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The longest oligothiophene ever examined by X-ray structure analysis

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Fractional atomic coordinates with estimated standard deviation in parentheses and equivalent isotropic displacement parameter.

Atom	x	y	z	Ueq
S1	0.663050	0.755030	0.100930	0.0401
S2	0.644460	0.526460	0.098750	0.0333
S3	0.558210	0.246110	0.163600	0.0339
S4	0.349410	0.082340	0.052270	0.0313
S5	0.270630	-0.209700	0.085780	0.0295
S6	0.014400	-0.347310	-0.017150	0.0309
C1	0.766040	0.834650	0.110960	0.0464
C2	0.879610	0.788460	0.144590	0.0403
C3	0.885790	0.688480	0.163470	0.0334
C4	0.775120	0.659380	0.142840	0.0320
C5	0.736770	0.565780	0.151310	0.0254
C6	0.764490	0.499770	0.200190	0.0404
C7	0.706610	0.415820	0.193270	0.0370
C8	0.639770	0.420250	0.141090	0.0245
C9	0.568380	0.351460	0.119480	0.0243
C10	0.512340	0.350490	0.065750	0.0330
C11	0.461990	0.267030	0.058380	0.0351
C12	0.478860	0.203560	0.107100	0.0233
C13	0.434810	0.109920	0.112740	0.0229
C14	0.451930	0.036590	0.159100	0.0241
C15	0.392790	-0.040300	0.143340	0.0287
C16	0.336040	-0.029670	0.088080	0.0223
C17	0.270290	-0.092470	0.056320	0.0229
C18	0.204490	-0.075710	0.002360	0.0275
C19	0.151150	-0.153280	-0.015320	0.0214
C20	0.180180	-0.232370	0.025980	0.0236
C21	0.147270	-0.327820	0.025800	0.0244
C22	0.207860	-0.413090	0.058980	0.0279
C23	0.146770	-0.492170	0.050350	0.0244
C24	0.040930	-0.468380	0.010590	0.0260
C25	1.000240	0.626240	0.201100	0.0377
C26	0.972520	0.648230	0.269060	0.0424
C27	1.065300	0.571190	0.310090	0.0543
C28	1.076950	0.599150	0.374490	0.0493
C29	1.163750	0.516050	0.412800	0.0574
C30	1.197770	0.540080	0.473650	0.0555
C31	1.279500	0.455560	0.512190	0.0540
C32	1.333110	0.477810	0.570650	0.0547
C33	1.402990	0.389390	0.609150	0.0548
C34	1.473830	0.405330	0.664090	0.0569
C35	1.526080	0.320630	0.705870	0.0720
C36	1.607900	0.332760	0.758790	0.0616
C37	0.529810	0.035290	0.215570	0.0426
C38	0.519880	-0.038630	0.265800	0.0425

C39	0.620950	-0.046700	0.314650	0.0482
C40	0.591640	-0.096910	0.373780	0.0518
C41	0.704730	-0.118420	0.418640	0.0499
C42	0.668260	-0.154080	0.481930	0.0568
C43	0.786850	-0.181390	0.524480	0.0515
C44	0.743710	-0.208520	0.590440	0.0534
C45	0.857850	-0.239250	0.632740	0.0505
C46	0.814350	-0.260860	0.698920	0.0553
C47	0.932550	-0.296270	0.740600	0.0447
C48	0.879660	-0.314150	0.806300	0.0658
C49	0.079910	-0.150770	-0.073730	0.0258
C50	0.078010	-0.063990	-0.118740	0.0286
C51	0.021060	-0.078350	-0.179200	0.0320
C52	-0.005590	0.012730	-0.222710	0.0330
C53	-0.057140	-0.007050	-0.282980	0.0366
C54	-0.093460	0.084220	-0.327470	0.0419
C55	-0.139470	0.062350	-0.388060	0.0404
C56	-0.175630	0.148820	-0.433640	0.0428
C57	-0.221300	0.123220	-0.493310	0.0441
C58	-0.260260	0.207010	-0.540470	0.0480
C59	-0.302980	0.178110	-0.599970	0.0487
C60	-0.342410	0.261280	-0.648200	0.0772