

Supplementary Material

Table 1. Atomic coordinates and isotropic parameters of the compound **3**.

Atom label	X	Y	Z	Uiso
O1	0.50093(4)	0.28765(8)	1.00481(3)	0.01587(16)
O2	0.70251(4)	0.44473(8)	1.03879(4)	0.01690(16)
O3	0.84654(4)	0.05020(8)	1.10251(3)	0.01509(16)
O4	0.91720(4)	0.03493(8)	1.00968(3)	0.01569(16)
O5	0.76804(4)	0.24955(8)	0.95385(3)	0.01611(16)
O6	0.63707(4)	0.03508(8)	0.96062(4)	0.01935(17)
C1	0.90231(8)	0.70857(13)	1.12947(7)	0.0311(3)
H1A	0.9069	0.6816	1.1702	0.047
H1B	0.8528	0.7092	1.1048	0.047
H1C	0.9219	0.799	1.13	0.047
C2	0.94264(6)	0.60649(12)	1.10307(5)	0.0197(2)
C3	0.91552(6)	0.45851(11)	1.10274(5)	0.0155(2)
C4	0.85183(5)	0.42876(11)	1.11235(5)	0.0143(2)
H4	0.8261	0.501	1.1209	0.017
C5	0.82453(5)	0.29488(11)	1.10973(4)	0.01292(19)
C6	0.75261(5)	0.27094(10)	1.11476(5)	0.01266(19)
C7	0.69294(5)	0.34415(10)	1.07753(4)	0.01308(19)

C8	0.62437(5)	0.30998(11)	1.07614(5)	0.0135(2)
C9	0.56039(5)	0.37773(11)	1.03006(5)	0.0147(2)
H9A	0.5454	0.4545	1.0494	0.018
H9B	0.5747	0.4144	0.9973	0.018
C10	0.51615(6)	0.17006(11)	0.97414(5)	0.0154(2)
H10A	0.4728	0.1166	0.9573	0.018
H10B	0.5507	0.1127	1.0037	0.018
C11	0.54490(5)	0.20483(11)	0.92342(5)	0.0135(2)
C12	0.51308(5)	0.30638(11)	0.88095(5)	0.0141(2)
H12	0.4736	0.3527	0.884	0.017
C13	0.53850(5)	0.34117(11)	0.83379(5)	0.0139(2)
C14	0.50275(6)	0.45706(11)	0.78953(5)	0.0174(2)
C15	0.53057(7)	0.46579(13)	0.73572(5)	0.0235(2)
H15A	0.5228	0.3794	0.7145	0.035
H15B	0.5807	0.4861	0.7505	0.035
H15C	0.5056	0.5373	0.7085	0.035
C16	0.51790(8)	0.59406(12)	0.82421(6)	0.0269(3)
H16A	0.4974	0.6681	0.7967	0.04
H16B	0.5685	0.6074	0.8416	0.04
H16C	0.4973	0.5923	0.856	0.04
C17	0.68926(6)	0.58246(12)	1.05462(6)	0.0237(2)

H17A	0.6388	0.5985	1.0417	0.036
H17B	0.7109	0.6468	1.0349	0.036
H17C	0.7093	0.5941	1.0979	0.036
C18	0.74142(5)	0.16943(10)	1.15297(4)	0.01335(19)
H18	0.7805	0.121	1.178	0.016
C19	0.67369(5)	0.13773(10)	1.15506(4)	0.01296(19)
C20	0.66543(6)	0.02234(11)	1.19701(5)	0.0154(2)
C21	0.71674(6)	0.04583(14)	1.26202(5)	0.0253(3)
H21A	0.705	0.1308	1.2774	0.038
H21B	0.7648	0.0501	1.2617	0.038
H21C	0.7124	-0.0287	1.2876	0.038
C22	0.68337(7)	-0.11591(12)	1.17350(6)	0.0261(3)
H22A	0.6773	-0.1891	1.1989	0.039
H22B	0.7319	-0.1145	1.1743	0.039
H22C	0.6521	-0.1304	1.1326	0.039
C23	0.58961(6)	0.01396(12)	1.19964(5)	0.0206(2)
H23A	0.5768	0.1011	1.2124	0.031
H23B	0.5877	-0.056	1.2281	0.031
H23C	0.5569	-0.0084	1.1601	0.031
C24	0.61583(5)	0.20878(11)	1.11569(5)	0.0139(2)
H24	0.5702	0.1883	1.1157	0.017

