)	1.5664(8)	C(6)–C(7)	1.5559(8)
C(17)–C(19)	1.4941(9)	C(21)–C(23)	1.5227(9)	C(23)–C(24)	1.5070(9)
C(24)–C(25)	1.3963(8)	C(24)–C(29)	1.3949(8)	C(25)–C(26)	1.3900(9)
C(26)–C(27)	1.3918(10)	C(27)–C(28)	1.3935(12)	C(28)–C(29)	1.3987(10)
N(20)–H(201)	1.0091	C(3)–H(31)	1.0989	C(5)–H(51)	1.0990
C(6)–H(61)	1.0991	C(10)–H(101)	1.0590	C(10)–H(102)	1.0590
C(10)–H(103)	1.0590	C(11)–H(111)	1.0590	C(11)–H(112)	1.0590
C(11)–H(113)	1.0590	C(15)–H(151)	1.0920	C(15)–H(152)	1.0920
C(19)–H(191)	1.0590	C(19)–H(192)	1.0590	C(19)–H(193)	1.0590
C(23)–H(231)	1.0920	C(23)–H(232)	1.0920	C(25)–H(251)	1.0830
C(26)–H(261)	1.0830	C(27)–H(271)	1.0830	C(28)–H(281)	1.0830
C(29)–H(291)	1.0830				

Tabelle A.22: Penamecillin, Bindungslängen in [Å].

C(2)–S(1)–C(5)	94.89(2)	C(12)–O(14)–C(15)	115.97(5)	C(15)–O(16)–C(17)	116.00(5)
C(3)–N(4)–C(5)	117.25(5)	C(3)–N(4)–C(7)	125.85(5)	C(5)–N(4)–C(7)	94.25(5)
C(6)–N(20)–C(21)	123.58(5)	S(1)–C(2)–C(3)	105.13(4)	S(1)–C(2)–C(10)	110.15(4)
S(1)–C(2)–C(11)	108.49(4)	C(3)–C(2)–C(10)	109.34(5)	C(3)–C(2)–C(11)	113.41(5)
C(10)–C(2)–C(11)	110.19(5)	N(4)–C(3)–C(2)	106.23(4)	N(4)–C(3)–C(12)	109.74(4)
C(2)–C(3)–C(12)	112.69(4)	S(1)–C(5)–N(4)	105.64(4)	S(1)–C(5)–C(6)	119.10(4)
N(4)–C(5)–C(6)	88.58(4)	N(20)–C(6)–C(5)	116.26(5)	N(20)–C(6)–C(7)	115.63(5)
C(5)–C(6)–C(7)	83.95(4)	O(8)–C(7)–N(4)	131.05(6)	O(8)–C(7)–C(6)	136.81(7)
N(4)–C(7)–C(6)	92.06(5)	O(13)–C(12)–O(14)	124.87(5)	O(13)–C(12)–C(3)	125.32(5)
O(14)–C(12)–C(3)	109.75(5)	O(14)–C(15)–O(16)	110.62(5)	O(16)–C(17)–O(18)	123.00(6)
O(16)–C(17)–C(19)	111.60(5)	O(18)–C(17)–C(19)	125.40(6)	O(22)–C(21)–N(20)	123.58(6)
O(22)–C(21)–C(23)	120.90(5)	N(20)–C(21)–C(23)	115.48(5)	C(21)–C(23)–C(24)	116.09(5)
C(23)–C(24)–C(25)	119.79(5)	C(23)–C(24)–C(29)	121.43(5)	C(25)–C(24)–C(29)	118.72(5)
C(24)–C(25)–C(26)	121.45(5)	C(25)–C(26)–C(27)	119.46(6)	C(26)–C(27)–C(28)	119.87(6)
C(27)–C(28)–C(29)	120.29(6)	C(24)–C(29)–C(28)	120.20(6)		
C(6)–N(20)–H(201)	113.31	C(21)–N(20)–H(201)	121.41	N(4)–C(3)–H(31)	108.57
C(2)–C(3)–H(31)	114.55	C(12)–C(3)–H(31)	105.00	S(1)–C(5)–H(51)	111.43
N(4)–C(5)–H(51)	115.06	C(6)–C(5)–H(51)	114.72	N(20)–C(6)–H(61)	106.89
C(5)–C(6)–H(61)	117.47	C(7)–C(6)–H(61)	115.75	C(2)–C(10)–H(101)	104.71
C(2)–C(10)–H(102)	108.06	C(2)–C(10)–H(103)	108.81	H(101)–C(10)–H(102)	109.43
H(101)–C(10)–H(103)	120.05	H(102)–C(10)–H(103)	105.35	C(2)–C(11)–H(111)	111.40
C(2) –C(11)–H(112)	104.16	C(2)–C(11)–H(113)	106.78	H(111)–C(11)–H(112)	101.94
H(111)–C(11)–H(113)	113.99	H(112)–C(11)–H(113)	118.18	O(14)–C(15)–H(151)	110.19
O(14)–C(15)–H(152)	105.93	O(16)–C(15)–H(151)	103.04	O(16)–C(15)–H(152)	112.06
H(151)–C(15)–H(152)	115.07	C(17)–C(19)–H(191)	112.61	C(17)–C(19)–H(192)	101.58
C(17)–C(19)–H(193)	110.99	H(191)–C(19)–H(192)	116.55	H(191)–C(19)–H(193)	103.37
H(192)–C(19)–H(193)	112.02	C(21)–C(23)–H(231)	111.93	C(21)–C(23)–H(232)	107.25
C(24)–C(23)–H(231)	110.68	C(24)–C(23)–H(232)	109.18	H(231)–C(23)–H(232)	100.46
C(24)–C(25)–H(251)	111.82	C(26)–C(25)–H(251)	126.50	C(25)–C(26)–H(261)	119.56
C(27)–C(26)–H(261)	120.44	C(26)–C(27)–H(271)	121.41	C(28)–C(27)–H(271)	118.64
C(27) –C(28)–H(281)	126.38	C(29)–C(28)–H(281)	113.33	C(24)–C(29)–H(291)	123.17

Tabelle A.23: Penamecillin, Bindungswinkel in [°].

C(5) S(1) C(2) C(3)	16.68(4)	C(5) S(1) C(2) C(10)	-101.01(5)	C(5) S(1) C(2) C(11)	138.30(5)
C(2) S(1) C(5) N(4)	1.57(4)	C(2) S(1) C(5) C(6)	98.83(4)	C(15) O(14) C(12) O(13)	-5.02(7)
C(15) O(14) C(12) C(3)	177.71(4)	C(12) O(14) C(15) O(16)	84.23(5)	C(17) O(16) C(15) O(14)	78.23(6)
C(15) O(16) C(17) O(18)	-3.14(9)	C(15) O(16) C(17) C(19)	176.10(6)	C(5) N(4) C(3) C(2)	36.15(6)
C(5) N(4) C(3) C(12)	-85.95(6)	C(7) N(4) C(3) C(2)	-82.21(6)	C(7) N(4) C(3) C(12)	155.69(5)
C(3) N(4) C(5) S(1)	-22.95(6)	C(3) N(4) C(5) C(6)	-142.84(5)	C(7) N(4) C(5) S(1)	111.39(4)
C(7) N(4) C(5) C(6)	-8.50(5)	C(3) N(4) C(7) O(8)	-40.31(11)	C(3) N(4) C(7) C(6)	136.89(6)
C(5) N(4) C(7) O(8)	-168.63(8)	C(5) N(4) C(7) C(6)	8.56(5)	C(21) N(20) C(6) C(5)	137.88(6)
C(21) N(20) C(6) C(7)	-126.01(6)	C(6) N(20) C(21) O(22)	4.61(10)	C(6) N(20) C(21) C(23)	-177.65(6)
S(1) C(2) C(3) N(4)	-30.57(5)	S(1) C(2) C(3) C(12)	89.62(4)	C(10) C(2) C(3) N(4)	87.66(6)
C(10) C(2) C(3) C(12)	-152.14(5)	C(11) C(2) C(3) N(4)	-148.93(5)	C(11) C(2) C(3) C(12)	-28.73(6)
N(4) C(3) C(12) O(13)	34.19(7)	N(4) C(3) C(12) O(14)	-148.55(4)	C(2) C(3) C(12) O(13)	-83.97(6)
C(2) C(3) C(12) O(14)	93.29(5)	S(1) C(5) C(6) N(20)	16.07(7)	S(1) C(5) C(6) C(7)	-99.57(4)
N(4) C(5) C(6) N(20)	123.22(5)	N(4) C(5) C(6) C(7)	7.57(4)	N(20) C(6) C(7) O(8)	52.61(11)
N(20) C(6) C(7) N(4)	-124.30(5)	C(5) C(6) C(7) O(8)	168.88(9)	C(5) C(6) C(7) N(4)	-8.03(4)
O(22) C(21) C(23) C(24)	-164.73(6)	N(20) C(21) C(23) C(24)	17.47(8)	C(21) C(23) C(24) C(25)	94.55(7)
C(21) C(23) C(24) C(29)	-82.61(7)	C(23) C(24) C(25) C(26)	-177.13(6)	C(29) C(24) C(25) C(26)	0.11(9)
C(23) C(24) C(29) C(28)	177.26(6)	C(25) C(24) C(29) C(28)	0.07(9)	C(24) C(25) C(26) C(27)	-0.07(10)
C(25) C(26) C(27) C(28)	-0.15(11)	C(26) C(27) C(28) C(29)	0.31(12)	C(27) C(28) C(29) C(24)	-0.27(11)
C(2) S(1) C(5) H(51)	-124.05	C(12) O(14) C(15) H(151)	-29.05	C(12) O(14) C(15) H(152)	-154.11
C(17) O(16) C(15) H(151)	-164.03	C(17) O(16) C(15) H(152)	-39.75	C(5) N(4) C(3) H(31)	159.81
C(7) N(4) C(3) H(31)	41.45	C(3) N(4) C(5) H(51)	100.39	C(7) N(4) C(5) H(51)	-125.27
C(21) N(20) C(6) H(61)	4.47	H(201) N(20) C(6) C(5)	-27.40	H(201) N(20) C(6) C(7)	68.71
H(201) N(20) C(6) H(61)	-160.81	H(201) N(20) C(21) O(22)	168.74	H(201) N(20) C(21) C(23)	-13.52
S(1) C(2) C(3) H(31)	-150.41	C(10) C(2) C(3) H(31)	-32.18	C(11) C(2) C(3) H(31)	91.23
S(1) C(2) C(10) H(101)	-57.75	S(1) C(2) C(10) H(102)	-174.32	S(1) C(2) C(10) H(103)	71.78
C(3) C(2) C(10) H(101)	-172.80	C(3) C(2) C(10) H(102)	70.63	C(3) C(2) C(10) H(103)	-43.28
C(11) C(2) C(10) H(101)	61.91	C(11) C(2) C(10) H(102)	-54.66	C(11) C(2) C(10) H(103)	-168.57
S(1) C(2) C(11) H(111)	179.53	S(1) C(2) C(11) H(112)	70.38	S(1) C(2) C(11) H(113)	-55.42
C(3) C(2) C(11) H(111)	-64.07	C(3) C(2) C(11) H(112)	-173.23	C(3) C(2) C(11) H(113)	60.98
C(10) C(2) C(11) H(111)	58.87	C(10) C(2) C(11) H(112)	-50.29	C(10) C(2) C(11) H(113)	-176.08
H(31) C(3) C(12) O(13)	150.70	H(31) C(3) C(12) O(14)	-32.04	S(1) C(5) C(6) H(61)	144.50
N(4) C(5) C(6) H(61)	-108.36	H(51) C(5) C(6) N(20)	-119.71	H(51) C(5) C(6) C(7)	124.64
H(51) C(5) C(6) H(61)	8.71	H(61) C(6) C(7) O(8)	-73.49	H(61) C(6) C(7) N(4)	109.60
O(16) C(17) C(19) H(191)	18.91	O(16) C(17) C(19) H(192)	-106.50	O(16) C(17) C(19) H(193)	134.26
O(18) C(17) C(19) H(191)	-161.87	O(18) C(17) C(19) H(192)	72.72	O(18) C(17) C(19) H(193)	-46.52
O(22) C(21) C(23) H(231)	-36.34	O(22) C(21) C(23) H(232)	72.92	N(20) C(21) C(23) H(231)	145.86
N(20) C(21) C(23) H(232)	-104.88	H(231) C(23) C(24) C(25)	-34.44	H(231) C(23) C(24) C(29)	148.40
H(232) C(23) C(24) C(25)	-144.12	H(232) C(23) C(24) C(29)	38.72	C(23) C(24) C(25) H(251)	-2.35
C(29) C(24) C(25) H(251)	174.89	C(23) C(24) C(29) H(291)	2.48	C(25) C(24) C(29) H(291)	-174.72
C(24) C(25) C(26) H(261)	-171.67	H(251) C(25) C(26) C(27)	-174.04	H(251) C(25) C(26) H(261)	14.35
C(25) C(26) C(27) H(271)	176.58	H(261) C(26) C(27) C(28)	171.39	H(261) C(26) C(27) H(271)	-11.89
C(26) C(27) C(28) H(281)	-179.32	H(271) C(27) C(28) C(29)	-176.50	H(271) C(27) C(28) H(281)	3.86
C(27) C(28) C(29) H(291)	174.85	H(281) C(28) C(29) C(24)	179.41	H(281) C(28) C(29) H(291)	-5.47

