Supporting Info file

for

Synthesis and Characterization of Carbonyl Functionalized

Organotellurium(IV) Derivatives

Puspendra Singh,*a Mariya Khan,^b Andrew Duthie,^c Ray J. Butcher^d

^aDepartment of Chemistry, Dr. Shakuntala Misra National Rehabilitation University, Lucknow, 226017, India.

^bDepartment of Chemistry, University of Lucknow, Lucknow, 226007, India.

^cDepartment of Chemistry, Indian Institute of Technology Kanpur, Kanpur, 208016, India

^dDepartment of Chemistry, Howard University, Washington DC20059, USA

*Corresponding Author, E-mail address: pushpendrasingh0612@gmail.com

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| | 1 | 4 | 5 |
|---|---|--|--|
| empirical formula | C ₁₆ H ₁₄ Cl ₂ O ₂ Te | $C_{19}H_{20}Cl_2O_2Te$ | $C_{14}H_{18}Cl_2O_2Te$ |
| formula mass (g mol ⁻¹) | 436.77 | 478.85 | 416.78 |
| Temp (K) | 100(2) | 123(2) | 100(2) |
| Wavelength, λ (Å) | 0.710 73 | 0.710 73 | 0.710 73 |
| cryst syst | monoclinic | monoclinic | monoclinic |
| cryst size (mm ³) | 0.55 x 0.10 x 0.09 | 0.77 x 0.55 x 0.35 | 0.44 x 0.27 x 0.23 |
| space group | $P2_{1}/c$ | $P2_{1}/c$ | $P2_1$ |
| <i>a</i> (Å) | 13.395(3) | 8.7845(4) | 8.389(5) |
| <i>b</i> (Å) | 13.251(3) | 19.5434(8) | 12.312(5) |
| <i>c</i> (Å) | 9.036(2) | 11.0751(5) | 8.461(5) |
| α (deg) | 90 | 90 | 90.000(5) |
| β (deg) | 98.213(4) | 97.679(4) | 116.320(5) |
| γ (deg) | 90 | 90 | 90.000(5) |
| Volume (Å ³) | 1587.5(7) | 1884.3(1) | 783.3(7) |
| Z | 4 | 4 | 2 |
| ρ_{calcd} (Mg m ³) | 1.827 | 1.688 | 1.767 |
| abs coeff (mm ⁻¹) | 2.211 | 1.871 | 2.235 |
| F(000) | 848 | 944 | 408 |
| θ range (deg) | 2.17-32.17 | 3.13-40.86 | 2.69-41.13 |
| index ranges | $-19 \le h \le 18$, | $-15 \le h \le 16$, | $-14 \le h \le 15$, |
| - | $-18 \le k \le 19$, | $-35 \le k \le 27$, | $-22 \le k \le 22$, |
| | $-13 \le 1 \le 12$ | $-20 \le 1 \le 19$ | - 15 ≤ 1 ≤ 11 |
| no. of rflns collected | 12748 | 24302 | 11130 |
| no. of indep rflns | 5046 | 11990 | 7370 |
| | (R(int) = 0.0344) | (R(int) = 0.0256) | (R(int) = 0.0295) |
| completeness to θ max (%) | 99.4 | 99.8 | 99.5 |
| abs cor | semiempirical | analytical | analytical |
| | from equivalents | | |
| max. min. transmission | 0.7464, 0.4720 | 0.593, 0.434 | 0.733, 0.564 |
| refinement method | full-matrix least | full-matrix least | full-matrix least |
| | squares on F ² | squares on F ² | squares on F ² |
| No. of data/restraints/ | 5046/0/194 | 11990/0/224 | 7370/1/179 |
| parameters | | | |
| goodness of fit on F^2 | 1.040 | 1.088 | 1.019 |
| final R indices $[I > 2, \sigma(I))$ | R1 = 0.0224. | R1 = 0.0345. | R1 = 0.0292. |
| | wR2 = 0.0570 | wR2 = 0.0652 | wR2 = 0.0569 |
| R indices (all data) | R1 = 0.0255. | R1 = 0.0515, | R1 = 0.0344. |
| | wR2 = 0.0586 | wR2 = 0.0707 | wR2 = 0.0601 |
| largest diff peak/hole (e Å ⁻ | 1.013/-0.549 | 0.687/-1.097 | 1.285/-0.985 |
| 3) | | | |
| <i>R</i> indices (all data) largest diff peak/hole (e Å ⁻ ³) | R1 = 0.0255, wR2 = 0.0586 1.013/-0.549 | R1 = 0.0515, wR2 = 0.0707 0.687/-1.097 | R1 = 0.0344, wR2 = 0.0601 1.285/-0.985 |

