Dalton Trans. – Full Paper

Diarylhalotelluronium(IV) Cations $[(8\text{-}Me_2NC_{10}H_6)_2TeX]^+$ (X = Cl, Br, I) Stabilized by Intramolecularly Coordinating N-Donor Substituents

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Supporting Information

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Table S1. Crystal data and structure refinement of **1 - 7**.

	1·Cl^-·H_2O·½THF	**1**·PF_6^-	**2**·Br^-
Formula	$C_{52}H_{56}Cl_4N_4O_3Te_2$	$C_{24}H_{24}ClF_6N_2PTe$	$C_{26}H_{27}Br_2N_3Te$
Formula weight, g mol^{-1}	1182.01	648.47	668.93
Crystal system	Monoclinic	Triclinic	Triclinic
Crystal size, mm	0.41 × 0.35 × 0.15	0.27 × 0.21 × 0.07	0.36 × 0.28 × 0.17
Space group	*P* $2_1/c$	*P* -1	*P* -1
a, Å	33.779(2)	9.2967(10)	8.785(8)
b, Å	8.8592(8)	10.2462(11)	11.671(13)
c, Å	17.7936(12)	13.4833(16)	14.197(12)
α, °	90.00	92.378(9)	105.03(9)
β, °	109.754(5)	98.203(9)	98.59(7)
γ, °	90.00	97.233(9)	109.95(8)
V, $Å^3$	5011.5(6)	1258.8(2)	1275(2)
Z	2	2	2
ρ_{calcd}, Mg m^{-3}	1.567	1.711	1.742
μ (Mo $K\alpha$), mm^{-1}	1.424	1.412	4.318
F(000)	1184	640	652
θ range, deg	2.39 to 29.32	2.01 to 29.18	2.05 to 29.23
Index ranges	–45 ≤ h ≤ 46	–11 ≤ h ≤ 12	–12 ≤ h ≤ 11
	–11 ≤ k ≤ 12	–14 ≤ k ≤ 14	–16 ≤ k ≤ 16
	–11 ≤ l ≤ 24	–18 ≤ l ≤ 16	–19 ≤ l ≤ 19
No. of reflns collected	10858	14301	13649
Completeness to θ_{max}	97.4%	98.6%	98.1%
No. indep. Reflns	5704	6712	6791
No. obsd reflns with ($I>2\sigma(I)$)	4370	4804	5311
No. refined params	286	316	289
GooF (F^2)	0.980	0.913	1.041
R_1 (F) ($I > 2\sigma(I)$)	0.0361	0.0411	0.0486
wR_2 (F^2) (all data)	0.0909	0.0953	0.1246
Largest diff peak/hole, e $Å^{-3}$	0.655 / –1.030	0.876 / –0.694	1.705 / –1.195
CCDC number	928259	928260	928261

Table S1. cont.

2$_2$·Br^-·PF_6^-	**3**·I_3^-	**3**·I_3^-·I_2	**4**
$C_{48}H_{48}Br_3F_6N_4PTe_2$	$C_{24}H_{24}I_4N_2Te$	$C_{24}H_{24}I_6N_2Te$	$C_{24}H_{20}Cl_6N_2Te$
1320.80	975.65	1229.45	676.72
Monoclinic	Monoclinic	Monoclinic	Tetragonal
0.31 × 0.25 × 0.18	0.18 × 0.15 × 0.06	0.49 × 0.17 × 0.04	0.50 × 0.20 × 0.12
P $2_1/c$	*P* $2_1/c$	*C* 2/*c*	*I* -4
15.915(18)	7.837(3)	31.471(5)	22.4140(11)
9.941(7)	17.587(9)	12.1929(17)	22.4140(11)
16.361(13)	19.891(11)	21.729(3)	10.7778(5)
90	90	90	90
110.84(8)	97.28(4)	132.577(2)	90
90	90	90	90
2419(4)	2719(2)	6139.8(15)	5414.6(5)
2	4	8	8
1.813	2.383	2.660	1.660
3.778	5.650	7.019	1.707
1284	1784	4416	2656
2.05 to 29.25	2.06 to 29.21	1.76 to 30.54	2.78 to 29.17
–18 ≤ h ≤ 21	–10 ≤ h ≤ 10	–42 ≤ h ≤ 44	– 30 ≤ h ≤ 30
–13 ≤ k ≤ 13	–24 ≤ k ≤ 24	–17 ≤ k ≤ 15	–30 ≤ k ≤ 30
–22 ≤ l ≤ 22	–27 ≤ l ≤ 22	–31 ≤ l ≤ 23	–14 ≤ l ≤ 14
18185	21035	9367	25830
98.7%	98.8%	99.6%	99.5%
6501	7292	9367	7259
2951	3531	7256	6514
290	280	307	298
0.846	0.802	1.018	1.013
0.0628	0.0434	0.0347	0.0318
0.1330	0.1129	0.0820	0.0852
1.584 / –0.969	0.853 / –1.709	2.177 / –2.108	0.897 / –0.638
928262	928263	928264	928265

Table S1. cont.

