Electronic Supplementary Information for Dalton Transactions

Acylmethyl(aryl)tellurium(IV, II) Derivatives: Intramolecular Secondary Bonding and Steric Rigidity

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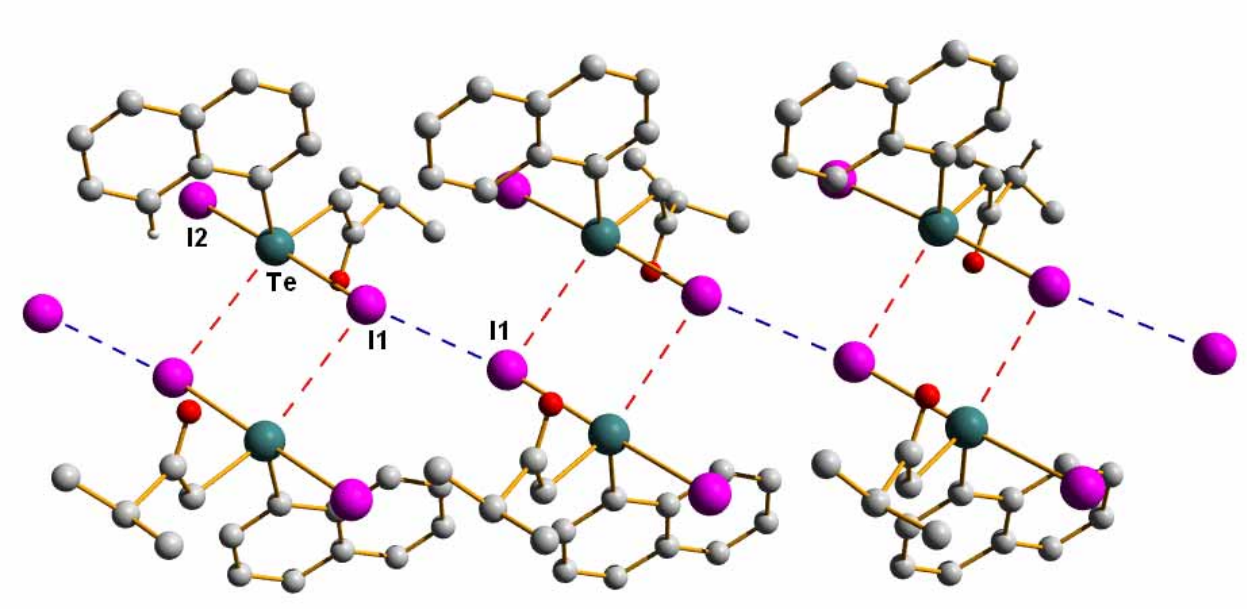
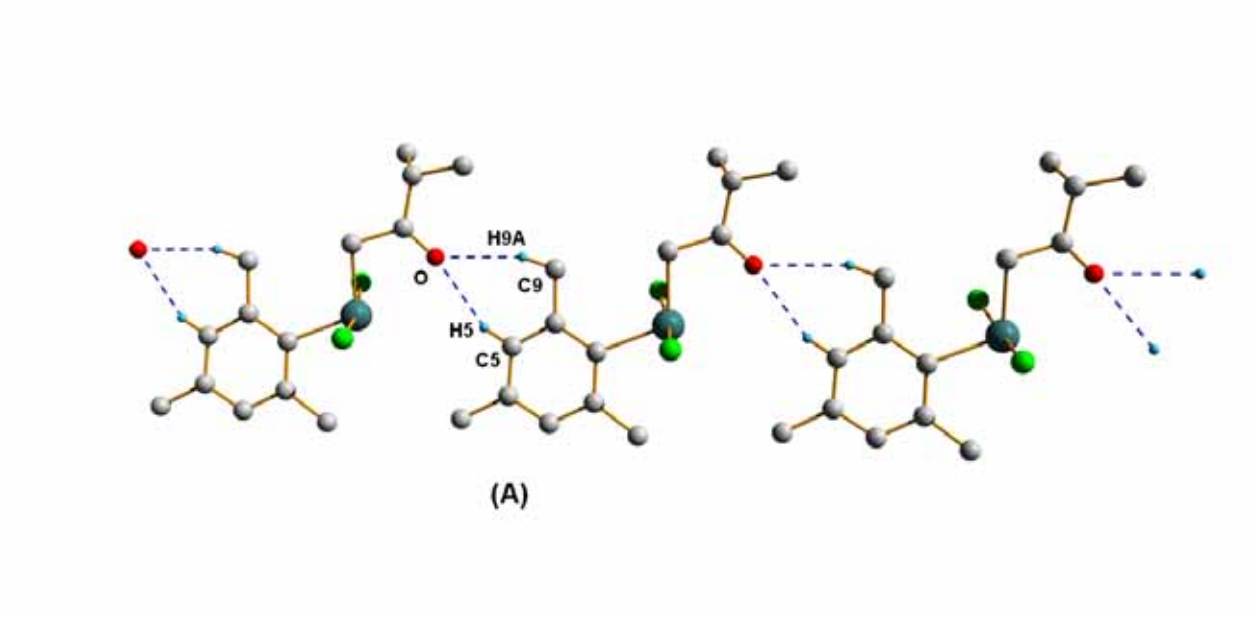
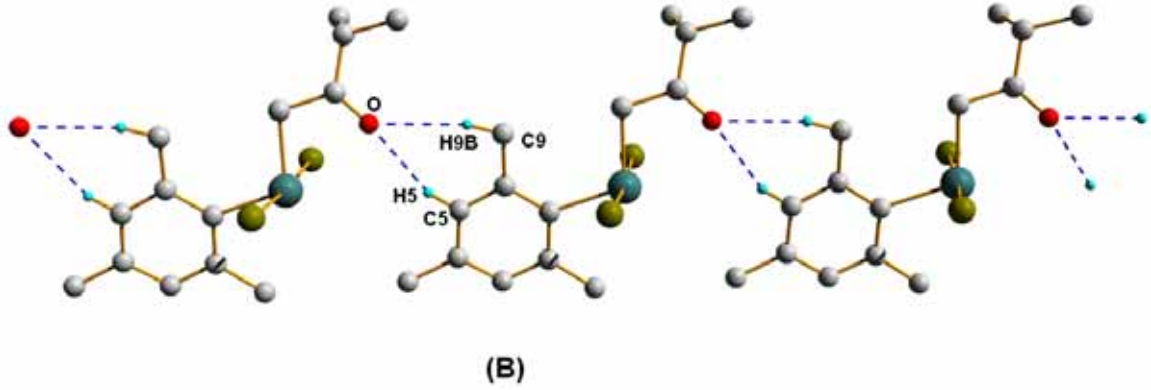