Table S1. Crystal Data and Structure Refinement Details of 1, 4 and 5

| | D-H···A | d(D-H) | d(H···A) | d(D····A) | ∠(DHA) | Symmetry |
|---|----------------------|---------|----------|-----------|--------|---------------------|
| 1 | O(2)-H(2)···O(1) | 0.80(3) | 1.824(3) | 2.559(2) | 154(3) | |
| | C(9)-H(9A)···Cl(1) | 0.95 | 2.667(1) | 3.541(2) | 153.1 | x,-y+1/2,z-1/2 |
| | C(6)-H(5A)···Cl(1) | 0.95 | 2.785(1) | 3.261(2) | 111.9 | -1+x, 0.5-y, -1.5+z |
| | C(9)-H(9A)···Cl(1) | 0.95 | 2.667(1) | 3.541(2) | 153.1 | 1-x, 0.5+y, 0.5-z |
| | C(15)-H(15A)···Cl(2) | 0.95 | 2.861(1) | 3.783(2) | 163.7 | -1-x, y, -1+z |
| | C(2)-H(2A)····Cl(2) | 0.95 | 2.853(1) | 3.302(2) | 110.1 | 1-x, 1-y, 1+z |
| | C(13)-H(13A)···O(1) | 0.95 | 2.427(1) | 3.339(2) | 160.9 | 1-x, 1-y, 1-z |
| 4 | O(2)-H(2)···O(1) | 0.75(2) | 1.854(2) | 2.541(1) | 151(3) | |
| | O(2)-H(2)···O(1) | 0.75(2) | 2.419(2) | 2.884(2) | 121(2) | -x+1,-y+1,-z+1 |
| | C(9)-H(9B)···Cl(2) | 0.98 | 2.881(0) | 3.629(2) | 133.8 | 1 -x, 1-y. 1-z |
| | C(7)-H(7B)···Cl(1) | 0.98 | 2.956(0) | 3.741(2) | 137.9 | 1 -x, 1-y. 1-z |
| | C(17)-H(17A)-Cl(1) | 0.95 | 2.902(0) | 3.717(2) | 144.6 | 1 -x, 1-y. 1-z |
| 5 | O(2)-H(2)···O(1) | 0.84 | 1.744(3) | 2.498(3) | 148.4 | |
| | C(12)-H(12)····Cl(2) | 0.95 | 2.911(1) | 3.704(3) | 141.8 | 1 -x+1,y-1/2,-z+1 |
| | C(7)-H(7B)····Cl(2) | 0.95 | 2.695(1) | 3.531(3) | 143.6 | 1-x, -0.5+y, 2-z |
| | C(14)-H(14A)···O(1) | 0.98 | 2.522(2) | 3.501(4) | 176.4 | -x+1,y-1/2,-z |
| | C(14)-H(14B)···Cl(1) | 0.98 | 2.843(1) | 3.803(4) | 166.8 | -x+2,y-1/2,-z+1 |
| | C(9)-H(9A)···Cl(1) | 0.98 | 2.872(1) | 3.749(3) | 149.6 | -x+2,y-1/2,-z+1 |
| | C(9)-H(9C)···Cl(1) | 0.98 | 2.778(1) | 3.462(3) | 127.5 | -x+2,y-1/2,-z+1 |

Table S2. Hydrogen bonds for 1, 4 and 5 (Å and °).



Fig. S1 Crystal lattices of compound **1** showing helical structure through C-H---Cl (green) hydrogen bonding interactions.



Fig. S2 Crystal lattices of compound **1** showing O-H---O (red), C-H---Cl and (green) hydrogen bonding interactions and Te---O (blue) & Te---Cl (black) secondary bonding interaction.



Fig. S3 Crystal lattices of compound 1 showing π --- π (brown) interaction.



Fig. S4. Centrosymmetric dimeric unit in the crystal lattices of compound **1** through C-H---Cl (green) hydrogen bonding interactions.



Fig. S5. Centrosymmetric dimeric unit in the crystal lattices of compound **4** through O-H---O (purple) hydrogen bonding interactions, Te---O (blue) secondary bonding interaction.



Fig. S6. Centrosymmetric dimeric unit in the crystal lattices of compound **4** through C-H---Cl (green) hydrogen bonding interactions.



Fig. S7. Supramolecular architecture along c axis of compound 4.



Fig. S8. Supramolecular architectures in the crystal lattices of compound **5** through O-H---O (purple) and C-H---Cl (green) hydrogen bonding interactions and Te---O (blue) secondary bonding interaction.