5	**6**·Br_3^-	**7**·Cl^-	**7**·Br^-·H_2O·THF
$C_{24}H_{22}Br_4N_2Te$	$C_{24}H_{22}Br_6N_2Te$	$C_{24}H_{25}ClN_2OTe$	$C_{28}H_{35}BrN_2O_3Te$
785.68	945.50	520.51	655.09
Orthorhombic	Triclinic	Orthorhombic	Monoclinic
0.10 × 0.10 × 0.05	0.39 × 0.14 × 0.12	0.42 × 0.39 × 0.13	0.50 × 0.11 × 0.06
P bca	*P* -1	*P* $ca2_1$	*P* $2_1/c$
14.315(6)	9.2192(12)	12.8089(18)	13.2151(13)
23.765(6)	12.0020(16)	10.4279(14)	9.0546(5)
14.779(12)	14.3375(18)	16.766(2)	23.424(2)
90	89.947(10)	90	90
90	108.386(10)	90	103.826(8)
90	110.917(10)	90	90
5028(5)	1395.0(3)	2239.4(5)	2721.7(4)
8	2	4	4
2.076	2.251	1.544	1.599
7.556	9.676	1.465	2.593
2976	884	1040	1312
2.16 to 29.27	1.83 to 29.20	1.95 to 30.50	1.79 to 29.24
0 ≤ h ≤ 19	–12 ≤ h ≤ 12	– 15 ≤ h ≤ 18	–18 ≤ h ≤ 17
0 ≤ k ≤ 32	–16 ≤ k ≤ 16	–14 ≤ k ≤ 14	–10 ≤ k ≤ 12
0 ≤ l ≤ 20	–19 ≤ l ≤ 19	–20 ≤ l ≤ 23	–32 ≤ l ≤ 32
6764	14896	17741	19661
98.6%	98.0%	99.9%	98.7%
6764	7426	5910	7309
4008	4811	5180	4080
280	298	266	328
0.928	0.964	1.069	0.873
0.0492	0.0514	0.0219	0.0451
0.0807	0.1048	0.0491	0.1116
0.721 / –1.040	0.885 / –0.954	0.680 / –0.475	0.980 / –0. 535
928266	928267	928268	928269

Table S1. cont.

7·I^-	**7**·I_3^-·H_2O
$C_{24}H_{25}IN_2OTe$	$C_{24}H_{25}I_3N_2OTe$
611.96	865.76
Orthorhombic	Monoclinic
0.21 × 0.17 × 0.12	0.33 × 0.21 × 0.08
P ca2_1	*P* $2_1/n$
11.496(5)	11.2981(10)
21.960(11)	12.4425(7)
18.202(9)	19.647(2)
90	90
90	94.176(8)
90	90
4595(4)	2754.6(4)
8	4
1.769	2.088
2.656	4.460
2368	1608
1.85 to 29.22	2.70 to 29.21
0 ≤ h ≤ 15	– 15 ≤ h ≤ 15
0 ≤ k ≤ 29	–14 ≤ k ≤ 17
–24 ≤ l ≤ 23	–19 ≤ l ≤ 26
9791	19462
98.0%	97.8%
9791	7311
4926	5035
524	280
0.859	0.849
0.0580	0.0354
0.1386	0.0864
0.847 / –0.977	1.522 / –1.244
928270	928271

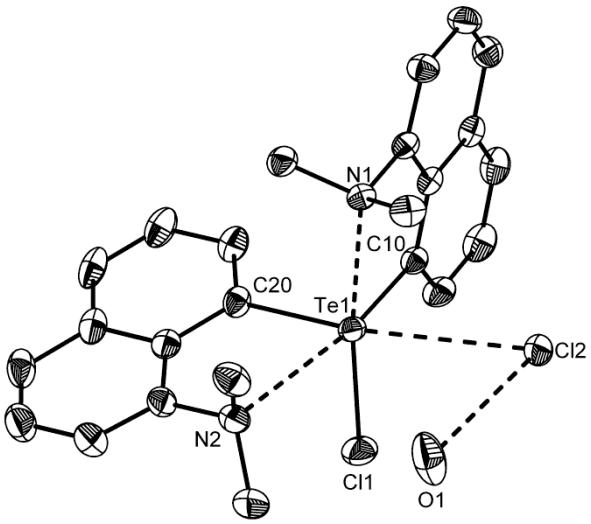

Figure S1. Molecular structure of **1**·Cl^{-}·H_2O·½THF showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Te1-Cl1 2.444(1), Te1-C10 2.141(3), Te1-C20 2.145(3), Te1···N1 2.445(3), Te1···N2 2.800(3), C10-Te1-C20 92.8(1), Cl1-Te1-C10 92.63(9), Cl1-Te1-C20 90.4(1), Ion contact: Te1···Cl2 3.173(1).

