

Chalcogen Bonds, Halogen Bonds and Halogen...Halogen Contacts in Di- and Tri-iododiorganyltellurium(IV) Derivatives

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Cartesian coordinates of the calculated CSD assemblies

BZTELI10.

C	-0.20880000	1.23340000	2.61850000
C	2.07200000	4.91420000	0.11200000
C	2.07680000	4.47580000	1.43410000
C	1.29050000	3.38460000	1.73300000
C	-0.91190000	0.19810000	3.18890000
C	-1.80320000	-0.49460000	2.36990000
C	-1.97890000	-0.13390000	1.05920000
C	-1.26590000	0.90690000	0.49540000
C	-0.34700000	1.61950000	1.26990000
C	0.47940000	2.74120000	0.80390000
C	0.49250000	3.22520000	-0.50870000
C	1.28460000	4.28440000	-0.83900000
H	2.49780000	5.79130000	-0.10440000
H	2.66640000	4.79810000	2.11650000
H	-0.85610000	0.02290000	4.08110000
H	-2.24940000	-1.55400000	2.70490000
H	-2.65560000	-0.68880000	0.40810000
H	-1.38620000	1.24190000	-0.37960000
H	-0.16490000	2.72330000	-1.11990000
H	1.37440000	4.45910000	-1.79380000
I	-1.01600000	4.26710000	4.36670000
I	3.36650000	0.67870000	2.82000000
Te	1.18500000	2.45620000	3.62850000
C	4.74900000	-0.19780000	6.87230000
C	2.46820000	-3.87860000	9.37880000
C	2.46340000	-3.44020000	8.05680000
C	3.24970000	-2.34890000	7.75780000
C	5.45210000	0.83750000	6.30190000
C	6.34340000	1.53030000	7.12100000
C	6.51920000	1.16950000	8.43170000
C	5.80610000	0.12870000	8.99540000
C	4.88720000	-0.58390000	8.22100000
C	4.06080000	-1.70550000	8.68700000
C	4.04770000	-2.18960000	9.99950000
C	3.25560000	-3.24870000	10.32980000
H	2.04240000	-4.75560000	9.59520000
H	1.87380000	-3.76250000	7.37440000
H	5.39630000	1.01280000	5.40980000
H	6.78960000	2.58970000	6.78590000
H	7.19580000	1.72440000	9.08270000
H	5.92640000	-0.20620000	9.87050000
H	4.70510000	-1.68770000	10.61080000
H	3.16580000	-3.42350000	11.28460000
I	5.55620000	-3.23150000	5.12410000
I	1.17370000	0.35700000	6.67080000
Te	3.35520000	-1.42060000	5.86230000
C	2.90150000	7.77290000	6.87230000
C	0.62070000	4.09210000	9.37880000
C	0.61590000	4.53050000	8.05680000
C	1.40220000	5.62180000	7.75780000
C	3.60460000	8.80820000	6.30190000
C	4.49590000	9.50090000	7.12100000
C	4.67160000	9.14020000	8.43170000
C	3.95860000	8.09940000	8.99540000
C	3.03970000	7.38680000	8.22100000
C	2.21330000	6.26520000	8.68700000
C	2.20020000	5.78110000	9.99950000
C	1.40810000	4.72200000	10.32980000
H	0.19490000	3.21500000	9.59520000
H	0.02630000	4.20820000	7.37440000
H	3.54880000	8.98340000	5.40980000
H	4.94210000	10.56040000	6.78590000
H	5.34830000	9.69510000	9.08270000
H	4.07890000	7.76450000	9.87050000
H	2.85760000	6.28300000	10.61080000
H	1.31830000	4.54720000	11.28460000
I	3.70870000	4.73920000	5.12410000