C25	1.02181(7)	0.61519(15)	1.14139(8)	0.0386(4)
H25A	1.0377	0.7088	1.1426	0.058
H25B	1.0489	0.5582	1.1236	0.058
H25C	1.0285	0.5841	1.1819	0.058
C26	0.93210(9)	0.64943(14)	1.03726(7)	0.0359(3)
H26A	0.9471	0.7431	1.0367	0.054
H26B	0.8826	0.6412	1.0131	0.054
H26C	0.96	0.5908	1.0209	0.054
C27	0.95180(5)	0.34757(11)	1.08805(5)	0.0158(2)
H27	0.9935	0.3645	1.0796	0.019
C28	0.92730(5)	0.21329(11)	1.08577(5)	0.0141(2)
C29	0.86475(5)	0.18615(10)	1.09882(4)	0.01286(19)
C30	0.78549(6)	0.00022(12)	1.05380(5)	0.0183(2)
H30A	0.7544	0.0758	1.0361	0.028
H30B	0.7603	-0.0659	1.0695	0.028
H30C	0.8011	-0.0425	1.0234	0.028
C31	0.96358(5)	0.09690(11)	1.06449(5)	0.0157(2)
H31A	1.0058	0.1319	1.0574	0.019
H31B	0.9787	0.0276	1.0961	0.019
C32	0.89953(5)	0.12590(11)	0.95837(5)	0.0152(2)
H32A	0.9359	0.1215	0.9393	0.018

H32B	0.8966	0.2199	0.9713	0.018
C33	0.82865(5)	0.08161(11)	0.91399(5)	0.0140(2)
C34	0.76562(5)	0.14638(11)	0.91256(5)	0.0138(2)
C35	0.76958(6)	0.38616(11)	0.93125(5)	0.0210(2)
H35A	0.8095	0.3952	0.9172	0.032
H35B	0.7741	0.4514	0.9632	0.032
H35C	0.7262	0.4034	0.8982	0.032
C36	0.69974(5)	0.10145(11)	0.87248(5)	0.0141(2)
C37	0.63256(5)	0.16960(11)	0.87323(5)	0.0141(2)
C38	0.60433(5)	0.13584(11)	0.91867(5)	0.0142(2)
C39	0.61038(7)	-0.09989(13)	0.94194(6)	0.0281(3)
H39A	0.5598	-0.1014	0.9337	0.042
H39B	0.633	-0.1643	0.9737	0.042
H39C	0.6204	-0.1247	0.9058	0.042
C40	0.59868(6)	0.27074(11)	0.83096(5)	0.0151(2)
H40	0.6166	0.292	0.8	0.018
C41	0.69839(6)	-0.01105(11)	0.83507(5)	0.0153(2)
H41	0.6548	-0.0399	0.8078	0.018
C42	0.76044(6)	-0.08227(11)	0.83714(5)	0.0146(2)
C43	0.75558(6)	-0.21483(11)	0.80028(5)	0.0178(2)
C44	0.72566(8)	-0.18425(14)	0.73186(6)	0.0318(3)

