

## Supplementary Information

### **Form III-like Conformation and Form I-like Packing in a Chloroform Channel Solvate of the Diuretic Drug Chlortalidone†**

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Table S1. Selected bond lengths (Å) of CTD Form I,<sup>10</sup> Form III,<sup>10</sup> and Form IV (this study).

Bond	Form I	Form III	Form IV	
			Conformer A	Conformer B
C1-C8	1.513(3)	1.517(3)	1.524(7)	1.532(7)
C2-C3	1.473(3)	1.467(3)	1.465(7)	1.460(7)
C3-C4	1.386(3)	1.384(3)	1.382(7)	1.376(7)
C4-C5	1.380(3)	1.377(3)	1.383(8)	1.363(8)
C5-C6	1.387(4)	1.389(4)	1.380(8)	1.385(9)
C6-C7	1.382(3)	1.391(3)	1.420(8)	1.383(8)
C7-C8	1.378(3)	1.379(3)	1.368(7)	1.376(7)
C3-C8	1.382(3)	1.381(3)	1.364(7)	1.385(7)
C1-C9	1.525(3)	1.520(3)	1.530(6)	1.504(6)
C9-C10	1.394(3)	1.391(3)	1.375(6)	1.380(6)
C10-C11	1.394(3)	1.388(3)	1.384(6)	1.400(6)
C11-C12	1.385(3)	1.397(3)	1.407(6)	1.403(7)
C12-C13	1.380(3)	1.383(3)	1.381(6)	1.357(7)
C13-C14	1.382(3)	1.381(3)	1.372(6)	1.377(7)
C9-C14	1.382(3)	1.386(3)	1.387(6)	1.383(6)
N1-C1	1.468(3)	1.466(3)	1.479(6)	1.470(6)
N1-C2	1.346(3)	1.342(3)	1.349(6)	1.352(6)
O1-C2	1.242(2)	1.242(3)	1.227(6)	1.250(6)
O2-C1	1.419(3)	1.411(3)	1.411(5)	1.406(5)
S1-C11	1.786(2)	1.781(2)	1.778(5)	1.762(5)
S1-N2	1.590(2)	1.595(2)	1.590(4)	1.536(5)
S1-O3	1.419(2)	1.428(2)	1.416(3)	1.435(4)
S1-O4	1.429(2)	1.431(2)	1.464(4)	1.537(5)
C11-C12	1.728(2)	1.727(2)	1.724(5)	1.742(5)
Cl1s-C1s	-	-		1.69(3)
Cl2s-C1s	-	-		1.47(2)
Cl3s-C1s	-	-		1.53(2)

Table S2. Selected valence angles (°) of CTD Form I,<sup>10</sup> Form III,<sup>10</sup> and Form IV (this study).

Angle	Form I	Form III	Form IV	
			Conformer A	Conformer B
C1-C8-C3	109.9(2)	109.6(2)	110.6(5)	110.3(6)
C1-C8-C7	129.1(2)	129.3(2)	128.2(6)	129.3(6)
C1-C9-C10	118.8(2)	118.9(2)	120.8(4)	121.1(4)
C1-C9-C14	122.0(2)	122.0(2)	119.3(4)	120.4(5)
C2-C3-C4	130.4(2)	129.9(2)	128.9(6)	130.1(6)
C2-C3-C8	108.2(2)	108.3(2)	109.2(6)	108.0(6)
C3-C4-C5	117.5(2)	117.5(2)	118.3(6)	117.4(7)
C3-C8-C7	120.9(2)	121.0(2)	121.1(6)	120.4(6)
C4-C5-C6	121.1(2)	120.9(2)	120.3(7)	121.4(7)
C4-C3-C8	121.4(2)	121.8(2)	121.9(6)	121.9(6)
C5-C6-C7	121.0(2)	121.3(2)	120.5(7)	121.1(7)
C6-C7-C8	118.1(2)	117.4(2)	117.8(6)	117.7(7)
C8-C1-C9	115.0(2)	114.3(2)	113.2(4)	112.2(5)
C9-C10-C11	120.5(2)	120.7(2)	120.8(4)	121.9(5)
C9-C14-C13	120.5(2)	120.7(2)	120.2(5)	121.1(5)
C10-C11-C12	119.2(2)	119.4(2)	119.1(5)	117.1(5)
C10-C9-C14	119.2(2)	119.1(2)	119.8(4)	118.4(5)
C11-C12-C13	120.4(2)	119.9(2)	119.4(5)	121.5(5)
C12-C13-C14	120.2(2)	120.2(2)	120.6(5)	119.9(5)
C1-N1-C2	113.7(2)	113.8(2)	114.7(5)	114.1(5)
N1-C1-C8	101.0(2)	100.7(2)	99.3(4)	100.0(4)
N1-C1-C9	110.6(2)	112.6(2)	111.8(4)	111.9(4)
N1-C2-C3	107.1(2)	107.2(2)	106.2(5)	107.7(5)
N1-C1-O2	111.9(2)	111.5(2)	111.2(4)	111.6(4)
N1-C2-O1	125.8(2)	125.7(2)	126.0(6)	124.0(6)
N2-S1-O3	107.7(1)	108.6(1)	109.0(3)	112.9(3)
N2-S1-O4	106.9(1)	108.6(1)	108.5(3)	108.5(3)
N2-S1-C11	106.6(1)	106.8(1)	108.0(3)	107.9(3)
O1-C2-C3	127.0(2)	127.0(2)	127.8(6)	128.3(6)
O2-C1-C8	112.4(2)	111.2(2)	113.3(4)	112.4(4)
O2-C1-C9	105.9(2)	106.5(2)	107.9(4)	108.7(4)
O3-S1-O4	119.6(2)	118.4(1)	117.6(3)	114.0(3)
O3-S1-C11	105.8(1)	106.1(1)	105.5(2)	106.1(2)
O4-S1-C11	109.5(1)	107.8(1)	107.9(3)	107.2(3)
C11-C12-C11	122.0(2)	121.8(2)	122.6(4)	120.8(4)

C11-C12-C13	117.6(2)	118.3(2)	118.0(4)	117.7(4)
S1-C11-C10	117.6(2)	118.2(2)	118.0(4)	118.8(4)
S1-C11-C12	123.1(2)	122.3(2)	122.9(4)	124.0(4)
C11s-C1s-C12s	-	-	104.1(16)	
C11s-C1s-C13s	-	-	102.9(14)	
C12s-C1s-C13s	-	-	129(2)	

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