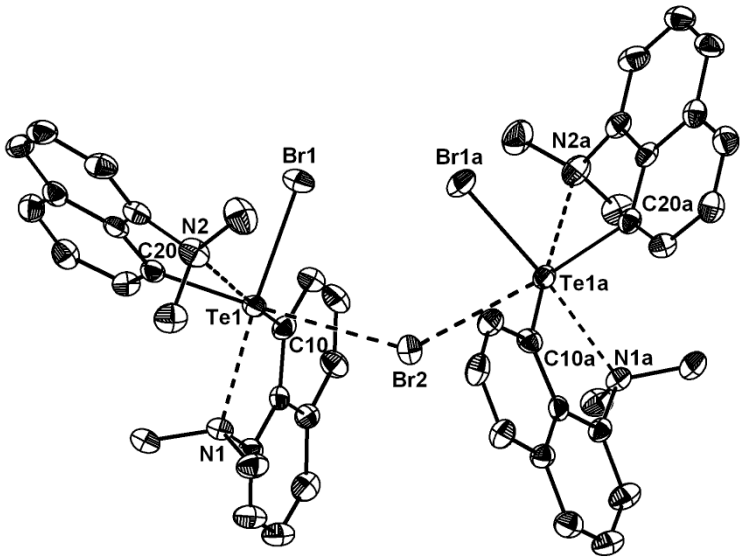

Figure S2. Molecular structure of **2**$_2$·Br^{-}·PF_6^{-} showing 30% probability ellipsoids and the crystallographic numbering scheme (symmetry code used to generate equivalent atoms: a = 1 – x, y, 0.5 – z). Selected bond parameters [Å, º]: Te1-Br1 2.582(2), Te1-C10 2.132(7), Te1-C20 2.137(8), Te1···N1 2.502(6), Te1···N2 2.732(8), Br1-Te1-C10 93.2(2), Br1-Te1-C20 89.7(2), C10-Te1-C20 95.5(3), Ion contact: Te1···Br2 3.272(4).

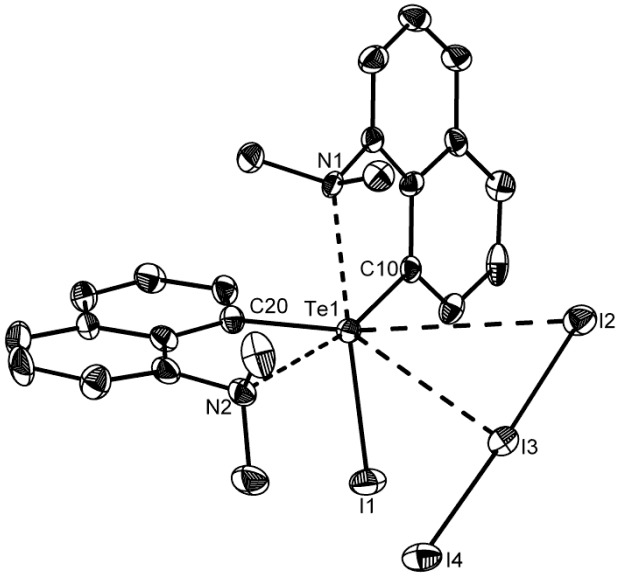

Figure S3. Molecular structure of **3**·I_3^- showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Te1-I1 2.780(2), Te1-C10 2.165(8), Te1-C20 2.136(8), Te1···N1 2.532(7), Te2···N2 2.743(7), I2-I3 2.921(2), I3-I4 2.918(1), I1-Te1-C10 95.2(2), I1-Te1-C20 91.8(3), C10-Te1-C20 96.7(3), Ion contacts: Te1···I2 4.037(2), Te1···I3 4.219(2).