Fig. S9. Supramolecular architectures in the crystal lattices of compound **5** through O-H---O (purple) and C-H---Cl (green) hydrogen bonding interactions.



Fig. S10. Supramolecular architectures in the crystal lattices of compound **5** through O-H---O (purple) and C-H---Cl (green) hydrogen bonding interactions.



Fig. S11. ¹H NMR spectrum of compound Ph[PhC(OH)CHC(O)CH₂]TeCl₂ (1) in CDCl₃.



Fig. S12. Expanded aryl region of ¹H NMR spectrum of compound Ph[PhC(OH)CHC(O)CH₂]TeCl₂ (1) in CDCl₃.



Fig. S13. ¹³C NMR spectrum of compound Ph[PhC(OH)CHC(O)CH₂]TeCl₂ (1) in CDCl₃.



Fig. S14. Expanded aryl region of ¹³C NMR spectrum of compound Ph[PhC(OH)CHC(O)CH₂]TeCl₂ (1) in CDCl₃.



Fig. S15. ¹²⁵Te NMR spectrum of compound Ph[PhC(OH)CHC(O)CH₂]TeCl₂ (1) in CDCl₃.



Fig. S16. ¹H NMR spectrum of compound *p*-Tol[PhC(OH)CHC(O)CH₂]TeCl₂ (2) in CDCl₃.



Fig. S17. Expanded aryl region of ¹H NMR spectrum of compound *p*-Tol[PhC(OH)CHC(O)CH₂]TeCl₂ (**2**) in CDCl₃.



Fig. S18. ¹³C NMR spectrum of compound *p*-Tol[PhC(OH)CHC(O)CH₂]TeCl₂ (2) in CDCl₃.



Fig. S19. Expanded aryl region of ¹³C NMR spectrum of compound *p*-Tol[PhC(OH)CHC(O)CH₂]TeCl₂ (**2**) in CDCl₃.



Fig. S20. ¹²⁵Te NMR spectrum of compound p-Tol[PhC(OH)CHC(O)CH₂]TeCl₂ (**2**) in CDCl₃.



Fig. S21. ¹H NMR spectrum of compound *1*-Nap[PhC(OH)CHC(O)CH₂]TeCl₂ (3) in CDCl₃.



Fig. S22. Expanded aryl region of ¹H NMR spectrum of compound *1*-Nap[PhC(OH)CHC(O)CH₂]TeCl₂ (**3**) in CDCl₃.



Fig. S23. ¹³C NMR spectrum of compound *1*-Nap[PhC(OH)CHC(O)CH₂]TeCl₂ (**3**) in CDCl₃.



Fig. S24. Expanded aryl region of ¹³C NMR spectrum of compound *1*-Nap[PhC(OH)CHC(O)CH₂]TeCl₂ (**3**) in CDCl₃.



Fig. S25. ¹²⁵Te NMR spectrum of compound *1*-Nap[PhC(OH)CHC(O)CH₂]TeCl₂ (**3**) in CDCl₃.



Fig. S26. ¹H NMR spectrum of compound Mes[PhC(OH)CHC(O)CH₂]TeCl₂ (4).



Fig. S27. Expanded aryl region of ¹H NMR spectrum of compound Mes[PhC(OH)CHC(O)CH₂]TeCl₂ (**4**).



Fig. S28. ¹³C NMR spectrum of compound Mes[PhC(OH)CHC(O)CH₂]TeCl₂ (4) in CDCl₃.



Fig. S29. Expanded aryl region of ¹³C NMR spectrum of compound Mes[PhC(OH)CHC(O)CH₂]TeCl₂ (**4**) in CDCl₃.



Fig. S30. ¹²⁵Te NMR spectrum of compound Mes[PhC(OH)CHC(O)CH₂]TeCl₂ (4) in CDCl₃.



Fig. S31. ¹H NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeCl₂ (**5**).



Fig. S32. Expanded aryl region of ¹H NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeCl₂ (**5**).



Fig. S33. ¹³C NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeCl₂ (5) in CDCl₃.



Fig. S34. Expanded alkyl region of ¹³C NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeCl₂ (**5**) in CDCl₃.



Fig. S35. ¹H NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeBr₂ (6).



Fig. S36. ¹H NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeBr₂ (6).



Fig. S37. Expanded aryl region of ¹³C NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeBr₂ (**6**) in CDCl₃.



Fig. S38. ¹²⁵Te NMR spectrum of compound Mes[CH₃(OH)CHC(O)CH₂]TeBr₂ (**6**) in CDCl₃.