I	-0.67380000	8.32760000	6.67080000
Te	1.50770000	6.55010000	5.86230000
DIDMTE01.			
Te	3.24650000	8.89270000	1.87510000
I	1.54770000	8.99660000	-0.49270000
C	4.55310000	10.30140000	0.94950000
H	4.06400000	10.79460000	0.25880000
H	5.30690000	9.82800000	0.54080000
H	4.88800000	10.92860000	1.62380000
I	4.94530000	8.99660000	4.24280000
C	1.93980000	10.30140000	2.80060000
H	2.42890000	10.79460000	3.49140000
H	1.18600000	9.82800000	3.20940000
H	1.60500000	10.92860000	2.12630000
Te	2.71940000	6.33030000	5.62520000
I	4.41820000	6.22640000	7.99300000
C	1.41280000	4.92160000	6.55080000
H	1.90190000	4.42840000	7.24150000
H	0.65900000	5.39500000	6.95950000
H	1.07790000	4.29440000	5.87650000
I	1.02060000	6.22640000	3.25750000
C	4.02610000	4.92160000	4.69970000
H	3.53700000	4.42840000	4.00890000
H	4.77990000	5.39500000	4.29090000
H	4.36090000	4.29440000	5.37400000
Te	3.77350000	6.33030000	-1.87510000
I	5.47230000	6.22640000	0.49270000
C	2.46690000	4.92160000	-0.94950000
H	2.95600000	4.42840000	-0.25880000
H	1.71310000	5.39500000	-0.54080000
H	2.13200000	4.29440000	-1.62380000
I	2.07470000	6.22640000	-4.24280000
C	5.08020000	4.92160000	-2.80060000
H	4.59110000	4.42840000	-3.49140000
H	5.83400000	5.39500000	-3.20940000
H	5.41500000	4.29440000	-2.12630000
DIDMTE01_B (Dimeric form).			
Te	3.77350000	6.33030000	-1.87510000
I	5.47230000	6.22640000	0.49270000
C	2.46690000	4.92160000	-0.94950000
H	2.95600000	4.42840000	-0.25880000
H	1.71310000	5.39500000	-0.54080000
H	2.13200000	4.29440000	-1.62380000
I	2.07470000	6.22640000	-4.24280000
C	5.08020000	4.92160000	-2.80060000
H	4.59110000	4.42840000	-3.49140000
H	5.83400000	5.39500000	-3.20940000
H	5.41500000	4.29440000	-2.12630000
Te	-2.19240000	6.33030000	-9.37540000
I	-0.49360000	6.22640000	-7.00760000
C	-3.49900000	4.92160000	-8.44980000
H	-3.00990000	4.42840000	-7.75910000
H	-4.25280000	5.39500000	-8.04110000
H	-3.83390000	4.29440000	-9.12410000
I	-3.89120000	6.22640000	-11.74310000
C	-0.88580000	4.92160000	-10.30090000
H	-1.37480000	4.42840000	-10.99170000
H	-0.13190000	5.39500000	-10.70970000
H	-0.55090000	4.29440000	-9.62660000
OPAXEJ.			
Te	2.39150000	2.36340000	2.06950000
I	0.13010000	1.53930000	3.75220000
I	4.66570000	3.03180000	0.40470000
C	2.02990000	0.65100000	0.80930000
H	2.87000000	0.19210000	0.65310000
H	1.44030000	0.03720000	1.27470000
C	1.40820000	1.00970000	-0.53150000
H	1.32250000	0.21710000	-1.06700000
H	1.96960000	1.64280000	-0.98480000
H	0.54100000	1.39490000	-0.38890000
C	3.67300000	1.18750000	3.35390000

H	3.29980000	0.29500000	3.42880000
H	4.54260000	1.10510000	2.93030000
C	3.86620000	1.74310000	4.73730000
H	4.47020000	1.17970000	5.22690000
H	3.02060000	1.77500000	5.18990000
H	4.23170000	2.62840000	4.67850000
Te	10.35470000	5.54300000	-2.06950000
I	12.61620000	6.36720000	-3.75220000
I	8.08050000	4.87470000	-0.40470000
C	10.71630000	7.25550000	-0.80930000
H	9.87620000	7.71440000	-0.65310000
H	11.30590000	7.86930000	-1.27470000
C	11.33810000	6.89680000	0.53150000
H	11.42370000	7.68930000	1.06700000
H	10.77660000	6.26370000	0.98480000
H	12.20530000	6.51160000	0.38890000
C	9.07320000	6.71890000	-3.35390000
H	9.44650000	7.61150000	-3.42880000
H	8.20360000	6.80130000	-2.93030000
C	8.88000000	6.16340000	-4.73730000
H	8.27600000	6.72670000	-5.22690000
H	9.72570000	6.13150000	-5.18990000
H	8.51460000	5.27810000	-4.67850000

OPUXEF.