H44A	0.7575	-0.1235	0.721	0.048
H44B	0.6797	-0.1415	0.7223	0.048
H44C	0.7211	-0.2686	0.7095	0.048
C45	0.70530(8)	-0.31504(14)	0.81652(8)	0.0375(3)
H45A	0.7029	-0.3996	0.7947	0.056
H45B	0.6586	-0.2752	0.8056	0.056
H45C	0.7229	-0.3331	0.8594	0.056
C46	0.82795(7)	-0.28571(13)	0.81396(6)	0.0262(3)
H46A	0.8605	-0.2245	0.8043	0.039
H46B	0.8223	-0.3677	0.7899	0.039
H46C	0.8465	-0.3094	0.8563	0.039
C47	0.82495(6)	-0.03185(11)	0.87632(5)	0.0151(2)
H47	0.867	-0.0752	0.8775	0.018
C48	0.42191(7)	0.43293(16)	0.76342(7)	0.0344(3)
H48A	0.4024	0.433	0.7959	0.052
H48B	0.4126	0.3457	0.7429	0.052
H48C	0.4001	0.5049	0.7351	0.052

Table 2. Atomic displacement parameters of the compound **3**.

Atom label	U11	U22	U33	U23	U13	U12
O1	0.0123(3)	0.0196(4)	0.0164(4)	0.0010(3)	0.0057(3)	0.0021(3)
O2	0.0193(4)	0.0142(4)	0.0186(4)	0.0060(3)	0.0083(3)	0.0021(3)
O3	0.0150(3)	0.0119(4)	0.0167(4)	0.0016(3)	0.0031(3)	-0.0004(3)
O4	0.0158(4)	0.0153(4)	0.0145(4)	-0.0005(3)	0.0031(3)	0.0013(3)
O5	0.0193(4)	0.0151(4)	0.0148(4)	-0.0009(3)	0.0068(3)	0.0014(3)
O6	0.0164(4)	0.0197(4)	0.0202(4)	0.0088(3)	0.0038(3)	0.0041(3)
C1	0.0367(7)	0.0158(6)	0.0467(8)	-0.0061(5)	0.0215(6)	-0.0060(5)
C2	0.0187(5)	0.0156(5)	0.0249(6)	-0.0012(4)	0.0073(4)	-0.0053(4)
C3	0.0163(5)	0.0147(5)	0.0147(5)	-0.0002(4)	0.0043(4)	-0.0029(4)
C4	0.0154(5)	0.0132(5)	0.0140(5)	-0.0005(4)	0.0046(4)	0.0007(4)
C5	0.0125(4)	0.0146(5)	0.0115(4)	0.0011(3)	0.0036(4)	0.0000(4)
C6	0.0130(4)	0.0126(4)	0.0127(4)	-0.0008(4)	0.0047(4)	-0.0001(4)
C7	0.0161(5)	0.0112(4)	0.0128(4)	0.0012(4)	0.0060(4)	0.0010(4)
C8	0.0142(5)	0.0135(5)	0.0127(4)	0.0004(4)	0.0044(4)	0.0031(4)
C9	0.0146(5)	0.0144(5)	0.0145(5)	0.0018(4)	0.0039(4)	0.0029(4)
C10	0.0152(5)	0.0162(5)	0.0150(5)	0.0008(4)	0.0056(4)	-0.0009(4)
C11	0.0122(4)	0.0149(5)	0.0125(4)	-0.0002(4)	0.0028(4)	-0.0016(4)
C12	0.0119(4)	0.0144(5)	0.0153(5)	-0.0012(4)	0.0036(4)	0.0010(4)
C13	0.0131(5)	0.0135(5)	0.0130(4)	0.0007(4)	0.0015(4)	0.0002(4)