Figure S1. 1-D Supramolecular motif via Te···I and I···I interactions in the lattices of **1Ac**.



(A)



(B)

Figure S2. 1-D Supramolecular motif via C─H···O H-Bonds in the lattices of **1Ba** (A) and **1Bb** (B). Only relevant H atoms are shown for clarity.

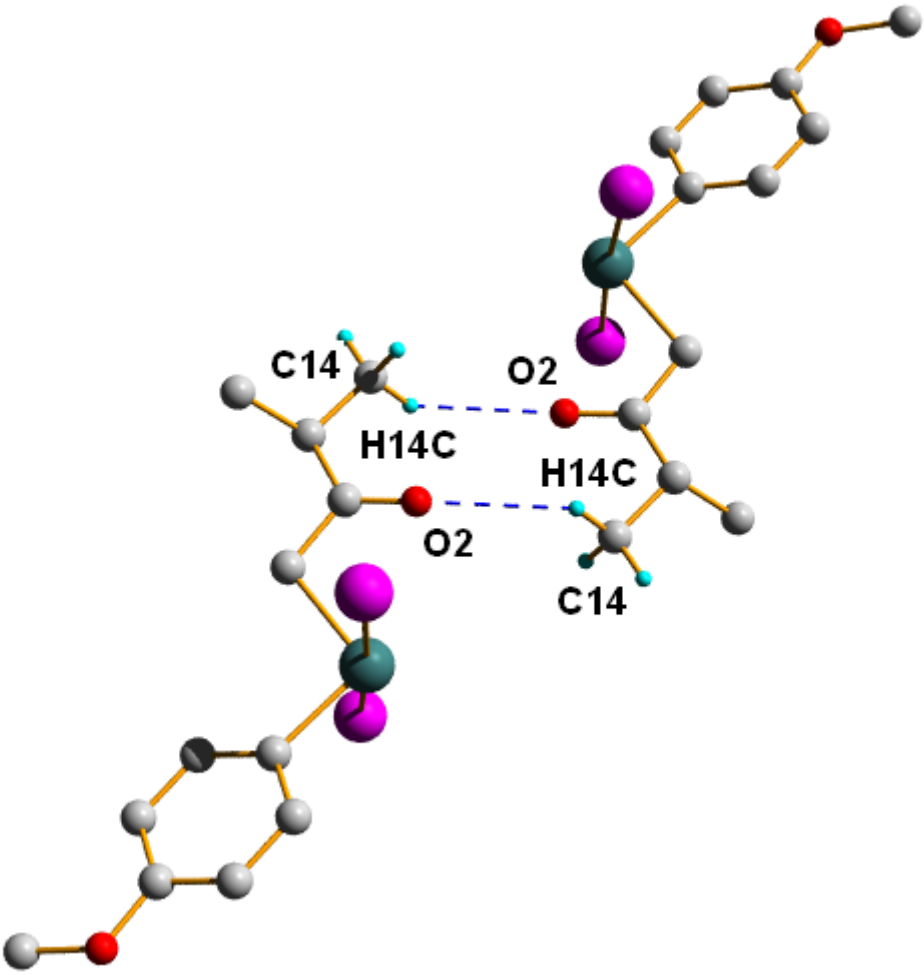


Figure S3. Centrosymmetric pair of **1Cc** molecules realized by means of a supramolecular synthon provided by isopropyl fragments.

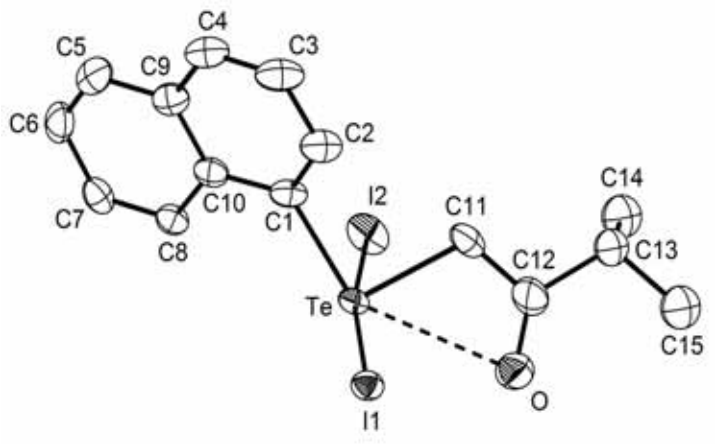


Figure S4. Molecular structure of **1Ac** showing 50% probability displacement ellipsoids and the atom numbering scheme. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Te─C1 = 2.131(5), Te─C11 = 2.141(5), Te─I1 = 2.8951(5), Te─I2 = 2.9499(4), Te···O = 2.958(4); C1─Te─C11 = 93.5(2), I1─Te─I2 = 169.01(2).