Tabelle A.24: Penamecillin, Torsionsswinkel in [°].

S(1)–O(9)	1.4932(8)	S(1)–C(2)	1.8616(6)	S(1)–C(5)	1.8334(7)
O(8)–C(7)	1.2009(9)	O(13)–C(12)	1.2091(6)	O(14)–C(12)	1.3333(6)
O(14)–C(15)	1.4477(7)	O(16)–C(15)	1.4067(8)	O(16)–C(17)	1.3659(13)
O(18)–C(17)	1.2046(12)	O(22)–C(21)	1.2282(6)	N(4)–C(3)	1.4567(7)
N(4)–C(5)	1.4706(8)	N(4)–C(7)	1.3956(8)	N(20)–C(6)	1.4278(7)
N(20)–C(21)	1.3586(6)	C(2)–C(3)	1.5678(11)	C(2)–C(10)	1.5260(10)
C(2)–C(11)	1.5354(9)	C(3)–C(12)	1.5205(7)	C(5)–C(6)	1.5689(9)
C(6)–C(7)	1.5426(9)	C(17)–C(19)	1.4950(13)	C(21)–C(23)	1.5175(7)
C(23)–C(24)	1.5070(7)	C(24)–C(25)	1.3942(7)	C(24)–C(29)	1.3990(9)
C(25)–C(26)	1.3961(11)	C(26)–C(27)	1.3922(14)	C(27)–C(28)	1.3947(13)
C(28)–C(29)	1.3878(12)				
N(20)–H(201)	1.0090	C(3)–H(31)	1.0991	C(5)–H(51)	1.0989
C(6)–H(61)	1.0990	C(10)–H(101)	1.0591	C(10)–H(102)	1.0588
C(10)–H(103)	1.0590	C(11)–H(111)	1.0590	C(11)–H(112)	1.0591
C(11)–H(113)	1.0590	C(15)–H(151)	1.0920	C(15)–H(152)	1.0919
C(19)–H(191)	1.0589	C(19)–H(192)	1.0590	C(19)–H(193)	1.0590
C(23)–H(231)	1.0919	C(23)–H(232)	1.0919	C(25)–H(251)	1.0829
C(26)–H(261)	1.0831	C(27)–H(271)	1.0830	C(28)–H(281)	1.0829
C(29)–H(291)	1.0830				

Tabelle A.25: Penamecillin-1β-sulfoxid, Bindungslängen in [Å].

O(9)–S(1)–C(2)	106.14(4)	O(9)–S(1)–C(5)	104.67(5)	C(2)–S(1)–C(5)	88.35(3)
C(12)–O(14)–C(15)	115.82(4)	C(15)–O(16)–C(17)	115.41(6)	C(3)–N(4)–C(5)	117.22(5)
C(3)–N(4)–C(7)	125.63(5)	C(5)–N(4)–C(7)	93.39(4)	C(6)–N(20)–C(21)	122.06(4)
S(1)–C(2)–C(3)	103.47(4)	S(1)–C(2)–C(10)	107.51(4)	S(1)–C(2)–C(11)	107.76(4)
C(3)–C(2)–C(10)	112.65(6)	C(3)–C(2)–C(11)	113.36(5)	C(10)–C(2)–C(11)	111.48(6)
N(4)–C(3)–C(2)	106.11(4)	N(4)–C(3)–C(12)	111.80(4)	C(2)–C(3)–C(12)	111.12(5)
S(1)–C(5)–N(4)	103.46(4)	S(1)–C(5)–C(6)	117.34(3)	N(4)–C(5)–C(6)	88.37(5)
N(20)–C(6)–C(5)	121.09(6)	N(20)–C(6)–C(7)	116.39(5)	C(5)–C(6)–C(7)	84.21(4)
O(8)–C(7)–N(4)	132.08(6)	O(8)–C(7)–C(6)	135.69(6)	N(4)–C(7)–C(6)	92.21(5)
O(13)–C(12)–O(14)	124.37(5)	O(13)–C(12)–C(3)	125.15(4)	O(14)–C(12)–C(3)	110.48(4)
O(14)–C(15)–O(16)	105.41(5)	O(16)–C(17)–O(18)	122.69(8)	O(16)–C(17)–C(19)	111.01(8)
O(18)–C(17)–C(19)	126.29(11)	O(22)–C(21)–N(20)	123.18(5)	O(22)–C(21)–C(23)	122.44(4)
N(20)–C(21)–C(23)	114.33(4)	C(21)–C(23)–C(24)	113.15(4)	C(23)–C(24)–C(25)	121.72(5)
C(23)–C(24)–C(29)	119.31(4)	C(25)–C(24)–C(29)	118.94(5)	C(24)–C(25)–C(26)	120.70(7)
C(25)–C(26)–C(27)	119.79(7)	C(26)–C(27)–C(28)	119.85(9)	C(27)–C(28)–C(29)	120.11(9)
C(24)–C(29)–C(28)	120.60(6)				
C(6)–N(20)–H(201)	117.60	C(21)–N(20)–H(201)	120.34	N(4)–C(3)–H(31)	111.62
C(2)–C(3)–H(31)	109.60	C(12)–C(3)–H(31)	106.64	S(1)–C(5)–H(51)	110.72
N(4)–C(5)–H(51)	116.65	C(6)–C(5)–H(51)	117.73	N(20)–C(6)–H(61)	107.66
C(5)–C(6)–H(61)	112.06	C(7)–C(6)–H(61)	114.18	C(2)–C(10)–H(101)	110.00
C(2)–C(10)–H(102)	101.63	C(2)–C(10)–H(103)	109.02	H(101)–C(10)–H(102)	115.32
H(101)–C(10)–H(103)	104.70	H(102)–C(10)–H(103)	116.09	C(2)–C(11)–H(111)	107.81
C(2)–C(11)–H(112)	112.61	C(2)–C(11)–H(113)	105.22	H(111)–C(11)–H(112)	111.11
H(111)–C(11)–H(113)	112.51	H(112)–C(11)–H(113)	107.49	O(14)–C(15)–H(151)	109.19
O(14)–C(15)–H(152)	108.90	O(16)–C(15)–H(151)	111.10	O(16)–C(15)–H(152)	104.32
H(151)–C(15)–H(152)	117.22	C(17)–C(19)–H(191)	107.12	C(17)–C(19)–H(192)	116.18
C(17)–C(19)–H(193)	111.31	H(191)–C(19)–H(192)	113.05	H(191)–C(19)–H(193)	104.50
H(192)–C(19)–H(193)	104.10	C(21)–C(23)–H(231)	107.80	C(21)–C(23)–H(232)	104.30
C(24)–C(23)–H(231)	111.24	C(24)–C(23)–H(232)	111.04	H(231)–C(23)–H(232)	109.01
C(24)–C(25)–H(251)	120.60	C(26)–C(25)–H(251)	118.65	C(25)–C(26)–H(261)	121.03
C(27)–C(26)–H(261)	119.14	C(26)–C(27)–H(271)	120.63	C(28)–C(27)–H(271)	119.41

Tabelle A.26: Penamecillin-1β-sulfoxid, Bindungswinkel in [°].