Te	6.08100000	1.93170000	17.10450000
I	8.52660000	3.03780000	16.67720000
I	7.10720000	-0.32310000	18.17840000
I	3.47280000	0.81110000	17.52130000
O	5.11760000	3.45000000	14.98780000
C	5.97500000	1.29180000	15.02090000
H	5.09480000	0.88350000	14.88260000
C	7.01380000	0.32190000	14.49030000
H	6.97140000	-0.51590000	14.97730000
H	7.90360000	0.69360000	14.59400000
C	6.70650000	0.09370000	13.02000000
H	5.86120000	-0.37650000	12.94490000
H	7.39450000	-0.47350000	12.63820000
C	6.62720000	1.38310000	12.21280000
H	7.49970000	1.80450000	12.19320000
H	6.37200000	1.17690000	11.30030000
C	5.61520000	2.34810000	12.81260000
H	5.62140000	3.18430000	12.32250000
H	4.72300000	1.96990000	12.76150000
C	5.99610000	2.58850000	14.25720000
H	6.90330000	2.96020000	14.28880000
C	5.18620000	4.83960000	14.61950000
H	4.72970000	4.98880000	13.77770000
H	6.11140000	5.11680000	14.52330000
C	4.51600000	5.61960000	15.72750000
H	3.62650000	5.28300000	15.86280000
H	4.47270000	6.54710000	15.48390000
H	5.02060000	5.52430000	16.53770000
Te	4.53490000	-2.14340000	20.47790000
I	2.08930000	-1.03740000	20.90510000
I	3.50870000	-4.39820000	19.40390000
I	7.14310000	-3.26400000	20.06100000
O	5.49830000	-0.62510000	22.59450000
C	4.64090000	-2.78330000	22.56140000
H	5.52110000	-3.19170000	22.69970000
C	3.60210000	-3.75320000	23.09210000
H	3.64450000	-4.59110000	22.60500000
H	2.71230000	-3.38160000	22.98840000
C	3.90940000	-3.98140000	24.56230000
H	4.75470000	-4.45170000	24.63750000
H	3.22140000	-4.54870000	24.94420000
C	3.98870000	-2.69200000	25.36960000
H	3.11620000	-2.27070000	25.38910000
H	4.24390000	-2.89820000	26.28210000
C	5.00070000	-1.72700000	24.76980000
H	4.99450000	-0.89080000	25.25980000

H	5.89290000	-2.10520000	24.82090000
C	4.61970000	-1.48660000	23.32510000
H	3.71260000	-1.11500000	23.29350000
C	5.42970000	0.76450000	22.96280000
H	5.88620000	0.91360000	23.80470000
H	4.50450000	1.04160000	23.05900000
C	6.09990000	1.54450000	21.85490000
H	6.98940000	1.20790000	21.71960000
H	6.14320000	2.47200000	22.09840000
H	5.59530000	1.44910000	21.04460000
ОТЕHEX.			
C	2.58120000	2.46450000	3.04130000
C	3.83120000	2.15430000	2.23930000
C	3.03900000	1.39290000	0.13460000
C	1.52860000	1.46460000	0.23010000
H	2.36730000	1.81780000	3.70070000
H	2.56200000	3.42840000	3.55270000
H	4.51170000	1.84970000	3.14900000
H	3.97730000	2.81450000	1.85710000
H	3.06570000	0.59800000	-0.44410000
H	3.32290000	2.03310000	-0.14800000
H	1.16460000	1.61850000	-0.71320000
H	1.15840000	0.63780000	0.26910000
I	-0.51240000	0.57210000	3.08980000
I	2.07630000	5.08960000	0.48380000
O	3.67690000	1.06280000	1.35240000
Te	0.83140000	2.76990000	1.78790000
C	-5.07690000	-1.52200000	3.68730000
C	-6.32680000	-1.83220000	4.48930000
C	-5.53460000	-2.59360000	6.59400000
C	-4.02420000	-2.52190000	6.49850000
H	-4.86290000	-2.16870000	3.02790000
H	-5.05760000	-0.55810000	3.17590000
H	-7.00740000	-2.13680000	3.57960000
H	-6.47290000	-1.17200000	4.87150000
H	-5.56140000	-3.38850000	7.17270000
H	-5.81860000	-1.95340000	6.87660000
H	-3.66020000	-2.36800000	7.44180000
H	-3.65410000	-3.34870000	6.45940000
I	-1.98320000	-3.41440000	3.63880000
I	-4.57190000	1.10310000	6.24480000
O	-6.17250000	-2.92370000	5.37610000
Te	-3.32710000	-1.21660000	4.94070000
PEBHEN01.			
Te	5.15810000	2.11270000	0.85770000
I	3.55180000	4.14590000	0.06770000
I	4.61190000	0.67250000	-1.63510000
I	5.86030000	3.37660000	3.35400000
Cl	7.54330000	0.28240000	0.94350000
C	7.21400000	4.09610000	-0.44240000
C	6.58910000	4.52600000	-1.63650000
H	6.08490000	3.92440000	-2.13590000
C	8.01650000	1.75320000	0.12150000
C	9.36310000	1.77880000	-0.37960000
C	7.06430000	2.71560000	0.01930000
C	7.93730000	5.01510000	0.31510000
H	8.33650000	4.75410000	1.11300000
C	8.05620000	6.32650000	-0.13320000
H	8.55600000	6.93360000	0.36270000
C	6.72550000	5.83150000	-2.06720000
H	6.33570000	6.10320000	-2.86700000
C	7.45110000	6.74060000	-1.29380000
H	7.52450000	7.62700000	-1.56540000
C	9.70220000	2.53020000	-1.49990000
H	9.05290000	3.05690000	-1.90680000
C	10.38000000	1.00580000	0.21620000
H	10.18720000	0.49520000	0.96820000
C	10.99990000	2.50850000	-2.02860000
H	11.19420000	3.00350000	-2.79230000
C	11.98580000	1.76500000	-1.42870000
H	12.85420000	1.76980000	-1.76180000