C14	0.0149(5)	0.0186(5)	0.0180(5)	0.0066(4)	0.0047(4)	0.0032(4)
C15	0.0282(6)	0.0257(6)	0.0169(5)	0.0078(4)	0.0080(5)	0.0067(5)
C16	0.0387(7)	0.0173(5)	0.0306(6)	0.0052(5)	0.0196(6)	0.0068(5)
C17	0.0222(5)	0.0130(5)	0.0334(6)	0.0055(5)	0.0057(5)	0.0018(4)
C18	0.0130(4)	0.0137(5)	0.0126(4)	0.0013(4)	0.0033(4)	0.0017(4)
C19	0.0148(5)	0.0127(5)	0.0114(4)	0.0005(4)	0.0045(4)	-0.0003(4)
C20	0.0142(5)	0.0160(5)	0.0160(5)	0.0043(4)	0.0051(4)	-0.0007(4)
C21	0.0216(6)	0.0354(7)	0.0164(5)	0.0085(5)	0.0031(4)	-0.0063(5)
C22	0.0316(6)	0.0164(5)	0.0345(7)	0.0059(5)	0.0168(5)	0.0032(5)
C23	0.0173(5)	0.0229(6)	0.0227(5)	0.0059(4)	0.0082(4)	-0.0020(4)
C24	0.0127(4)	0.0157(5)	0.0140(5)	0.0004(4)	0.0056(4)	0.0006(4)
C25	0.0218(6)	0.0236(6)	0.0606(10)	-0.0019(6)	0.0010(6)	-0.0081(5)
C26	0.0533(9)	0.0247(6)	0.0327(7)	0.0023(5)	0.0183(6)	-0.0138(6)
C27	0.0122(4)	0.0196(5)	0.0157(5)	-0.0003(4)	0.0046(4)	-0.0020(4)
C28	0.0123(4)	0.0169(5)	0.0118(4)	0.0002(4)	0.0022(4)	0.0016(4)
C29	0.0132(4)	0.0129(5)	0.0110(4)	0.0007(4)	0.0020(4)	-0.0009(4)
C30	0.0182(5)	0.0177(5)	0.0183(5)	-0.0028(4)	0.0049(4)	-0.0047(4)
C31	0.0122(4)	0.0187(5)	0.0147(5)	-0.0006(4)	0.0026(4)	0.0025(4)
C32	0.0140(5)	0.0170(5)	0.0147(5)	0.0003(4)	0.0049(4)	0.0001(4)
C33	0.0137(5)	0.0156(5)	0.0129(4)	0.0017(4)	0.0048(4)	-0.0001(4)
C34	0.0161(5)	0.0140(5)	0.0120(4)	0.0016(4)	0.0057(4)	0.0010(4)

C35	0.0258(6)	0.0156(5)	0.0226(5)	-0.0010(4)	0.0094(5)	-0.0002(4)
C36	0.0134(5)	0.0152(5)	0.0145(5)	0.0035(4)	0.0058(4)	0.0022(4)
C37	0.0114(4)	0.0152(5)	0.0144(5)	-0.0008(4)	0.0027(4)	0.0012(4)
C38	0.0122(4)	0.0142(5)	0.0136(5)	0.0018(4)	0.0009(4)	0.0006(4)
C39	0.0320(7)	0.0170(6)	0.0369(7)	0.0087(5)	0.0137(6)	0.0020(5)
C40	0.0149(5)	0.0175(5)	0.0128(5)	0.0006(4)	0.0047(4)	0.0006(4)
C41	0.0142(5)	0.0166(5)	0.0145(5)	0.0007(4)	0.0041(4)	-0.0006(4)
C42	0.0171(5)	0.0132(5)	0.0148(5)	0.0009(4)	0.0069(4)	0.0002(4)
C43	0.0179(5)	0.0136(5)	0.0225(5)	-0.0029(4)	0.0077(4)	-0.0007(4)
C44	0.0403(7)	0.0271(6)	0.0225(6)	-0.0082(5)	0.0034(5)	0.0062(6)
C45	0.0393(8)	0.0182(6)	0.0674(10)	-0.0065(6)	0.0342(8)	-0.0067(5)
C46	0.0230(6)	0.0226(6)	0.0326(6)	-0.0081(5)	0.0090(5)	0.0040(5)
C47	0.0141(5)	0.0161(5)	0.0162(5)	0.0012(4)	0.0064(4)	0.0021(4)
C48	0.0162(6)	0.0450(8)	0.0360(7)	0.0224(6)	0.0007(5)	0.0024(5)

Table 3. Bond lengths of the compound **3**.