O(9) S(1) C(2) C(3)	62.97(6)	O(9) S(1) C(2) C(10)	-56.42(7)	O(9) S(1) C(2) C(11)	-176.71(6)
C(5) S(1) C(2) C(3)	-41.83(4)	C(5) S(1) C(2) C(10)	-161.23(6)	C(5) S(1) C(2) C(11)	78.49(5)
O(9) S(1) C(5) N(4)	-67.74(5)	O(9) S(1) C(5) C(6)	27.48(6)	C(2) S(1) C(5) N(4)	38.52(4)
C(2) S(1) C(5) C(6)	133.73(5)	C(15) O(14) C(12) O(13)	8.02(9)	C(15) O(14) C(12) C(3)	-171.57(5)
C(12) O(14) C(15) O(16)	164.72(6)	C(17) O(16) C(15) O(14)	-77.25(6)	C(15) O(16) C(17) O(18)	0.09(10)
C(15) O(16) C(17) C(19)	178.92(6)	C(5) N(4) C(3) C(2)	-4.93(6)	C(5) N(4) C(3) C(12)	-126.22(5)
C(7) N(4) C(3) C(2)	-121.71(6)	C(7) N(4) C(3) C(12)	117.00(6)	C(3) N(4) C(5) S(1)	-26.12(5)
C(3) N(4) C(5) C(6)	-143.87(4)	C(7) N(4) C(5) S(1)	107.25(4)	C(7) N(4) C(5) C(6)	-10.49(4)
C(3) N(4) C(7) O(8)	-40.39(11)	C(3) N(4) C(7) C(6)	138.00(6)	C(5) N(4) C(7) O(8)	-167.71(7)
C(5) N(4) C(7) C(6)	10.68(4)	C(21) N(20) C(6) C(5)	118.36(6)	C(21) N(20) C(6) C(7)	-141.98(6)
C(6) N(20) C(21) O(22)	0.66(9)	C(6) N(20) C(21) C(23)	-176.60(5)	S(1) C(2) C(3) N(4)	33.15(4)
S(1) C(2) C(3) C(12)	154.88(3)	C(10) C(2) C(3) N(4)	148.95(5)	C(10) C(2) C(3) C(12)	-89.33(5)
C(11) C(2) C(3) N(4)	-83.28(5)	C(11) C(2) C(3) C(12)	38.45(6)	N(4) C(3) C(12) O(13)	11.91(9)
N(4) C(3) C(12) O(14)	-168.50(5)	C(2) C(3) C(12) O(13)	-106.43(6)	C(2) C(3) C(12) O(14)	73.16(5)
S(1) C(5) C(6) N(20)	22.61(7)	S(1) C(5) C(6) C(7)	-94.81(5)	N(4) C(5) C(6) N(20)	126.94(5)
N(4) C(5) C(6) C(7)	9.52(4)	N(20) C(6) C(7) O(8)	46.30(11)	N(20) C(6) C(7) N(4)	-131.99(6)
C(5) C(6) C(7) O(8)	168.25(8)	C(5) C(6) C(7) N(4)	-10.04(4)	O(22) C(21) C(23) C(24)	59.35(7)
N(20) C(21) C(23) C(24)	-123.36(5)	C(21) C(23) C(24) C(25)	-104.39(6)	C(21) C(23) C(24) C(29)	77.72(6)
C(23) C(24) C(25) C(26)	-177.10(6)	C(29) C(24) C(25) C(26)	0.80(9)	C(23) C(24) C(29) C(28)	177.29(6)
C(25) C(24) C(29) C(28)	-0.66(9)	C(24) C(25) C(26) C(27)	-0.14(11)	C(25) C(26) C(27) C(28)	-0.67(12)
C(26) C(27) C(28) C(29)	0.81(13)	C(27) C(28) C(29) C(24)	-0.14(12)		
O(9) S(1) C(5) H(51)	166.55	C(2) S(1) C(5) H(51)	-87.19	C(12) O(14) C(15) H(151)	45.29
C(12) O(14) C(15) H(152)	-83.84	C(17) O(16) C(15) H(151)	40.90	C(17) O(16) C(15) H(152)	168.09
C(5) N(4) C(3) H(31)	114.42	C(7) N(4) C(3) H(31)	-2.36	C(3) N(4) C(5) H(51)	95.69
C(7) N(4) C(5) H(51)	-130.93	C(21) N(20) C(6) H(61)	-12.35	H(201) N(20) C(6) C(5)	-61.56
H(201) N(20) C(6) C(7)	38.10	H(201) N(20) C(6) H(61)	167.73	H(201) N(20) C(21) O(22)	-179.42
H(201) N(20) C(21) C(23)	3.32	S(1) C(2) C(3) H(31)	-87.51	C(10) C(2) C(3) H(31)	28.29
C(11) C(2) C(3) H(31)	156.06	S(1) C(2) C(10) H(101)	60.22	S(1) C(2) C(10) H(102)	-62.43
S(1) C(2) C(10) H(103)	174.49	C(3) C(2) C(10) H(101)	-53.13	C(3) C(2) C(10) H(102)	-175.78
C(3) C(2) C(10) H(103)	61.14	C(11) C(2) C(10) H(101)	178.12	C(11) C(2) C(10) H(102)	55.47
C(11) C(2) C(10) H(103)	-67.61	S(1) C(2) C(11) H(111)	60.23	S(1) C(2) C(11) H(112)	-62.70
S(1) C(2) C(11) H(113)	-179.49	C(3) C(2) C(11) H(111)	174.11	C(3) C(2) C(11) H(112)	51.17
C(3) C(2) C(11) H(113)	-65.62	C(10) C(2) C(11) H(111)	-57.52	C(10) C(2) C(11) H(112)	179.55
C(10) C(2) C(11) H(113)	62.76	H(31) C(3) C(12) O(13)	134.17	H(31) C(3) C(12) O(14)	-46.24
S(1) C(5) C(6) H(61)	151.41	N(4) C(5) C(6) H(61)	-104.26	H(51) C(5) C(6) N(20)	-113.58
H(51) C(5) C(6) C(7)	128.99	H(51) C(5) C(6) H(61)	15.22	H(61) C(6) C(7) O(8)	-80.14
H(61) C(6) C(7) N(4)	101.57	O(16) C(17) C(19) H(191)	-77.86	O(16) C(17) C(19) H(192)	154.69
O(16) C(17) C(19) H(193)	35.80	O(18) C(17) C(19) H(191)	100.92	O(18) C(17) C(19) H(192)	-26.53
O(18) C(17) C(19) H(193)	-145.42	O(22) C(21) C(23) H(231)	-177.21	O(22) C(21) C(23) H(232)	-61.43
N(20) C(21) C(23) H(231)	0.08	N(20) C(21) C(23) H(232)	115.85	H(231) C(23) C(24) C(25)	134.09
H(231) C(23) C(24) C(29)	-43.81	H(232) C(23) C(24) C(25)	12.49	H(232) C(23) C(24) C(29)	-165.40
C(23) C(24) C(25) H(251)	0.36	C(29) C(24) C(25) H(251)	178.26	C(23) C(24) C(29) H(291)	0.26
C(25) C(24) C(29) H(291)	-177.69	C(24) C(25) C(26) H(261)	177.79	H(251) C(25) C(26) C(27)	-177.65
H(251) C(25) C(26) H(261)	0.28	C(25) C(26) C(27) H(271)	175.47	H(261) C(26) C(27) C(28)	-178.64
H(261) C(26) C(27) H(271)	-2.50	C(26) C(27) C(28) H(281)	-177.09	H(271) C(27) C(28) C(29)	-175.37
H(271) C(27) C(28) H(281)	6.73	C(27) C(28) C(29) H(291)	176.86	H(281) C(28) C(29) C(24)	177.87
H(281) C(28) C(29) H(291)	-5.13				

Tabelle A.27: Penamecillin-1β-sulfoxid, Torsionsswinkel in [°].

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S(1)–C(2)	0.9872	0.8698	-5.90	-4.38	9.36	-0.9(1)	1.03(1)	0.35
S(1)–C(5)	0.9185	0.9006	-7.08	-5.65	9.04	-3.7(1)	1.21(3)	0.25
C(7)–O(8)	0.4414	0.7685	-31.43	-27.79	23.70	-35.5(4)	3.06(7)	0.13
C(12)–O(13)	0.4191	0.7844	-31.35	-30.20	33.50	-28.1(3)	2.99(5)	0.04
C(17)–O(18)	0.4212	0.7866	-30.99	-29.86	31.85	-29.0(1)	2.97(1)	0.04
C(21)–O(22)	0.4509	0.7734	-27.28	-23.24	18.66	-31.9(4)	3.09(7)	0.17
C(12)–O(14)	0.5740	0.7828	-19.11	-18.20	18.94	-18.4(2)	2.25(4)	0.05
C(15)–O(14)	0.5737	0.8461	-14.58	-12.03	15.36	-11.2(1)	1.79(3)	0.21
C(15)–O(16)	0.5849	0.8330	-13.80	-13.01	17.11	-9.7(2)	1.85(4)	0.06
C(17)–O(16)	0.5738	0.7840	-19.25	-18.24	18.71	-18.8(1)	2.26(1)	0.06
C(3)–N(4)	0.6269	0.8158	-14.73	-12.65	17.08	-10.3(2)	1.94(5)	0.16
C(5)–N(4)	0.6478	0.8179	-15.70	-13.22	15.77	-13.1(2)	1.92(4)	0.19
C(7)–N(4)	0.6175	0.7678	-19.33	-16.03	18.14	-17.2(2)	2.20(5)	0.21
C(6)–N(20)	0.6281	0.8003	-16.02	-15.07	16.91	-14.2(2)	2.00(5)	0.06
C(21)–N(20)	0.5848	0.7705	-19.99	-17.59	14.66	-23.0(2)	2.34(5)	0.14
C(2)–C(10)	0.7582	0.7723	-10.16	-9.30	12.28	-7.2(1)	1.58(3)	0.09
C(2)–C(11)	0.7585	0.7724	-10.25	-9.22	12.29	-7.2(1)	1.57(1)	0.11
C(2)–C(3)	0.7785	0.7933	-10.79	-9.86	10.95	-9.7(1)	1.47(4)	0.10
C(3)–C(12)	0.7517	0.7667	-15.44	-14.04	13.39	-16.1(1)	1.93(4)	0.10
C(17)–C(19)	0.7803	0.7140	-12.34	-11.75	12.83	-11.3(1)	1.83(1)	0.05
C(5)–C(6)	0.8058	0.7617	-10.69	-10.31	11.93	-9.1(1)	1.56(4)	0.04
C(6)–C(7)	0.7595	0.8038	-13.29	-12.07	14.16	-11.2(1)	1.76(4)	0.10
C(21)–C(23)	0.8352	0.6878	-12.92	-11.73	11.47	-13.1(1)	1.71(3)	0.10
C(23)–C(24)	0.7064	0.8014	-11.89	-11.76	12.23	-11.4(1)	1.71(3)	0.01
C(24)–C(25)	0.6639	0.7325	-15.61	-14.09	12.10	-17.6(1)	2.08(3)	0.11
C(25)–C(26)	0.6940	0.6962	-18.16	-15.83	12.22	-21.8(1)	2.28(1)	0.15
C(26)–C(27)	0.6960	0.6958	-18.11	-15.79	12.29	-21.6(1)	2.28(1)	0.15
C(27)–C(28)	0.6972	0.6963	-18.05	-15.73	12.32	-21.5(1)	2.27(1)	0.15
C(28)–C(29)	0.6997	0.6990	-17.84	-15.58	12.42	-21.0(1)	2.26(1)	0.14
C(29)–C(24)	0.7317	0.6632	-15.67	-14.10	12.07	-17.7(1)	2.09(3)	0.11