C	11.65310000	0.99790000	-0.30170000
H	12.30650000	0.47610000	0.10610000
Te	6.05020000	-2.11270000	-3.33190000
I	4.44390000	-4.14590000	-4.12190000
I	5.50390000	-0.67250000	-5.82480000
I	6.75240000	-3.37660000	-0.83570000
Cl	8.43530000	-0.28240000	-3.24610000
C	8.10600000	-4.09610000	-4.63210000
C	7.48120000	-4.52600000	-5.82610000
H	6.97690000	-3.92440000	-6.32550000
C	8.90860000	-1.75320000	-4.06810000
C	10.25520000	-1.77880000	-4.56920000
C	7.95630000	-2.71560000	-4.17040000
C	8.82940000	-5.01510000	-3.87460000
H	9.22850000	-4.75410000	-3.07670000
C	8.94830000	-6.32650000	-4.32290000
H	9.44800000	-6.93360000	-3.82700000
C	7.61760000	-5.83150000	-6.25680000
H	7.22780000	-6.10320000	-7.05660000
C	8.34310000	-6.74060000	-5.48340000
H	8.41660000	-7.62700000	-5.75510000
C	10.59420000	-2.53020000	-5.68950000
H	9.94500000	-3.05690000	-6.09650000
C	11.27210000	-1.00580000	-3.97340000
H	11.07930000	-0.49520000	-3.22150000
C	11.89190000	-2.50850000	-6.21830000
H	12.08620000	-3.00350000	-6.98190000
C	12.87780000	-1.76500000	-5.61830000
H	13.74620000	-1.76980000	-5.95150000
C	12.54520000	-0.99790000	-4.49130000
H	13.19860000	-0.47610000	-4.08350000

Cartesian coordinates for the MEP surface calculations

BZTELI10.

C	2.90150000	7.77290000	6.87230000
C	0.62070000	4.09210000	9.37880000
C	0.61590000	4.53050000	8.05680000
C	1.40220000	5.62180000	7.75780000
C	3.60460000	8.80820000	6.30190000
C	4.49590000	9.50090000	7.12100000
C	4.67160000	9.14020000	8.43170000
C	3.95860000	8.09940000	8.99540000
C	3.03970000	7.38680000	8.22100000
C	2.21330000	6.26520000	8.68700000
C	2.20020000	5.78110000	9.99950000
C	1.40810000	4.72200000	10.32980000
H	0.19490000	3.21500000	9.59520000
H	0.02630000	4.20820000	7.37440000
H	3.54880000	8.98340000	5.40980000
H	4.94210000	10.56040000	6.78590000
H	5.34830000	9.69510000	9.08270000
H	4.07890000	7.76450000	9.87050000
H	2.85760000	6.28300000	10.61080000
H	1.31830000	4.54720000	11.28460000
I	3.70870000	4.73920000	5.12410000
I	-0.67380000	8.32760000	6.67080000
Te	1.50770000	6.55010000	5.86230000

DIDMTE01.

Te	3.77350000	6.33030000	-1.87510000
I	5.47230000	6.22640000	0.49270000
C	2.46690000	4.92160000	-0.94950000
H	2.95600000	4.42840000	-0.25880000
H	1.71310000	5.39500000	-0.54080000
H	2.13200000	4.29440000	-1.62380000
I	2.07470000	6.22640000	-4.24280000
C	5.08020000	4.92160000	-2.80060000
H	4.59110000	4.42840000	-3.49140000
H	5.83400000	5.39500000	-3.20940000
H	5.41500000	4.29440000	-2.12630000

OPAXEJ.