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
O1	C9	1.4308(13)	C21	H21B	0.96
O1	C10	1.4340(13)	C21	H21C	0.96
O2	C7	1.3878(12)	C22	H22A	0.96
O2	C17	1.4365(14)	C22	H22B	0.96
O3	C29	1.3804(12)	C22	H22C	0.96
O3	C30	1.4421(13)	C23	H23A	0.96
O4	C32	1.4345(13)	C23	H23B	0.96
O4	C31	1.4355(13)	C23	H23C	0.96
O5	C34	1.3807(12)	C24	H24	0.93
O5	C35	1.4329(13)	C25	H25A	0.96
O6	C38	1.3839(12)	C25	H25B	0.96
O6	C39	1.4275(15)	C25	H25C	0.96
C1	C2	1.5300(17)	C26	H26A	0.96
C1	H1A	0.96	C26	H26B	0.96
C1	H1B	0.96	C26	H26C	0.96
C1	H1C	0.96	C27	C28	1.3881(15)
C2	C25	1.5317(17)	C27	H27	0.93
C2	C3	1.5354(15)	C28	C29	1.4028(14)
C2	C26	1.5372(18)	C28	C31	1.5130(14)

C3	C4	1.3902(15)	C30	H30A	0.96
C3	C27	1.4029(15)	C30	H30B	0.96
C4	C5	1.4036(14)	C30	H30C	0.96
C4	H4	0.93	C31	H31A	0.97
C5	C29	1.3999(14)	C31	H31B	0.97
C5	C6	1.4935(14)	C32	C33	1.5066(14)
C6	C18	1.3973(14)	C32	H32A	0.97
C6	C7	1.4073(14)	C32	H32B	0.97
C7	C8	1.3948(14)	C33	C34	1.3942(14)
C8	C24	1.3981(14)	C33	C47	1.3970(15)
C8	C9	1.5147(14)	C34	C36	1.4014(14)
C9	H9A	0.97	C35	H35A	0.96
C9	H9B	0.97	C35	H35B	0.96
C10	C11	1.5163(14)	C35	H35C	0.96
C10	H10A	0.97	C36	C41	1.3940(15)
C10	H10B	0.97	C36	C37	1.4978(14)
C11	C12	1.3918(14)	C37	C40	1.3960(14)
C11	C38	1.3964(14)	C37	C38	1.3962(15)
C12	C13	1.3987(15)	C39	H39A	0.96
C12	H12	0.93	C39	H39B	0.96
C13	C40	1.4005(14)	C39	H39C	0.96

C13	C14	1.5330(14)	C40	H40	0.93
C14	C16	1.5349(17)	C41	C42	1.4028(15)
C14	C48	1.5358(16)	C41	H41	0.93
C14	C15	1.5360(16)	C42	C47	1.3923(15)
C15	H15A	0.96	C42	C43	1.5343(15)
C15	H15B	0.96	C43	C46	1.5309(16)
C15	H15C	0.96	C43	C45	1.5327(17)
C16	H16A	0.96	C43	C44	1.5354(17)
C16	H16B	0.96	C44	H44A	0.96
C16	H16C	0.96	C44	H44B	0.96
C17	H17A	0.96	C44	H44C	0.96
C17	H17B	0.96	C45	H45A	0.96
C17	H17C	0.96	C45	H45B	0.96
C18	C19	1.3996(14)	C45	H45C	0.96
C18	H18	0.93	C46	H46A	0.96
C19	C24	1.3924(14)	C46	H46B	0.96
C19	C20	1.5339(14)	C46	H46C	0.96
C20	C23	1.5333(15)	C47	H47	0.93
C20	C21	1.5362(15)	C48	H48A	0.96
C20	C22	1.5381(16)	C48	H48B	0.96
C21	H21A	0.96	C48	H48C	0.96