Tabelle A.28: Bindungstopologische Parameter von Penamecillin (Experiment)

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S1–C2	0.9883	0.8643	-6.21	-5.66	6.32	-5.5	1.15	0.10
S1–C5	0.9501	0.8683	-6.65	-5.88	6.11	-6.4	1.21	0.13
C7–O8	0.4145	0.7928	-26.14	-24.67	46.18	-4.6	2.80	0.06
C12–O13	0.4130	0.7902	-27.02	-24.95	47.20	-4.8	2.85	0.08
C17–O18	0.4153	0.7931	-26.79	-24.73	45.17	-6.4	2.83	0.08
C21–O22	0.4225	0.8023	-24.90	-23.32	39.12	-9.1	2.73	0.07
C12–O14	0.4718	0.8837	-15.18	-14.85	18.08	-11.9	2.00	0.02
C15–O14	0.4964	0.9235	-12.21	-10.31	12.03	-10.5	1.71	0.18
C15–O16	0.4982	0.9199	-12.55	-10.59	11.83	-11.3	1.73	0.19
C17–O16	0.4712	0.8855	-15.24	-14.79	18.22	-11.8	1.99	0.03
C3–N4	0.5690	0.8732	-12.63	-12.15	7.61	-17.2	1.82	0.04
C5–N4	0.6000	0.8660	-12.56	-12.08	8.42	-16.2	1.80	0.04
C7–N4	0.5318	0.8523	-16.01	-14.61	9.23	-21.4	2.10	0.10
C6–N20	0.5532	0.8722	-13.11	-12.59	7.48	-18.2	1.88	0.04
C21–N20	0.5021	0.8524	-16.82	-15.15	10.45	-21.5	2.17	0.11
C2–C10	0.7891	0.7414	-10.90	-10.88	8.73	-13.0	1.64	0.00
C2–C11	0.7904	0.7403	-10.86	-10.68	8.64	-12.9	1.63	0.02
C2–C3	0.7712	0.7993	-10.06	-9.86	8.84	-11.1	1.53	0.02
C3–C12	0.7308	0.7870	-12.68	-11.86	9.15	-15.4	1.75	0.07
C17–C19	0.7925	0.7025	-12.59	-11.77	8.50	-15.8	1.77	0.07
C5–C6	0.7915	0.7765	-10.53	-10.27	9.15	-11.7	1.57	0.03
C6–C7	0.7652	0.7918	-11.38	-10.76	9.48	-12.7	1.62	0.06
C21–C23	0.7821	0.7409	-11.91	-11.07	8.91	-14.1	1.68	0.08
C23–C24	0.7465	0.7607	-11.64	-11.31	8.55	-14.4	1.70	0.03
C24–C25	0.7041	0.6921	-15.70	-13.02	8.00	-20.7	2.09	0.21
C25–C26	0.6985	0.6914	-15.65	-13.05	7.79	-20.9	2.09	0.20
C26–C27	0.6957	0.6962	-15.66	-13.04	7.83	-20.9	2.09	0.20
C27–C28	0.6928	0.7006	-15.56	-12.98	7.85	-20.7	2.08	0.20
C28–C29	0.6980	0.7003	-15.58	-12.99	8.02	-20.6	2.08	0.20
C29–C24	0.6971	0.6978	-15.61	-12.94	7.93	-20.6	2.08	0.21

Tabelle A.29: Bindungstopologische Parameter von Penamecillin (B3LYP / 6-311++(d,p))

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S1–C2	0.9885	0.8640	-6.38	-5.86	5.82	-6.4	1.18	0.09
S1–C5	0.9469	0.8715	-6.88	-6.09	5.54	-7.4	1.24	0.13
C7–O8	0.4152	0.7921	-29.46	-26.84	44.73	-11.6	2.91	0.10
C12–O13	0.4137	0.7895	-30.45	-27.29	45.76	-12.0	2.95	0.12
C17–O18	0.4161	0.7922	-30.14	-27.03	43.70	-13.5	2.93	0.12
C21–O22	0.4237	0.8011	-27.94	-25.45	37.94	-15.4	2.82	0.10
C12–O14	0.4731	0.8824	-17.12	-16.68	17.84	-16.0	2.06	0.03
C15–O14	0.4981	0.9218	-13.67	-11.72	12.39	-13.0	1.75	0.17
C15–O16	0.4999	0.9181	-13.97	-11.98	12.22	-13.7	1.77	0.17
C17–O16	0.4726	0.8839	-17.06	-16.80	17.95	-15.9	2.05	0.02
C3–N4	0.5701	0.8721	-13.40	-12.88	8.06	-18.2	1.85	0.04
C5–N4	0.6021	0.8637	-13.14	-12.57	8.77	-16.9	1.82	0.05
C7–N4	0.5366	0.8475	-17.62	-15.52	9.34	-23.8	2.15	0.14
C6–N20	0.5564	0.8690	-14.03	-13.47	7.97	-19.5	1.91	0.04
C21–N20	0.5060	0.8486	-18.79	-16.35	10.49	-24.7	2.23	0.15
C2–C10	0.7873	0.7432	-11.23	-11.17	8.58	-13.8	1.66	0.01
C2–C11	0.7887	0.7419	-11.19	-10.98	8.50	-13.7	1.65	0.02
C2–C3	0.7711	0.7994	-10.26	-10.07	8.69	-11.6	1.55	0.02
C3–C12	0.7281	0.7897	-13.17	-12.24	9.14	-16.3	1.77	0.08
C17–C19	0.7942	0.7009	-13.12	-12.19	8.50	-16.8	1.80	0.08
C5–C6	0.7911	0.7767	-10.79	-10.51	8.98	-12.3	1.58	0.03
C6–C7	0.7617	0.7952	-11.73	-11.00	9.45	-13.3	1.64	0.07
C21–C23	0.7842	0.7387	-12.33	-11.42	8.84	-14.9	1.71	0.08
C23–C24	0.7445	0.7627	-11.99	-11.67	8.42	-15.2	1.73	0.03
C24–C25	0.7035	0.6927	-16.44	-13.72	7.89	-22.3	2.14	0.20
C25–C26	0.6989	0.6910	-16.52	-13.79	7.61	-22.7	2.14	0.20
C26–C27	0.6955	0.6964	-16.49	-13.77	7.68	-22.6	2.14	0.20
C27–C28	0.6920	0.7014	-16.41	-13.71	7.69	-22.4	2.13	0.20
C28–C29	0.6983	0.7001	-16.32	-13.70	7.89	-22.1	2.12	0.19
C29–C24	0.6981	0.6968	-16.41	-13.65	7.79	-22.3	2.13	0.20

Tabelle A.30: Bindungstopologische Parameter von Penamecillin (B3LYP / 6-311++(3df,3pd))