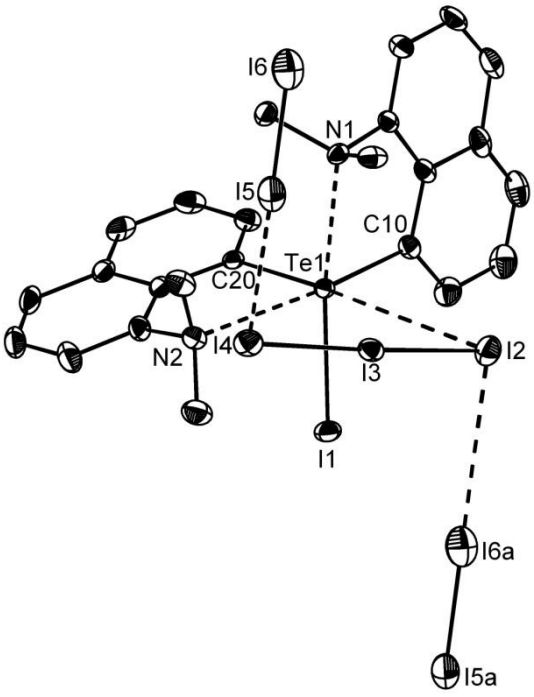

Figure S4. Molecular structure of **3**·I_3^-·I_2 showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Te1-I1 2.7827(8), Te1-C10 2.16(1), Te1-C20 2.138(6), Te1···N1 2.515(7), Te1···N2 2.80(1), I1-Te1-C10 94.9(2), I1-Te1-C20 91.6(2), C10-Te1-C20 96.2(3), Ion contact: Te1···I2 3.8606(8).

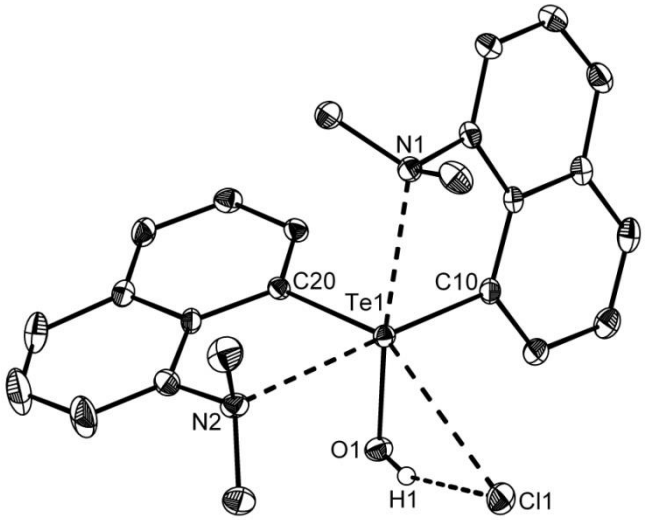

Figure S5. Molecular structure of **7**·Cl^- showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Te1-O1 1.951(2), Te1-C10 2.134(2), Te1-C20 2.123(2), Te1···N1 2.596(2), Te1···N2 2.682(2), O1-H1 0.70(3), O1···Cl1 2.960(2), Cl1···H1 2.32(3), O1-Te1-C10 91.25(9), O1-Te1-C20 89.00(8), C10-Te1-C20 96.81(9). Ion contact: Te1···Cl1 3.2535(7).

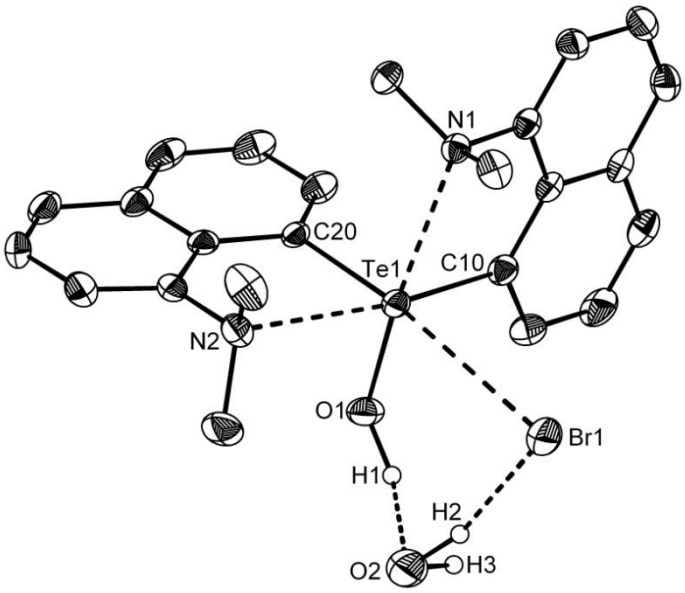

Figure S6. Molecular structure of **7**·Br^-·H_2O·THF showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Te1-O1 1.957(3), Te1-C10 2.130(5), Te1-C20 2.127(5), Te1···N1 2.586(3), Te1···N2 2.709(4), O1-H1 1.07(9), O2···H1 1.71(9), O1···O2 2.729(8), O2-H2 1.05(6), O2-H3 1.02(4), Br1···H2 2.20(6), O2···Br1 3.232(5), O1-Te1-C10 92.2(2), O1-Te1-C20 87.6(2), C10-Te1-C20 94.9(2), Ion contact: Te1···Br1 3.4777(9).