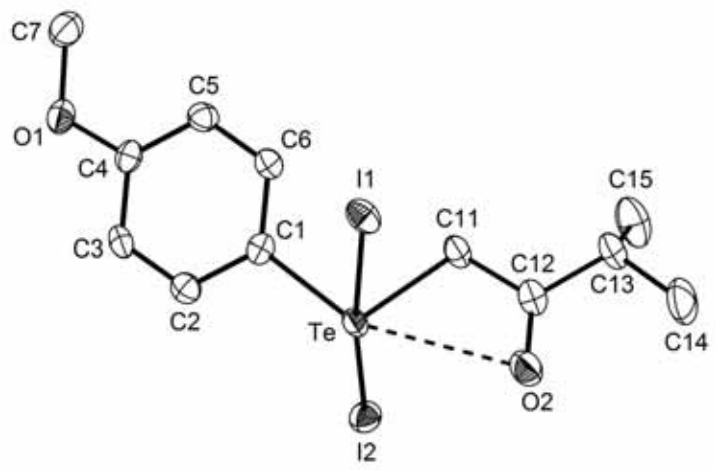


Figure S5. Molecular structure of **1Cc** showing 50% probability displacement ellipsoids and the atom numbering scheme. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Te─C1 = 2.103(4), Te─C11 = 2.129(4), Te─I1 = 2.9513(4), Te─I2 = 2.8690(4), Te···O = 2.874(3); C1─Te─C11 = 98.4(2), I1─Te─I2 = 173.26(1).

Table S1. Bond parameters for D─H···A interactions[a]

	D─H...A	d(D─H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (°)
1Aa	C4A─H4A··· OA^{i}	0.95	2.611	3.448	147.3
	C5A─H5A··· OA^{i}	0.95	2.688	3.505	144.4
1Ac	C3─H3··· O^{ii}	0.95	2.561	3.397	146.9
1Ba	C5─H5···O^{iii}	0.95	2.499	3.402	158.9
	C9─H9A···O^{iii}	0.98	2.656	3.577	156.7
	C3─H3···Cl1^{iv}	0.95	2.904	3.741	147.6
1Bb	C5─H5···O^{v}	0.95	2.567	3.449	154.8
	C9─H9B···O^{v}	0.98	2.519	3.472	163.9
	C7─H7A···Br1^{vi}	0.98	3.124	3.650	115.1
	C14─H14C···Br2^{vii}	0.98	3.147	4.093	162.6
1Ca	C2A─H2A···O2A^{viii}	0.95	2.733	3.550	144.6
	C7B─H7B1··· O2A^{viii}	0.98	2.547	3.350	139.2
	C2B─H2B···O2B^{ix}	0.95	2.635	3.395	137.2
	C14A─H14A··· O2B^{x}	0.98	2.768	3.642	148.8
	C2B─H2B···Cl1B^{xi}	0.95	2.921	3.463	117.4
	C5B─H5B···Cl2A^{xii}	0.95	2.937	3.864	165.1
	C11B─H11C···Cl1A^{iii}	0.99	2.839	3.816	169.1
	C11B─H11D···Cl1B^{xiii}	0.99	2.874	3.646	135.4
	C14B─H14F···Cl1A^{iii}	0.98	2.930	3.805	149.2
1Cc	C14─H14C···O2^{iv}	0.98	2.678	3.498	141.5
	C7─H7B···O1^{xiv}	0.98	2.700	3.380	127.0
	C2─H2···I2 ^{xiv}	0.95	3.153	4.020	152.6
	C7─H7A···I2^{xv}	0.98	3.159	3.912	134.7
	C11─H11A···I1^{xvi}	0.99	3.068	4.005	158.4
	C11─H11B···I1^{xvii}	0.99	3.151	3.995	144.1

[a] Symmetry operations used to generate equivalent atoms: (i) 1.5-x, y, 1.5+z; (ii) 1.5+x, 1.5-y, 1.5+z; (iii) 1+x, y, z; (iv) 2-x, -y, -z; (v) -1+x, y, z; (vi) -x, -1.5+y, 1.5-z; (vii) -x, 1-y, -z; (viii) -1.5+x, 1.5-y, 2-z; (ix) -1.5+x, 1.5-y, 2-z; (x) 1-x, 1.5+y, 1.5-z; (xi) -1.5+x, 1.5-y, 2-z; (xii) ½+x, 1.5-y, 2-z; (xiii) 1.5+x, 1.5-y, 2-z; (xiv) x, 1.5-y, 1.5+z; (xv) -1.5+x, 1.5-y, -½+z; (xvi) x, y, 1+z; (xvii) 1-x, -y, -z;.