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S(1)–C(2)	0.9698	0.8952	-6.82	-6.19	7.13	-5.9(1)	1.18(2)	0.10
S(1)–C(5)	0.9376	0.8977	-7.56	-5.53	8.54	-4.6(1)	1.24(3)	0.37
S(1)–O(9)	0.6883	0.8090	-18.39	-13.22	9.56	-22.1(1)	2.41(7)	0.39
C(7)–O(8)	0.4940	0.7074	-30.62	-25.80	24.42	-32.0(4)	3.18(87)	0.19
C(12)–O(13)	0.4642	0.7449	-25.01	-21.43	21.84	-24.6(3)	2.82(5)	0.17
C(17)–O(18)	0.4604	0.7444	-25.21	-21.76	22.42	-24.6(1)	2.84(1)	0.16
C(21)–O(22)	0.4931	0.7353	-29.38	-23.75	18.97	-34.2(4)	2.99(8)	0.24
C(12)–O(14)	0.5565	0.7771	-18.54	-16.11	20.43	-14.2(2)	2.20(5)	0.15
C(15)–O(14)	0.6417	0.8082	-12.26	-10.72	19.57	-3.4(1)	1.65(4)	0.14
C(15)–O(16)	0.6298	0.7771	-14.13	-13.82	22.36	-5.6(1)	1.92(4)	0.02
C(17)–O(16)	0.5873	0.7788	-16.88	-15.11	22.13	-9.9(1)	2.09(1)	0.12
C(3)–N(4)	0.6748	0.7832	-15.46	-11.82	17.64	-9.6(2)	1.82(5)	0.31
C(5)–N(4)	0.6655	0.8062	-15.37	-13.96	17.09	-12.2(2)	1.92(5)	0.10
C(7)–N(4)	0.6010	0.7947	-19.99	-16.00	19.49	-16.5(3)	2.20(6)	0.25
C(6)–N(20)	0.6685	0.7637	-13.90	-10.31	19.55	-4.7(2)	1.73(5)	0.35
C(21)–N(20)	0.6104	0.7484	-22.18	-19.31	18.32	-23.2(3)	2.42(6)	0.15
C(2)–C(10)	0.7833	0.7428	-11.87	-11.08	11.52	-11.4(1)	1.75(3)	0.07
C(2)–C(11)	0.7865	0.7490	-11.64	-10.88	11.60	-10.9(1)	1.71(1)	0.07
C(2)–C(3)	0.7891	0.7817	-9.97	-9.55	12.35	-7.2(1)	1.48(5)	0.04
C(3)–C(12)	0.7539	0.7666	-12.65	-9.68	13.17	-9.2(1)	1.61(4)	0.31
C(17)–C(19)	0.7572	0.7379	-12.00	-11.65	11.85	-11.8(1)	1.73(1)	0.03
C(5)–C(6)	0.8095	0.7601	-9.50	-8.36	12.64	-5.2(2)	1.37(5)	0.14
C(6)–C(7)	0.7696	0.7748	-13.42	-10.89	14.81	-9.5(2)	1.69(4)	0.23
C(21)–C(23)	0.7935	0.7252	-11.54	-10.76	12.65	-9.6(1)	1.60(4)	0.07
C(23)–C(24)	0.7622	0.7464	-12.09	-10.23	13.11	-9.2(1)	1.66(5)	0.18
C(24)–C(25)	0.7109	0.6838	-17.84	-15.15	12.36	-20.6(1)	2.23(3)	0.18
C(25)–C(26)	0.6986	0.6974	-17.32	-15.03	12.15	-20.2(1)	2.18(2)	0.15
C(26)–C(27)	0.6962	0.6961	-17.46	-15.13	12.07	-20.5(1)	2.19(1)	0.15
C(27)–C(28)	0.6973	0.6974	-17.38	-15.06	12.12	-20.3(1)	2.18(1)	0.15
C(28)–C(29)	0.6935	0.6942	-17.59	-15.28	11.97	-20.9(1)	2.21(1)	0.15
C(29)–C(24)	0.6864	0.7132	-17.66	-15.02	12.47	-20.2(1)	2.21(3)	0.18

Tabelle A.31: Bindungstopologische Parameter von Penamecillin-1β-sulfoxid (Experiment)

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S1–C2	1.0040	0.8572	-6.75	-6.45	7.15	-6.1	1.19	0.05
S1–C5	0.9712	0.8626	-7.18	-6.82	6.99	-7.0	1.25	0.05
S1–O9	0.5865	0.9065	-9.97	-9.78	35.81	16.1	1.81	0.02
C7–O8	0.4125	0.7892	-26.72	-25.07	48.01	-3.8	2.84	0.07
C12–O13	0.4159	0.7936	-26.48	-24.30	44.46	-6.3	2.82	0.09
C17–O18	0.4139	0.7915	-27.16	-25.02	46.45	-5.7	2.84	0.09
C21–O22	0.4242	0.8050	-24.42	-23.00	37.92	-9.5	2.70	0.06
C12–O14	0.4566	0.8768	-16.11	-15.73	22.68	-9.2	2.07	0.02
C15–O14	0.5202	0.9280	-11.45	-9.64	9.94	-11.1	1.62	0.19
C15–O16	0.4886	0.9184	-13.19	-11.06	13.04	-11.2	1.77	0.19
C17–O16	0.4778	0.8886	-14.78	-14.44	16.64	-12.6	1.96	0.02
C3–N4	0.5841	0.8726	-12.24	-11.81	7.78	-16.3	1.77	0.04
C5–N4	0.6082	0.8631	-12.32	-11.75	8.59	-15.5	1.78	0.05
C7–N4	0.5452	0.8513	-15.66	-14.25	9.19	-20.7	2.05	0.10
C6–N20	0.5612	0.8665	-13.01	-12.90	7.59	-18.3	1.87	0.01
C21–N20	0.5045	0.8543	-16.65	-15.03	10.23	-21.5	2.15	0.11
C2–C10	0.7954	0.7309	-10.81	-10.61	8.51	-12.9	1.63	0.02
C2–C11	0.7934	0.7420	-10.58	-10.34	8.51	-12.4	1.61	0.02
C2–C3	0.7714	0.7965	-10.06	-9.83	8.76	-11.1	1.53	0.02
C3–C12	0.7353	0.7854	-12.64	-11.48	9.21	-14.9	1.73	0.10
C17–C19	0.7926	0.7027	-12.58	-11.73	8.43	-15.9	1.76	0.07
C5–C6	0.8082	0.7627	-10.17	-9.85	8.92	-11.1	1.53	0.03
C6–C7	0.7669	0.7773	-11.90	-11.08	9.54	-13.4	1.67	0.07
C21–C23	0.7854	0.7321	-12.01	-11.41	8.93	-14.5	1.70	0.05
C23–C24	0.7562	0.7507	-11.60	-11.23	8.52	-14.3	1.69	0.03
C24–C25	0.7014	0.6928	-15.66	-12.90	7.91	-20.7	2.09	0.21
C25–C26	0.6974	0.6986	-15.54	-12.95	7.89	-20.6	2.08	0.20
C26–C27	0.6955	0.6973	-15.68	-13.03	7.85	-20.9	2.09	0.20
C27–C28	0.6943	0.6999	-15.58	-13.02	7.85	-20.8	2.08	0.20
C28–C29	0.6911	0.6965	-15.90	-13.19	7.81	-21.3	2.11	0.21
C29–C24	0.6947	0.7046	-15.53	-12.86	7.98	-20.4	2.07	0.21

Tabelle A.32: Bindungstopologische Parameter von Penamecillin-1β-sulfoxid (B3LYP / 6-311++(d,p))

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S1–C2	1.0030	0.8583	-7.09	-6.66	6.50	-7.3	1.22	0.07
S1–C5	0.9673	0.8665	-7.54	-7.06	6.28	-8.3	1.28	0.07
S1–O9	0.5926	0.9003	-10.95	-10.85	33.90	12.1	1.88	0.01
C7–O8	0.4129	0.7888	-30.07	-27.30	46.69	-10.7	2.94	0.10
C12–O13	0.4167	0.7929	-29.84	-26.60	43.15	-13.3	2.92	0.12
C17–O18	0.4148	0.7907	-30.56	-27.33	44.93	-13.0	2.95	0.12
C21–O22	0.4256	0.8036	-27.41	-25.11	36.70	-15.8	2.80	0.09
C12–O14	0.4581	0.8754	-18.35	-17.80	22.19	-13.9	2.14	0.03
C15–O14	0.5197	0.9285	-12.67	-10.71	10.38	-13.0	1.66	0.18
C15–O16	0.4911	0.9158	-14.68	-12.56	13.36	-13.9	1.82	0.17
C17–O16	0.4790	0.8874	-16.55	-16.27	16.50	-16.3	2.01	0.02
C3–N4	0.5843	0.8724	-12.89	-12.46	8.10	-17.2	1.80	0.04
C5–N4	0.6091	0.8620	-12.85	-12.20	8.87	-16.2	1.80	0.05
C7–N4	0.5494	0.8471	-17.11	-15.06	9.26	-22.9	2.10	0.14
C6–N20	0.5632	0.8644	-13.84	-13.73	8.01	-19.6	1.91	0.01
C21–N20	0.5085	0.8503	-18.58	-16.20	10.29	-24.5	2.21	0.15
C2–C10	0.7930	0.7333	-11.15	-10.92	8.37	-13.7	1.66	0.02
C2–C11	0.7909	0.7445	-10.87	-10.64	8.36	-13.1	1.63	0.02
C2–C3	0.7711	0.7968	-10.25	-10.01	8.62	-11.6	1.55	0.02
C3–C12	0.7325	0.7882	-13.15	-11.85	9.18	-15.8	1.76	0.11
C17–C19	0.7941	0.7012	-13.12	-12.17	8.42	-16.9	1.80	0.08
C5–C6	0.8077	0.7630	-10.45	-10.11	8.75	-11.8	1.55	0.03
C6–C7	0.7631	0.7811	-12.28	-11.36	9.50	-14.1	1.69	0.08
C21–C23	0.7882	0.7294	-12.45	-11.75	8.88	-15.3	1.73	0.06
C23–C24	0.7539	0.7529	-11.98	-11.63	8.37	-15.2	1.72	0.03
C24–C25	0.7005	0.6937	-16.46	-13.62	7.76	-22.3	2.14	0.21
C25–C26	0.6971	0.6988	-16.34	-13.66	7.75	-22.3	2.13	0.20
C26–C27	0.6954	0.6973	-16.50	-13.76	7.74	-22.5	2.14	0.20
C27–C28	0.6940	0.7002	-16.41	-13.74	7.73	-22.4	2.13	0.19
C28–C29	0.6910	0.6966	-16.73	-13.94	7.67	-23.0	2.16	0.20
C29–C24	0.6957	0.7036	-16.27	-13.54	7.86	-22.0	2.12	0.20

Tabelle A.33: Bindungstopologische Parameter von Penamecillin-1β-sulfoxid (B3LYP / 6-311++(3df,3pd))