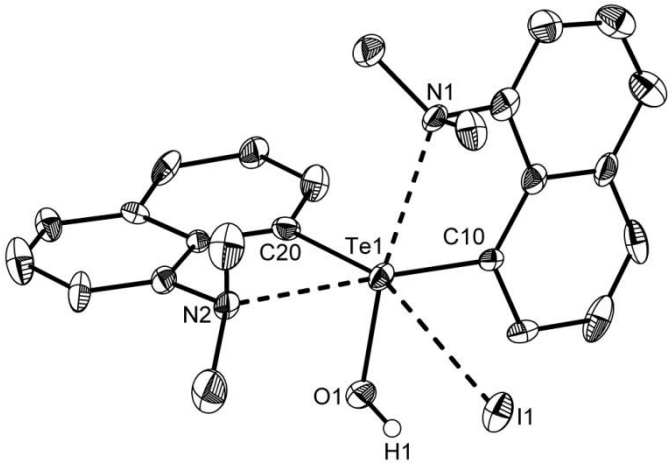

Figure S7. Molecular structure of **7**·I⁻ showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Conformer 1 (shown): Te1-O1 1.969(9), Te1-C10 2.15(1), Te1-C20 2.13(1), Te1···N1 2.61(1), Te1···N2 2.67(1), O1-Te1-C10 91.9(4), O1-Te1-C20 89.9(4), C10-Te1-C20 97.4(5). Ion contact: Te1···I1 3.595(2). Conformer 2 (not shown): Te2-O2 1.933(9), Te2-C30 2.15(1), Te2-C40 2.14(1), Te2-N3 2.595(9), Te2-N4 2.70(1), O2-Te2-C30 94.3(6), O2-Te2-C40 90.7(4), Ion contact: Te2···I2 3.591(2).

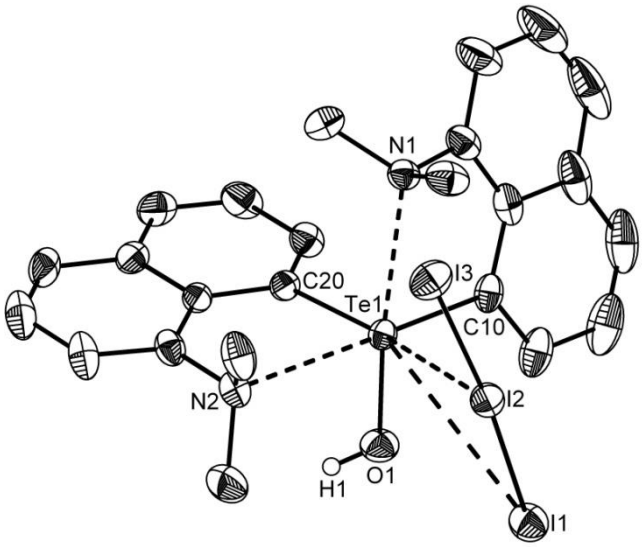

Figure S8. Molecular structure of **7**·I_3^-·H_2O showing 30% probability ellipsoids and the crystallographic numbering scheme. Selected bond parameters [Å, º]: Te1-O1 1.967(3), Te1-C10 2.118(5), Te1-C20 2.108(4), Te1···N1 2.566(4), Te1···N2 2.656(4), O1-H1 0.821(4), O1-Te1-C10 91.2(2), O1-Te1-C20 90.7(2). Ion contacts: Te1···I1 3.9635(5), Te1···I2 4.0977(5).

Table S2. Absolute energies and zero-point corrections together with point groups applied.