Table 3. Bond angles of the compound **3**.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C9	O1	C10	114.17(8)	C19	C24	C8	121.87(9)
C7	O2	C17	114.30(8)	C19	C24	H24	119.1
C29	O3	C30	116.28(8)	C8	C24	H24	119.1
C32	O4	C31	112.97(8)	C2	C25	H25A	109.5
C34	O5	C35	114.57(8)	C2	C25	H25B	109.5
C38	O6	C39	113.29(9)	H25A	C25	H25B	109.5
C2	C1	H1A	109.5	C2	C25	H25C	109.5
C2	C1	H1B	109.5	H25A	C25	H25C	109.5
H1A	C1	H1B	109.5	H25B	C25	H25C	109.5
C2	C1	H1C	109.5	C2	C26	H26A	109.5
H1A	C1	H1C	109.5	C2	C26	H26B	109.5
H1B	C1	H1C	109.5	H26A	C26	H26B	109.5
C1	C2	C25	107.75(11)	C2	C26	H26C	109.5
C1	C2	C3	112.23(9)	H26A	C26	H26C	109.5
C25	C2	C3	110.24(10)	H26B	C26	H26C	109.5
C1	C2	C26	108.21(11)	C28	C27	C3	121.93(10)
C25	C2	C26	109.74(11)	C28	C27	H27	119
C3	C2	C26	108.63(10)	C3	C27	H27	119
C4	C3	C27	116.87(10)	C27	C28	C29	119.65(9)

C4	C3	C2	122.16(10)	C27	C28	C31	121.01(9)
C27	C3	C2	120.81(10)	C29	C28	C31	119.15(9)
C3	C4	C5	123.13(10)	O3	C29	C5	122.21(9)
C3	C4	H4	118.4	O3	C29	C28	117.67(9)
C5	C4	H4	118.4	C5	C29	C28	120.08(9)
C29	C5	C4	118.10(9)	O3	C30	H30A	109.5
C29	C5	C6	121.24(9)	O3	C30	H30B	109.5
C4	C5	C6	120.56(9)	H30A	C30	H30B	109.5
C18	C6	C7	117.98(9)	O3	C30	H30C	109.5
C18	C6	C5	121.51(9)	H30A	C30	H30C	109.5
C7	C6	C5	120.36(9)	H30B	C30	H30C	109.5
O2	C7	C8	119.98(9)	O4	C31	C28	111.80(8)
O2	C7	C6	119.14(9)	O4	C31	H31A	109.3
C8	C7	C6	120.72(9)	C28	C31	H31A	109.3
C7	C8	C24	119.15(9)	O4	C31	H31B	109.3
C7	C8	C9	119.77(9)	C28	C31	H31B	109.3
C24	C8	C9	121.02(9)	H31A	C31	H31B	107.9
O1	C9	C8	114.15(8)	O4	C32	C33	108.01(8)
O1	C9	H9A	108.7	O4	C32	H32A	110.1
C8	C9	H9A	108.7	C33	C32	H32A	110.1
O1	C9	H9B	108.7	O4	C32	H32B	110.1

C8	C9	H9B	108.7	C33	C32	H32B	110.1
H9A	C9	H9B	107.6	H32A	C32	H32B	108.4
O1	C10	C11	114.25(9)	C34	C33	C47	118.98(10)
O1	C10	H10A	108.7	C34	C33	C32	121.01(9)
C11	C10	H10A	108.7	C47	C33	C32	119.87(9)
O1	C10	H10B	108.7	O5	C34	C33	119.40(9)
C11	C10	H10B	108.7	O5	C34	C36	119.89(9)
H10A	C10	H10B	107.6	C33	C34	C36	120.57(10)
C12	C11	C38	118.64(9)	O5	C35	H35A	109.5
C12	C11	C10	120.91(9)	O5	C35	H35B	109.5
C38	C11	C10	120.45(9)	H35A	C35	H35B	109.5
C11	C12	C13	122.27(10)	O5	C35	H35C	109.5
C11	C12	H12	118.9	H35A	C35	H35C	109.5
C13	C12	H12	118.9	H35B	C35	H35C	109.5
C12	C13	C40	117.39(9)	C41	C36	C34	118.68(9)
C12	C13	C14	119.98(9)	C41	C36	C37	121.64(9)
C40	C13	C14	122.57(9)	C34	C36	C37	119.59(9)
C13	C14	C16	108.48(9)	C40	C37	C38	118.72(9)
C13	C14	C48	110.07(9)	C40	C37	C36	121.65(9)
C16	C14	C48	109.65(11)	C38	C37	C36	119.57(9)
C13	C14	C15	112.26(9)	O6	C38	C37	119.35(9)