Bindung	d_1 [Å]	d_2 [Å]	λ_1	λ_2	λ_3	$\nabla^2\rho$ [eÅ^{-5}]	ρ [eÅ^{-3}]	ϵ
S1–C2	1.0220	0.8397	-7.78	-7.31	5.33	-9.8	1.30	0.06
S1–C5	0.9741	0.8599	-8.32	-7.78	4.97	-11.1	1.37	0.07
S1–O9	0.5809	0.9120	-12.49	-12.35	39.73	14.9	1.92	0.01
C7–O8	0.4002	0.8015	-33.06	-29.72	55.30	-7.5	2.98	0.11
C12–O13	0.4030	0.8066	-32.77	-28.98	51.67	-10.1	2.95	0.13
C17–O18	0.4014	0.8040	-33.54	-29.75	53.65	-9.6	2.98	0.13
C21–O22	0.4107	0.8185	-30.01	-27.80	43.98	-13.8	2.84	0.08
C12–O14	0.4326	0.9008	-20.78	-19.77	30.61	-9.9	2.15	0.05
C15–O14	0.4671	0.9811	-13.10	-10.15	15.30	-8.0	1.62	0.29
C15–O16	0.4521	0.9549	-15.80	-12.61	20.49	-7.9	1.80	0.25
C17–O16	0.4454	0.9209	-18.83	-17.57	23.53	-12.9	2.02	0.07
C3–N4	0.5233	0.9334	-13.20	-13.01	5.72	-20.5	1.84	0.01
C5–N4	0.5620	0.9093	-13.21	-12.93	5.49	-20.7	1.85	0.02
C7–N4	0.4982	0.8984	-18.20	-17.24	7.58	-27.9	2.16	0.06
C6–N20	0.5053	0.9224	-14.84	-14.30	6.72	-22.4	1.95	0.04
C21–N20	0.4650	0.8938	-20.09	-18.80	13.21	-25.7	2.25	0.07
C2–C10	0.8074	0.7189	-11.90	-11.70	6.84	-16.8	1.74	0.02
C2–C11	0.8017	0.7337	-11.62	-11.41	6.90	-16.1	1.71	0.02
C2–C3	0.7655	0.8024	-11.07	-10.84	7.24	-14.7	1.63	0.02
C3–C12	0.7133	0.8074	-14.34	-12.93	7.43	-19.8	1.86	0.11
C17–C19	0.8201	0.6752	-14.09	-13.11	6.47	-20.7	1.89	0.08
C5–C6	0.8181	0.7531	-11.33	-10.89	7.30	-14.9	1.64	0.04
C6–C7	0.7497	0.7949	-13.36	-12.45	7.86	-17.9	1.79	0.07
C21–C23	0.8077	0.7099	-13.48	-12.79	7.17	-19.1	1.83	0.05
C23–C24	0.7530	0.7539	-12.82	-12.49	6.94	-18.4	1.81	0.03
C24–C25	0.7028	0.6913	-17.47	-14.07	6.13	-25.4	2.21	0.24
C25–C26	0.6960	0.7000	-17.35	-14.19	6.13	-25.4	2.20	0.22
C26–C27	0.6953	0.6975	-17.50	-14.25	6.11	-25.6	2.21	0.23
C27–C28	0.6915	0.7027	-17.41	-14.27	6.10	-25.6	2.21	0.22
C28–C29	0.6897	0.6979	-17.75	-14.45	6.03	-26.2	2.24	0.23
C29–C24	0.6934	0.7058	-17.27	-14.04	6.23	-25.1	2.19	0.23

Tabelle A.34: Bindungstopologische Parameter von Penamecillin-1β-sulfoxid (HF/6-311++(3df,3pd))

A.3 Fulleren

2θ	ω	χ	ϕ	Scan	Δ	Frames	t
0°	47°	-54°	30°	ω	-0.3°	260	1 s
0°	47°	-54°	120°	ω	-0.3°	260	1 s
0°	47°	0°	210°	ω	-0.3°	260	1 s
0°	47°	0°	300°	ω	-0.3°	260	1 s
-30°	45°	-54°	0°	ω	-0.3°	300	4 s
-30°	45°	-54°	90°	ω	-0.3°	300	4 s
-30°	45°	-54°	180°	ω	-0.3°	300	4 s
-30°	45°	-54°	270°	ω	-0.3°	300	4 s
-30°	45°	0°	30°	ω	-0.3°	300	4 s
-30°	0°	0°	0°	ϕ	-0.3°	600	4 s
30°	46°	54°	0°	ω	-0.3°	300	6 s
30°	46°	54°	90°	ω	-0.3°	300	6 s
30°	46°	54°	180°	ω	-0.3°	300	6 s
30°	46°	54°	270°	ω	-0.3°	300	6 s
30°	46°	10°	30°	ω	-0.3°	300	6 s
30°	-20°	-54°	0°	ϕ	-0.3°	600	6 s
-60°	24°	-54°	0°	ω	-0.3°	236	8 s
-60°	24°	-54°	90°	ω	-0.3°	236	8 s
-60°	24°	-54°	180°	ω	-0.3°	236	8 s
-60°	24°	-54°	270°	ω	-0.3°	236	8 s
-60°	24°	0°	30°	ω	-0.3°	236	8 s
-60°	24°	0°	120°	ω	-0.3°	236	8 s
-60°	24°	0°	210°	ω	-0.3°	236	8 s
-60°	0°	0°	180°	ϕ	-0.3°	600	8 s
-60°	24°	0°	60°	ω	-0.3°	236	8 s
-60°	24°	0°	150°	ω	-0.3°	236	8 s
-60°	24°	0°	240°	ω	-0.3°	236	8 s
-60°	-46°	-54°	0°	ϕ	-0.3°	600	8 s
-60°	-46°	60°	0°	ϕ	-0.3°	1200	8 s
-60°	-20°	20°	0°	ϕ	-0.3°	1200	8 s
-60°	23°	-54°	0°	ω	-0.3°	207	12 s
-60°	23°	-54°	90°	ω	-0.3°	207	12 s
-60°	23°	-54°	180°	ω	-0.3°	207	12 s
-60°	23°	-54°	270°	ω	-0.3°	207	12 s

Tabelle A.35: Fulleren, Meßstrategie. Detektorabstand für 0° Stellung 6.5 cm, sonst 4 cm.

Schale $\sin\theta/\lambda_{max}$ [Å^{-1}]	Schale d_{min} [Å]	gemessene Reflexe	fehlende Reflexe	Vollständigkeit [%]
0.4636	1.078	3493	1	99.9
0.5841	0.856	3460	0	100.0
0.6686	0.748	3495	0	100.0
0.7359	0.679	3480	0	100.0
0.7928	0.631	3469	2	99.9
0.8424	0.594	3451	12	99.7
0.8868	0.564	3491	21	99.4
0.9272	0.539	3458	35	99.0
0.9643	0.518	3441	49	98.6
0.9988	0.501	3365	76	97.8
1.0311	0.485	3394	84	97.6
1.0614	0.471	3361	112	96.8
1.0901	0.459	3383	137	96.1
1.1174	0.447	3298	155	95.5
1.1434	0.437	3294	182	94.8
1.1682	0.428	3256	223	93.6
1.1921	0.419	3262	242	93.1
1.2150	0.412	3215	268	92.3
1.2371	0.404	3174	304	91.3
1.2584	0.397	1649	1609	50.6

Tabelle A.36: Fulleren, Vollständigkeit des Datensatzes in Schalen unterschiedlicher Auflösung (nach Mittelung).

O(101)–C(101)	1.2061	O(102)–C(101)	1.3378	O(102)–C(102)	1.4607	O(111)–C(111)	1.2085
O(112)–C(111)	1.3373	O(112)–C(112)	1.4579	O(201)–C(201)	1.2100	O(202)–C(201)	1.3352
O(202)–C(202)	1.4597	O(211)–C(211)	1.2073	O(212)–C(211)	1.3417	O(212)–C(212)	1.4582
O(301)–C(301)	1.2045	O(302)–C(301)	1.3451	O(302)–C(302)	1.4610	O(311)–C(311)	1.2066
O(312)–C(311)	1.3340	O(312)–C(312)	1.4620	C(1)–C(2)	1.5984	C(1)–C(6)	1.4947
C(1)–C(9)	1.4896	C(1)–C(100)	1.5193	C(2)–C(3)	1.4946	C(2)–C(12)	1.4958
C(2)–C(100)	1.5143	C(3)–C(4)	1.3951	C(3)–C(14)	1.4332	C(4)–C(5)	1.4755
C(4)–C(17)	1.4323	C(5)–C(6)	1.3998	C(5)–C(19)	1.4375	C(6)–C(7)	1.4356
C(7)–C(8)	1.4732	C(7)–C(21)	1.3929	C(8)–C(9)	1.4281	C(8)–C(24)	1.3991
C(9)–C(10)	1.3918	C(10)–C(11)	1.4746	C(10)–C(35)	1.4310	C(11)–C(12)	1.4021
C(11)–C(37)	1.4340	C(12)–C(13)	1.4349	C(13)–C(14)	1.4768	C(13)–C(39)	1.3966
C(14)–C(15)	1.3978	C(15)–C(16)	1.4319	C(15)–C(23)	1.4978	C(16)–C(17)	1.3976
C(16)–C(34)	1.4760	C(17)–C(18)	1.4937	C(18)–C(19)	1.5008	C(18)–C(36)	1.5906
C(18)–C(300)	1.5245	C(19)–C(20)	1.3964	C(20)–C(21)	1.4355	C(20)–C(38)	1.4724
C(21)–C(22)	1.4911	C(22)–C(23)a	1.5937	C(22)–C(39)a	1.4909	C(23)–C(24)a	1.5011
C(24)–C(34)a	1.4372	C(34)–C(35)a	1.3997	C(35)–C(36)a	1.4936	C(36)–C(37)a	1.4931
C(37)–C(38)a	1.3938	C(38)–C(39)a	1.4313	C(100)–C(101)	1.5207	C(100)–C(111)	1.5126
C(102)–C(103)	1.5139	C(112)–C(113)	1.5097	C(200)–C(22)	1.5236	C(200)–C(201)	1.5155
C(200)–C(211)	1.5265	C(200)–C(23)a	1.5231	C(202)–C(203)	1.5063	C(212)–C(213)	1.5118
C(300)–C(36)	1.5189	C(300)–C(301)	1.5114	C(300)–C(311)	1.5207	C(302)–C(303)	1.4959
C(312)–C(313)	1.5079	O(332)–C(301)	1.3239	O(332)–C(332)	1.4657	C(332)–C(333)	1.5103
C(102)–H(10A)	1.0798	C(102)–H(10B)	1.0801	C(103)–H(10C)	1.0798	C(103)–H(10D)	1.0803
C(103)–H(10E)	1.0802	C(112)–H(11A)	1.0804	C(112)–H(11B)	1.0803	C(113)–H(11C)	1.0794
C(113)–H(11D)	1.0810	C(113)–H(11E)	1.0801	C(202)–H(20A)	1.0799	C(202)–H(20B)	1.0798
C(203)–H(20C)	1.0798	C(203)–H(20D)	1.0802	C(203)–H(20E)	1.0800	C(212)–H(21A)	1.0802
C(212)–H(21B)	1.0800	C(213)–H(21C)	1.0799	C(213)–H(21D)	1.0805	C(213)–H(21E)	1.0800
C(302)–H(30A)	1.0810	C(302)–H(30B)	1.0799	C(303)–H(30C)	1.0815	C(303)–H(30D)	1.0817
C(303)–H(30E)	1.0779	C(312)–H(31A)	1.0801	C(312)–H(31B)	1.0801	C(313)–H(31C)	1.0799
C(313)–H(31D)	1.0806	C(313)–H(31E)	1.0802	C(332)–H(33A)	1.0811	C(332)–H(33B)	1.0768
C(333)–H(33C)	1.0808	C(333)–H(33D)	1.0800	C(333)–H(33E)	1.0811		
F(1)–C(81)	1.3552	F(2)–C(82)	1.3558	C(81)–C(82)	1.3965	C(81)–C(86)	1.3864
C(82)–C(83)	1.3895	C(83)–C(84)	1.4046	C(84)–C(85)	1.3976	C(85)-C(86)	1.4028
C(83)–H(83A)	1.0390	C(84)–H(84A)	1.0394	C(85)–H(85A)	1.0391	C(86)–H(86A)	1.0390

Tabelle A.37: Fulleren, Bindungslängen in [Å].