Molecule	Point group applied	Absolute energy	Zero-point correction	Sum of electronic and zero-point Energies
Cl^-	O_h	-460.245171	–	-460.245171
Br^-	O_h	-2574.212038	–	-2574.212038
I^-	O_h	-11.535524	–	-11.535524
Cl_2	$D_{\infty h}$	-920.315118	0.001291	-920.313827
Br_2	$D_{\infty h}$	-5148.247583	0.000745	-5148.246838
I_2	$D_{\infty h}$	-22.914513	0.000503	-22.914010
Ph_2Te	C_1	-471.350831	0.180020	-471.170811
$Ph_2Te\cdots Cl_2$ (**MC**)	C_1	-1391.681932	0.182266	-1391.499666
$Ph_2Te\cdots Br_2$ (**MC**)	C_1	-5619.617927	0.181646	-5619.436281
$Ph_2Te\cdots I_2$ (**MC**)	C_1	-494.283836	0.181374	-494.102462
Ph_2TeCl^+ (**CI**)	C_1	-931.288508	0.182130	-931.106379
Ph_2TeBr^+ (**CI**)	C_1	-3045.247463	0.181623	-3045.065840
Ph_2TeI^+ (**CI**)	C_1	-482.573006	0.181405	-482.391601
Ph_2TeCl_2 (**TB**)	C_2	-1391.741067	0.183049	-1391.558018
Ph_2TeBr_2 (**TB**)	C_2	-5619.653186	0.182297	-5619.470889
Ph_2TeI_2 (**TB**)	C_2	-494.294924	0.181776	-494.113148
$(8\text{-}Me_2NC_{10}H_6)_2Te$	C_2	-1046.498262	0.418257	-1046.080006
$(8\text{-}Me_2NC_{10}H_6)_2Te\cdots Cl_2$ (**MC**)	C_1	-1966.838221	0.421286	-1966.416935
$(8\text{-}Me_2NC_{10}H_6)_2Te\cdots Br_2$ (**MC**)	C_1	-6194.772312	0.420651	-6194.351662
$(8\text{-}Me_2NC_{10}H_6)_2Te\cdots I_2$ (**MC**)	C_1	-1069.436712	0.420439	-1069.016273
$(8\text{-}Me_2NC_{10}H_6)_2TeCl^+$ (**CI**)	C_1	-1506.492473	0.422667	-1506.069806
$(8\text{-}Me_2NC_{10}H_6)_2TeBr^+$ (**CI**)	C_1	-3620.447711	0.422128	-3620.025583
$(8\text{-}Me_2NC_{10}H_6)_2TeI^+$ (**CI**)	C_1	-1057.767340	0.421604	-1057.345735
$(8\text{-}Me_2NC_{10}H_6)_2TeCl_2$ (**TB**)	C_2	-1966.896775	0.422026	-1966.474749
$(8\text{-}Me_2NC_{10}H_6)_2TeBr_2$ (**TB**)	C_2	-6194.809041	0.421505	-6194.387535
$(8\text{-}Me_2NC_{10}H_6)_2TeI_2$ (**TB**)	C_2	-1069.449474	0.420988	-1069.028486

Table S3. Coordinates of the optimized gas-phase structures.

Ph_2Te:

Te	0.7252595126	0.7684946418	-0.9244993704
C	0.7388242144	0.7624972347	1.1877181593
C	1.9611310558	0.8368416391	1.8514938261
C	-0.4434368630	0.7383264330	1.9247564800
C	1.9988326313	0.8971940904	3.2390860916
H	2.8884296632	0.8364999209	1.2886038005
C	-0.3977846104	0.7747169268	3.3112147683
H	-1.4009405485	0.6908460728	1.4184100451
C	0.8214390065	0.8607841566	3.9721123144
H	2.9556627980	0.9584791232	3.7465961240
H	-1.3229109634	0.7479694989	3.8773111969
H	0.8521853719	0.8977341401	5.0554324466
C	-0.7213463732	-0.7439325237	-1.2100595372
C	-0.6818781328	-1.9361501532	-0.4898567213
C	-1.7040151764	-0.5589823173	-2.1797491655
C	-1.6257572244	-2.9243308312	-0.7312001309
H	0.0847744586	-2.0951704620	0.2600870457
C	-2.6314326604	-1.5620568422	-2.4332444456
H	-1.7560751670	0.3728150514	-2.7326959749
C	-2.5984126851	-2.7436834045	-1.7069227407
H	-1.5921035071	-3.8464242305	-0.1605459641
H	-3.3906994412	-1.4098074932	-3.1929647569
H	-3.3287964104	-3.5220094450	-1.8983600927

$Ph_2Te\cdots Cl_2$ (MC):

Te	0.0215969309	0.0481038342	0.4962079019
C	2.0500676887	0.0020032959	-0.1016068399
C	-0.3275476550	2.0956831308	0.1361720629
C	2.3980409574	0.4179224834	-1.3838793009
C	3.0153571016	-0.4894589273	0.7693370869
C	-1.3883922123	2.4597361027	-0.6874172671
C	0.4632012886	3.0663264944	0.7434376413
C	3.7235161885	0.3504245050	-1.7881353114
C	4.3381882490	-0.5633513102	0.3492738321
C	-1.6547566243	3.8054681660	-0.9076688127
C	0.1947823659	4.4068111852	0.5087464953
C	4.6931480066	-0.1430750060	-0.9241007387
C	-0.8626359074	4.7771440244	-0.3133637893
H	2.7482575018	-0.7957943230	1.7740403651
H	1.2741273553	2.7826562154	1.4043252171
H	5.0923309172	-0.9436613450	1.0292982904
H	0.8093986886	5.1651581391	0.9809299945
H	5.7274070966	-0.1977274538	-1.2451485555
H	-1.0712726419	5.8268856413	-0.4871875457
H	3.9970857929	0.6812637577	-2.7840416684
H	1.6456957921	0.7988269439	-2.0657740201
H	-2.4824155175	4.0907197988	-1.5475860296
H	-2.0056346718	1.7032635634	-1.1600930689
Cl	0.4974050730	0.2415367951	3.1144569325
Cl	0.9684200712	0.4582726361	5.2917623159