Te	10.35470000	5.54300000	-2.06950000
I	12.61620000	6.36720000	-3.75220000
I	8.08050000	4.87470000	-0.40470000
C	10.71630000	7.25550000	-0.80930000
H	9.87620000	7.71440000	-0.65310000
H	11.30590000	7.86930000	-1.27470000
C	11.33810000	6.89680000	0.53150000
H	11.42370000	7.68930000	1.06700000
H	10.77660000	6.26370000	0.98480000
H	12.20530000	6.51160000	0.38890000
C	9.07320000	6.71890000	-3.35390000
H	9.44650000	7.61150000	-3.42880000
H	8.20360000	6.80130000	-2.93030000
C	8.88000000	6.16340000	-4.73730000
H	8.27600000	6.72670000	-5.22690000
H	9.72570000	6.13150000	-5.18990000
H	8.51460000	5.27810000	-4.67850000

OPUXEF.

Te	4.53490000	-2.14340000	20.47790000
I	2.08930000	-1.03740000	20.90510000
I	3.50870000	-4.39820000	19.40390000
I	7.14310000	-3.26400000	20.06100000
O	5.49830000	-0.62510000	22.59450000
C	4.64090000	-2.78330000	22.56140000
H	5.52110000	-3.19170000	22.69970000
C	3.60210000	-3.75320000	23.09210000
H	3.64450000	-4.59110000	22.60500000
H	2.71230000	-3.38160000	22.98840000
C	3.90940000	-3.98140000	24.56230000
H	4.75470000	-4.45170000	24.63750000
H	3.22140000	-4.54870000	24.94420000
C	3.98870000	-2.69200000	25.36960000

H	3.11620000	-2.27070000	25.38910000
H	4.24390000	-2.89820000	26.28210000
C	5.00070000	-1.72700000	24.76980000
H	4.99450000	-0.89080000	25.25980000
H	5.89290000	-2.10520000	24.82090000
C	4.61970000	-1.48660000	23.32510000
H	3.71260000	-1.11500000	23.29350000
C	5.42970000	0.76450000	22.96280000
H	5.88620000	0.91360000	23.80470000
H	4.50450000	1.04160000	23.05900000
C	6.09990000	1.54450000	21.85490000
H	6.98940000	1.20790000	21.71960000
H	6.14320000	2.47200000	22.09840000
H	5.59530000	1.44910000	21.04460000
OTEXEX.			
C	-5.07690000	-1.52200000	3.68730000
C	-6.32680000	-1.83220000	4.48930000
C	-5.53460000	-2.59360000	6.59400000
C	-4.02420000	-2.52190000	6.49850000
H	-4.86290000	-2.16870000	3.02790000
H	-5.05760000	-0.55810000	3.17590000
H	-7.00740000	-2.13680000	3.57960000
H	-6.47290000	-1.17200000	4.87150000
H	-5.56140000	-3.38850000	7.17270000
H	-5.81860000	-1.95340000	6.87660000
H	-3.66020000	-2.36800000	7.44180000
H	-3.65410000	-3.34870000	6.45940000
I	-1.98320000	-3.41440000	3.63880000
I	-4.57190000	1.10310000	6.24480000
O	-6.17250000	-2.92370000	5.37610000
Te	-3.32710000	-1.21660000	4.94070000
PEBHEN01.			
Te	6.05020000	-2.11270000	-3.33190000
I	4.44390000	-4.14590000	-4.12190000
I	5.50390000	-0.67250000	-5.82480000
I	6.75240000	-3.37660000	-0.83570000
Cl	8.43530000	-0.28240000	-3.24610000
C	8.10600000	-4.09610000	-4.63210000
C	7.48120000	-4.52600000	-5.82610000
H	6.97690000	-3.92440000	-6.32550000
C	8.90860000	-1.75320000	-4.06810000
C	10.25520000	-1.77880000	-4.56920000
C	7.95630000	-2.71560000	-4.17040000
C	8.82940000	-5.01510000	-3.87460000
H	9.22850000	-4.75410000	-3.07670000
C	8.94830000	-6.32650000	-4.32290000
H	9.44800000	-6.93360000	-3.82700000
C	7.61760000	-5.83150000	-6.25680000
H	7.22780000	-6.10320000	-7.05660000
C	8.34310000	-6.74060000	-5.48340000
H	8.41660000	-7.62700000	-5.75510000
C	10.59420000	-2.53020000	-5.68950000
H	9.94500000	-3.05690000	-6.09650000
C	11.27210000	-1.00580000	-3.97340000
H	11.07930000	-0.49520000	-3.22150000
C	11.89190000	-2.50850000	-6.21830000
H	12.08620000	-3.00350000	-6.98190000
C	12.87780000	-1.76500000	-5.61830000
H	13.74620000	-1.76980000	-5.95150000
C	12.54520000	-0.99790000	-4.49130000
H	13.19860000	-0.47610000	-4.08350000