C(101)–O(102)–C(102)	115.97	C(111)–O(112)–C(112)	117.74	C(201)–O(202)–C(202)	116.72
C(211)–O(212)–C(212)	116.33	C(301)–O(302)–C(302)	116.91	C(311)–O(312)–C(312)	116.23
C(2)–C(1)–C(6)	115.54	C(2)–C(1)–C(9)	117.39	C(2)–C(1)–C(100)	58.05
C(6)–C(1)–C(9)	104.94	C(6)–C(1)–C(100)	126.72	C(9)–C(1)–C(100)	125.35
C(1)–C(2)–C(3)	116.78	C(1)–C(2)–C(12)	114.86	C(1)–C(2)–C(100)	58.36
C(3)–C(2)–C(12)	105.10	C(3)–C(2)–C(100)	128.41	C(12)–C(2)–C(100)	123.86
C(2)–C(3)–C(4)	122.32	C(2)–C(3)–C(14)	108.75	C(4)–C(3)–C(14)	119.45
C(3)–C(4)–C(5)	120.91	C(3)–C(4)–C(17)	120.35	C(5)–C(4)–C(17)	108.20
C(4)–C(5)–C(6)	121.17	C(4)–C(5)–C(19)	108.28	C(6)–C(5)–C(19)	120.37
C(1)–C(6)–C(5)	122.77	C(1)–C(6)–C(7)	108.22	C(5)–C(6)–C(7)	119.49
C(6)–C(7)–C(8)	108.65	C(6)–C(7)–C(21)	120.44	C(8)–C(7)–C(21)	120.53
C(7)–C(8)–C(9)	107.71	C(7)–C(8)–C(24)	121.76	C(9)–C(8)–C(24)	120.67
C(1)–C(9)–C(8)	109.27	C(1)–C(9)–C(10)	122.27	C(8)–C(9)–C(10)	120.11
C(9)–C(10)–C(11)	120.63	C(9)–C(10)–C(35)	119.91	C(11)–C(10)–C(35)	108.76
C(10)–C(11)–C(12)	121.33	C(10)–C(11)–C(37)	107.76	C(12)–C(11)–C(37)	120.52
C(2)–C(12)–C(11)	122.80	C(2)–C(12)–C(13)	108.54	C(11)–C(12)–C(13)	119.42
C(12)–C(13)–C(14)	108.32	C(12)–C(13)–C(39)	119.98	C(14)–C(13)–C(39)	121.00
C(3)–C(14)–C(13)	108.14	C(3)–C(14)–C(15)	120.53	C(13)–C(14)–C(15)	120.73
C(14)–C(15)–C(16)	119.42	C(14)–C(15)–C(23)	122.56	C(16)–C(15)–C(23)	108.96
C(15)–C(16)–C(17)	120.30	C(15)–C(16)–C(34)	108.27	C(17)–C(16)–C(34)	120.70
C(4)–C(17)–C(16)	119.70	C(4)–C(17)–C(18)	108.97	C(16)–C(17)–C(18)	122.57
C(17)–C(18)–C(19)	104.88	C(17)–C(18)–C(36)	116.55	C(17)–C(18)–C(300)	125.20
C(19)–C(18)–C(36)	115.59	C(19)–C(18)–C(300)	127.17	C(36)–C(18)–C(300)	58.32
C(5)–C(19)–C(18)	108.53	C(5)–C(19)–C(20)	119.23	C(18)–C(19)–C(20)	122.51
C(19)–C(20)–C(21)	120.64	C(19)–C(20)–C(38)	121.24	C(21)–C(20)–C(38)	108.00
C(7)–C(21)–C(20)	119.50	C(7)–C(21)–C(22)	122.26	C(20)–C(21)–C(22)	108.76
C(21)–C(22)–C(200)	127.95	C(21)–C(22)–C(23)a	117.55	C(21)–C(22)–C(39)a	105.02
C(200)–C(22)–C(23)a	58.45	C(200)–C(22)–C(39)a	123.47	C(23)a–C(22)–C(39)a	116.22
C(15)–C(23)–C(22)a	116.04	C(15)–C(23)–C(24)a	104.69	C(15)–C(23)–C(200)a	124.97
C(22)a–C(23)–C(24)a	114.96	C(22)a–C(23)–C(200)a	58.48	C(24)a–C(23)–C(200)a	128.00
C(8)–C(24)–C(23)a	122.49	C(8)–C(24)–C(34)a	118.72	C(23)a–C(24)–C(34)a	108.69
C(16)–C(34)–C(24)a	108.22	C(16)–C(34)–C(35)a	120.80	C(24)a–C(34)–C(35)a	120.54
C(10)–C(35)–C(34)a	119.77	C(10)–C(35)–C(36)a	108.33	C(34)a–C(35)–C(36)a	122.97
C(18)–C(36)–C(300)	58.66	C(18)–C(36)–C(35)a	115.71	C(18)–C(36)–C(37)a	116.92
C(300)–C(36)–C(35)a	124.03	C(300)–C(36)–C(37)a	127.63	C(35)a–C(36)–C(37)a	105.17
C(11)–C(37)–C(36)a	108.83	C(11)–C(37)–C(38)a	119.38	C(36)a–C(37)–C(38)a	122.25
C(20)–C(38)–C(37)a	121.02	C(20)–C(38)–C(39)a	108.33	C(37)a–C(38)–C(39)a	120.37
C(13)–C(39)–C(22)a	122.69	C(13)–C(39)–C(38)a	120.07	C(22)a–C(39)–C(38)a	108.73
C(1)–C(100)–C(2)	63.59	C(1)–C(100)–C(101)	118.94	C(1)–C(100)–C(111)	115.03
C(2)–C(100)–C(101)	116.53	C(2)–C(100)–C(111)	121.90	C(101)–C(100)–C(111)	112.63
O(101)–C(101)–O(102)	125.66	O(101)–C(101)–C(100)	125.57	O(102)–C(101)–C(100)	108.77
O(102)–C(102)–C(103)	109.65	O(111)–C(111)–O(112)	125.84	O(111)–C(111)–C(100)	125.56
O(112)–C(111)–C(100)	108.46	O(112)–C(112)–C(113)	106.25	C(22)–C(200)–C(201)	117.67
C(22)–C(200)–C(211)	115.23	C(22)–C(200)–C(23)a	63.08	C(201)–C(200)–C(211)	113.58
C(201)–C(200)–C(23)a	118.99	C(211)–C(200)–C(23)a	119.15	O(201)–C(201)–O(202)	125.07
O(201)–C(201)–C(200)	124.54	O(202)–C(201)–C(200)	110.37	O(202)–C(202)–C(203)	106.37
O(211)–C(211)–O(212)	125.51	O(211)–C(211)–C(200)	124.91	O(212)–C(211)–C(200)	109.56
O(212)–C(212)–C(213)	107.24	C(18)–C(300)–C(36)	63.02	C(18)–C(300)–C(301)	118.41
C(18)–C(300)–C(311)	118.47	C(36)–C(300)–C(301)	118.98	C(36)–C(300)–C(311)	115.98
C(301)–C(300)–C(311)	113.26	O(301)–C(301)–O(302)	125.80	O(301)–C(301)–C(300)	124.25
O(301)–C(301)–O(332)	123.17	O(302)–C(301)–C(300)	109.69	C(300)–C(301)–O(332)	111.87
O(302)–C(302)–C(303)	110.05	O(311)–C(311)–O(312)	125.80	O(311)–C(311)–C(300)	124.48
O(312)–C(311)–C(300)	109.71	O(312)–C(312)–C(313)	110.82	C(301)–O(332)–C(332)	115.87
O(332)–C(332)–C(333)	106.26				

Tabelle A.38: Fulleren, Bindungswinkel in [°] (Teil 1).