$Ph_2Te\cdots Br_2$ (MC):

Te	-0.0017833057	0.0388936472	-0.0046883571
C	-0.0012593677	0.0161010267	2.1108469098
C	2.0899438012	0.0076901024	-0.2772651030
C	0.6654173738	-1.0037472895	2.7846897453
C	-0.7081451356	0.9838161034	2.8147771199
C	2.6374505040	-0.9427876306	-1.1334676590
C	2.9043916842	0.9399026257	0.3581676247
C	0.6315870077	-1.0432911648	4.1711058189
C	-0.7455340984	0.9273939405	4.2030054442
C	4.0096452160	-0.9604287683	-1.3508005650
C	4.2742257002	0.9064155309	0.1432505428
C	-0.0763617387	-0.0812081071	4.8806534854
C	4.8271359429	-0.0403383095	-0.7106857888
H	-1.2117605562	1.7886135361	2.2915196514
H	2.4754417325	1.6935772183	1.0083776572
H	-1.2943216560	1.6841793907	4.7524723071
H	4.9107043306	1.6316323033	0.6380357725
H	-0.1036842917	-0.1180907344	5.9639913770
H	5.8980510778	-0.0573976983	-0.8796020704
H	1.1571283822	-1.8327401017	4.6971416602
H	1.2142244413	-1.7621218078	2.2372955568
H	4.4372056791	-1.6993375143	-2.0194629145
H	2.0038159941	-1.6710801865	-1.6281959642
Br	-0.4291923982	2.8177971127	-0.3730016736
Br	-0.7563920045	5.2682067636	-0.6470786730

$Ph_2Te\cdots I_2$ (MC):

Te	0.0383232714	0.3577483168	-0.0269307736
C	0.0153889262	0.1725111503	2.0805794127
C	2.1175723620	0.1092155534	-0.3043190267
C	0.2274048449	-1.0829864633	2.6459976765
C	-0.2454591671	1.2733226674	2.8881663046
C	2.5510623974	-0.5411092545	-1.4556429873
C	3.0376467716	0.6050881732	0.6129011444
C	0.1913782821	-1.2289614801	4.0253030537
C	-0.2896244155	1.1146311499	4.2683370777
C	3.9118825784	-0.6896950640	-1.6897634391
C	4.3949058619	0.4407454080	0.3758100220
C	-0.0695387802	-0.1316169570	4.8363997338
C	4.8339720747	-0.2028242874	-0.7742534895
H	-0.4082252978	2.2509731280	2.4482796873
H	2.7038585688	1.1196945664	1.5065928430
H	-0.4936017129	1.9737797981	4.8977669299
H	5.1123000260	0.8262329058	1.0919481357
H	-0.1030995935	-0.2502469077	5.9137470672
H	5.8958737159	-0.3235452160	-0.9566785634
H	0.3613727729	-2.2053189115	4.4656053303
H	0.4212616392	-1.9448856992	2.0171986222
H	4.2485184553	-1.1945271704	-2.5885423456
H	1.8368781682	-0.9372800905	-2.1698716665
I	-0.1676875687	3.4321923516	-0.3599080667
I	-0.3388091994	6.2417122057	-0.6487245584

Ph_2TeCl^+ (CI):

Te	0.1217887651	0.1717608867	-0.2628030151
C	2.2090020046	0.0378121643	-0.2607712098
C	-0.1604898774	2.2390739507	-0.2445627786
C	2.7875560677	-0.3888373080	-1.4536504066
C	2.9705576442	0.3432468346	0.8622295922
C	-1.4674552729	2.6775756083	-0.4621337463
C	0.8928354269	3.1306418191	-0.0606871392
C	4.1703136731	-0.4864506013	-1.5239648099
C	4.3498063310	0.2285570214	0.7741512591
C	-1.7189086538	4.0400890576	-0.4796184739
C	0.6216773706	4.4896576582	-0.0872433612
C	4.9454592863	-0.1794117030	-0.4141588691
C	-0.6773166806	4.9406823196	-0.2922137282
H	2.5077353070	0.6467277949	1.7941307534
H	1.9069058074	2.7812089913	0.0916424758
H	4.9602153013	0.4547280364	1.6406546261
H	1.4292557044	5.1989586672	0.0509851623
H	6.0241754762	-0.2680464263	-0.4712257851
H	-0.8789073491	6.0055284699	-0.3116058592
H	4.6370957482	-0.8153700189	-2.4448608171
H	2.1866160645	-0.6498193847	-2.3192682348
H	-2.2834968999	1.9782175425	-0.6138227716
H	-2.7286258547	4.3972896176	-0.6438513996
Cl	-0.2657754488	-0.2779683241	1.9665623126