C16	C14	C15	108.83(10)	O6	C38	C11	119.61(9)
C48	C14	C15	107.52(10)	C37	C38	C11	121.01(9)
C14	C15	H15A	109.5	O6	C39	H39A	109.5
C14	C15	H15B	109.5	O6	C39	H39B	109.5
H15A	C15	H15B	109.5	H39A	C39	H39B	109.5
C14	C15	H15C	109.5	O6	C39	H39C	109.5
H15A	C15	H15C	109.5	H39A	C39	H39C	109.5
H15B	C15	H15C	109.5	H39B	C39	H39C	109.5
C14	C16	H16A	109.5	C37	C40	C13	121.93(10)
C14	C16	H16B	109.5	C37	C40	H40	119
H16A	C16	H16B	109.5	C13	C40	H40	119
C14	C16	H16C	109.5	C36	C41	C42	122.26(10)
H16A	C16	H16C	109.5	C36	C41	H41	118.9
H16B	C16	H16C	109.5	C42	C41	H41	118.9
O2	C17	H17A	109.5	C47	C42	C41	117.17(10)
O2	C17	H17B	109.5	C47	C42	C43	122.34(9)
H17A	C17	H17B	109.5	C41	C42	C43	120.39(9)
O2	C17	H17C	109.5	C46	C43	C45	108.02(10)
H17A	C17	H17C	109.5	C46	C43	C42	112.52(9)
H17B	C17	H17C	109.5	C45	C43	C42	108.57(9)
C6	C18	C19	122.64(9)	C46	C43	C44	108.29(10)

C6	C18	H18	118.7	C45	C43	C44	108.83(11)
C19	C18	H18	118.7	C42	C43	C44	110.53(9)
C24	C19	C18	117.47(9)	C43	C44	H44A	109.5
C24	C19	C20	122.82(9)	C43	C44	H44B	109.5
C18	C19	C20	119.61(9)	H44A	C44	H44B	109.5
C23	C20	C19	112.48(9)	C43	C44	H44C	109.5
C23	C20	C21	107.79(9)	H44A	C44	H44C	109.5
C19	C20	C21	110.14(9)	H44B	C44	H44C	109.5
C23	C20	C22	108.51(9)	C43	C45	H45A	109.5
C19	C20	C22	108.86(9)	C43	C45	H45B	109.5
C21	C20	C22	109.00(10)	H45A	C45	H45B	109.5
C20	C21	H21A	109.5	C43	C45	H45C	109.5
C20	C21	H21B	109.5	H45A	C45	H45C	109.5
H21A	C21	H21B	109.5	H45B	C45	H45C	109.5
C20	C21	H21C	109.5	C43	C46	H46A	109.5
H21A	C21	H21C	109.5	C43	C46	H46B	109.5
H21B	C21	H21C	109.5	H46A	C46	H46B	109.5
C20	C22	H22A	109.5	C43	C46	H46C	109.5
C20	C22	H22B	109.5	H46A	C46	H46C	109.5
H22A	C22	H22B	109.5	H46B	C46	H46C	109.5
C20	C22	H22C	109.5	C42	C47	C33	122.26(10)

H22A	C22	H22C	109.5	C42	C47	H47	118.9
H22B	C22	H22C	109.5	C33	C47	H47	118.9
C20	C23	H23A	109.5	C14	C48	H48A	109.5
C20	C23	H23B	109.5	C14	C48	H48B	109.5
H23A	C23	H23B	109.5	H48A	C48	H48B	109.5
C20	C23	H23C	109.5	C14	C48	H48C	109.5
H23A	C23	H23C	109.5	H48A	C48	H48C	109.5
H23B	C23	H23C	109.5	H48B	C48	H48C	109.5