O(102)–C(102)–H(10A)	110.04	O(102)–C(102)–H(10B)	109.75	C(103)–C(102)–H(10A)	109.79
C(103)–C(102)–H(10B)	109.44	H(10A)–C(102)–H(10B)	108.15	C(102)–C(103)–H(10C)	109.63
C(102)–C(103)–H(10D)	109.48	C(102)–C(103)–H(10E)	108.86	H(10C)–C(103)–H(10D)	110.17
H(10C)–C(103)–H(10E)	109.21	H(10D)–C(103)–H(10E)	109.47	O(112)–C(112)–H(11A)	110.57
O(112)–C(112)–H(11B)	110.78	C(113)–C(112)–H(11A)	110.60	C(113)–C(112)–H(11B)	110.56
H(11A)–C(112)–H(11B)	108.10	C(112)–C(113)–H(11C)	109.42	C(112)–C(113)–H(11D)	109.05
C(112)–C(113)–H(11E)	109.28	H(11C)–C(113)–H(11D)	109.29	H(11C)–C(113)–H(11E)	109.91
H(11D)–C(113)–H(11E)	109.87	O(202)–C(202)–H(20A)	110.64	O(202)–C(202)–H(20B)	110.65
C(203)–C(202)–H(20A)	110.69	C(203)–C(202)–H(20B)	110.10	H(20A)–C(202)–H(20B)	108.40
C(202)–C(203)–H(20C)	109.83	C(202)–C(203)–H(20D)	110.11	C(202)–C(203)–H(20E)	109.41
H(20C)–C(203)–H(20D)	109.38	H(20C)–C(203)–H(20E)	108.82	H(20D)–C(203)–H(20E)	109.27
O(212)–C(212)–H(21A)	110.53	O(212)–C(212)–H(21B)	110.55	C(213)–C(212)–H(21A)	110.36
C(213)–C(212)–H(21B)	110.40	H(21A)–C(212)–H(21B)	107.78	C(212)–C(213)–H(21C)	109.53
C(212)–C(213)–H(21D)	109.41	C(212)–C(213)–H(21E)	109.30	H(21C)–C(213)–H(21D)	109.66
H(21C)–C(213)–H(21E)	109.15	H(21D)–C(213)–H(21E)	109.76	O(302)–C(302)–H(30A)	108.44
O(302)–C(302)–H(30B)	109.59	C(303)–C(302)–H(30A)	109.39	C(303)–C(302)–H(30B)	110.97
H(30A)–C(302)–H(30B)	108.33	C(302)–C(303)–H(30C)	107.03	C(302)–C(303)–H(30D)	108.13
C(302)–C(303)–H(30E)	107.44	H(30C)–C(303)–H(30D)	110.55	H(30C)–C(303)–H(30E)	111.74
H(30D)–C(303)–H(30E)	111.72	O(312)–C(312)–H(31A)	109.78	O(312)–C(312)–H(31B)	109.60
C(313)–C(312)–H(31A)	109.67	C(313)–C(312)–H(31B)	109.33	H(31A)–C(312)–H(31B)	107.57
C(312)–C(313)–H(31C)	109.81	C(312)–C(313)–H(31D)	109.44	C(312)–C(313)–H(31E)	108.97
H(31C)–C(313)–H(31D)	109.94	H(31C)–C(313)–H(31E)	109.50	H(31D)–C(313)–H(31E)	109.16
O(332)–C(332)–H(33A)	110.60	O(332)–C(332)–H(33B)	113.87	C(333)–C(332)–H(33A)	104.79
C(333)–C(332)–H(33B)	110.81	H(33A)–C(332)–H(33B)	110.07	C(332)–C(333)–H(33C)	108.96
C(332)–C(333)–H(33D)	110.89	C(332)–C(333)–H(33E)	108.01	H(33C)–C(333)–H(33D)	107.63
H(33C)–C(333)–H(33E)	110.79	H(33D)–C(333)–H(33E)	110.57		
F(1)–C(81)–C(82)	118.56	F(1)–C(81)–C(86)	120.77	C(82)–C(81)–C(86)	120.65
F(2)–C(82)–C(81)	118.22	F(2)–C(82)–C(83)	120.70	C(81)–C(82)–C(83)	121.07
C(82)–C(83)–C(84)	118.57	C(83)–C(84)–C(85)	120.31	C(84)–C(85)–C(86)	120.59
C(81)–C(86)–C(85)	118.81				
C(82)–C(83)–H(83A)	120.31	C(84)–C(83)–H(83A)	121.12	C(83)–C(84)–H(84A)	119.53
C(85)–C(84)–H(84A)	120.15	C(84)–C(85)–H(85A)	119.86	C(86)–C(85)–H(85A)	119.54
C(81)–C(86)–H(86A)	120.56	C(85)–C(86)–H(86A)	120.63		

Tabelle A.39: Fulleren, Bindungswinkel in [°] (Teil 2).

Atom	Elektronen [e]	Ladung [e]	Volumen [Å^3]	Atom	Elektronen [e]	Ladung [e]	Volumen [Å^3]
C(1)	6.0498497	-0.0498497	7.9099858	O(111)	9.0257038	-1.0257038	17.3391249
C(2)	6.0525624	-0.0525624	8.0022879	O(112)	9.1330047	-1.1330047	14.3165042
C(3)	5.9342312	0.0657688	10.6508428	O(201)	9.0248953	-1.0248953	19.0662695
C(4)	5.9172164	0.0827836	11.4027066	O(202)	9.1390424	-1.1390424	14.7121715
C(5)	5.9170899	0.0829101	10.1242681	O(211)	9.0349542	-1.0349542	19.2835075
C(6)	5.9360574	0.0639426	10.4098738	O(212)	9.1290765	-1.1290765	14.4643290
C(7)	5.9159260	0.0840740	10.1265665	O(301)	9.0365523	-1.0365523	17.6723182
C(8)	5.9161170	0.0838830	9.6485245	O(302)	9.1128528	-1.1128528	14.3864548
C(9)	5.9356735	0.0643265	9.2601332	O(311)	9.0481328	-1.0481328	17.3114876
C(10)	5.9160761	0.0839239	9.8672282	O(312)	9.1416539	-1.1416539	14.8665584
C(11)	5.9153122	0.0846878	10.0353382	H(10A)	0.8138896	0.1861104	6.1439476
C(12)	5.9408813	0.0591187	10.2779975	H(10B)	0.8174236	0.1825764	7.3398494
C(13)	5.9203253	0.0796747	11.1170709	H(10C)	0.8884389	0.1115611	6.7296281
C(14)	5.9166450	0.0833550	10.6499870	H(10D)	0.8808431	0.1191569	6.9627266
C(15)	5.9364207	0.0635793	10.4399629	H(10E)	0.8788575	0.1211425	8.3401152
C(16)	5.9164930	0.0835070	10.6465874	H(11A)	0.8054401	0.1945599	5.9804422
C(17)	5.9354274	0.0645726	10.6479590	H(11B)	0.8159369	0.1840631	8.0831961
C(18)	6.0466302	-0.0466302	7.6192505	H(11C)	0.8891850	0.1108150	6.8280828
C(19)	5.9364294	0.0635706	10.7788959	H(11D)	0.8820409	0.1179591	8.3315605
C(20)	5.9154641	0.0845359	9.7196985	H(11E)	0.8819699	0.1180301	8.4732418
C(21)	5.9361782	0.0638218	10.6037568	H(20A)	0.8050727	0.1949273	6.8749497
C(22)	6.0472848	-0.0472848	7.9192139	H(20B)	0.8159575	0.1840425	6.4852119
C(23)	6.0519357	-0.0519357	7.9044177	H(20C)	0.8887805	0.1112195	7.7318522
C(24)	5.9360621	0.0639379	10.9899899	H(20D)	0.8806361	0.1193639	7.1226934
C(34)	5.9182904	0.0817096	10.6877927	H(20E)	0.8825800	0.1174200	7.8029684
C(35)	5.9393018	0.0606982	10.7670184	H(21A)	0.8038374	0.1961626	8.0751857
C(36)	6.0486169	-0.0486169	7.5931438	H(21B)	0.8171233	0.1828767	7.5498234
C(37)	5.9336769	0.0663231	9.7503842	H(21C)	0.8818957	0.1181043	7.7909679
C(38)	5.9170158	0.0829842	9.9333847	H(21D)	0.8819647	0.1180353	7.1361284
C(39)	5.9357389	0.0642611	9.8722871	H(21E)	0.8808526	0.1191474	8.4017736
C(100)	6.0093014	-0.0093014	7.5240145	H(30A)	0.8348151	0.1651849	6.5755489
C(101)	4.5262719	1.4737281	4.7579258	H(30B)	0.8334331	0.1665669	7.5896148
C(102)	5.9182457	0.0817543	9.0037137	H(30C)	0.8086107	0.1913893	6.8949409
C(103)	6.3376847	-0.3376847	12.6701322	H(30D)	0.7960010	0.2039990	6.8298001
C(111)	4.5367931	1.4632069	5.2706782	H(30E)	0.8013017	0.1986983	7.6522176
C(112)	5.9254902	0.0745098	9.5423569	H(31A)	0.8439480	0.1560520	8.4195939
C(113)	6.3354245	-0.3354245	14.4568009	H(31B)	0.9443911	0.0556089	6.6068154
C(200)	6.0098098	-0.0098098	7.7266332	H(31C)	0.9169653	0.0830347	7.3232545
C(201)	4.5441531	1.4558469	5.8880145	H(31D)	1.0107309	-0.0107309	9.9787327
C(202)	5.9259863	0.0740137	10.1001425	H(31E)	0.9262294	0.0737706	8.7369265
C(203)	6.3350157	-0.3350157	13.1932760	C(81)	5.3220536	0.6779464	9.6583739
C(211)	4.5304782	1.4695218	4.8310961	C(82)	5.3177430	0.6822570	8.8349071
C(212)	5.9174739	0.0825261	9.1780868	C(83)	6.1412331	-0.1412331	11.6477606
C(213)	6.3346423	-0.3346423	13.8526477	C(84)	5.9652479	0.0347521	12.0028858
C(300)	6.0091571	-0.0091571	7.4032510	C(85)	5.9637889	0.0362111	11.6548884
C(301)	4.5514928	1.4485072	5.2106546	C(86)	6.1440510	-0.1440510	12.7449072
C(302)	5.8730062	0.1269938	9.9714609	F(1)	9.4695978	-0.4695978	15.3669049
C(303)	6.5756430	-0.5756430	17.3332256	F(2)	9.4669297	-0.4669297	15.7729247
C(311)	4.5180030	1.4819970	4.6904056	H(83A)	1.0839647	-0.0839647	8.2037422
C(312)	5.7496537	0.2503463	9.1266966	H(84A)	1.0306993	-0.0306993	7.6173828
C(313)	6.1214999	-0.1214999	12.4930895	H(85A)	1.0340350	-0.0340350	7.5246062
O(101)	9.0453568	-1.0453568	17.8119407	H(86A)	1.0882397	-0.0882397	8.5983675
O(102)	9.1389217	-1.1389217	13.8779010				

Tabelle A.40: Fulleren, Gesamtzahl der Elektronen, atomare Ladungen und Volumina nach Integration mit TOPXD.