Ph_2TeBr^+ (CI):

Te	-0.0036235607	-0.0131841653	-0.0014052225
C	0.0029709379	0.0017179152	2.0934145064
C	2.0451467183	0.0040109540	-0.4171271765
C	-0.4019852904	-1.1842423672	2.7007784515
C	0.3734795856	1.1199489597	2.8322307293
C	2.4005027089	-0.1927334001	-1.7518294309
C	3.0009602294	0.1539348807	0.5832921622
C	-0.4115441966	-1.2522208883	4.0873610572
C	0.3483167422	1.0343807965	4.2161955064
C	3.7448968301	-0.2234433305	-2.0860009385
C	4.3409565278	0.1134656203	0.2296091791
C	-0.0384299653	-0.1469514445	4.8392991365
C	4.7099295000	-0.0702090344	-1.0977442979
H	0.6603155057	2.0469409346	2.3491366487
H	2.7159520214	0.2906995625	1.6194096274
H	0.6272084191	1.8977126382	4.8090801555
H	5.0994751139	0.2250210682	0.9955590085
H	-0.0580716713	-0.2016104437	5.9216043864
H	5.7602753323	-0.0992626314	-1.3638782341
H	-0.7230936753	-2.1680466623	4.5755634961
H	-0.7127488418	-2.0465714748	2.1192939789
H	1.6510824409	-0.3184030798	-2.5267340727
H	4.0376323732	-0.3720229815	-3.1186371664
Br	-0.5494806738	2.3560598804	-0.4329226874

Ph_2TeI^+ (CI):

Te	-0.0173652641	0.0455091790	-0.0093316088
C	-0.0093885176	0.0316137712	2.0909570976
C	2.0403968161	0.0186339656	-0.4140705872
C	-0.3953902861	-1.1708625235	2.6776047037
C	0.3524959962	1.1377685238	2.8508660607
C	2.4044203276	-0.1725909006	-1.7462924895
C	2.9877246419	0.1333102853	0.5975043136
C	-0.3948154922	-1.2666624900	4.0627969612
C	0.3401156258	1.0243752786	4.2331469917
C	3.7515013850	-0.2379414609	-2.0655721226
C	4.3307475052	0.0597589338	0.2584368522
C	-0.0284509361	-0.1734033418	4.8350850210
C	4.7099131691	-0.1212943276	-1.0659353789
H	0.6257480984	2.0777840821	2.3851612811
H	2.6949174903	0.2683100552	1.6316506000
H	0.6146095926	1.8786510622	4.8410399664
H	5.0826185515	0.1432000220	1.0344795971
H	-0.0389010603	-0.2508458265	5.9161217084
H	5.7618236884	-0.1764894449	-1.3213425482
H	-0.6921351783	-2.1961653355	4.5338296358
H	-0.6978728567	-2.0255734879	2.0809801530
H	1.6607709229	-0.2688907525	-2.5307729485
H	4.0510001639	-0.3842611745	-3.0966675271
I	-0.5893200855	2.6239050254	-0.4978923499

Ph_2TeCl_2 (TB):

Te	0.2273741531	0.0000000019	0.0142121525
C	1.6071973212	-1.6123120760	0.1000933247
C	1.6071518150	1.6123120759	0.1008214321
C	1.3403301179	-2.6703698996	0.9586331080
C	1.4492711375	2.6703699002	-0.7842674640
C	2.2095351846	-3.7532152243	0.9885236967
C	2.3154328772	3.7532152224	-0.7056879431
C	3.3315453823	3.7664191975	0.2390782267
H	4.0095110488	4.6110212101	0.2937370678
C	3.4820125071	2.6993986470	1.1150180521
H	4.2762579777	2.7067371557	1.8531818091
C	2.6127307177	1.6190123106	1.0580716880
H	2.7155698890	0.8003989422	1.7600219239
C	2.7241505679	-1.6190123137	-0.7244868271
H	2.9135994015	-0.8003989457	-1.4081674316
C	3.5937575380	-2.6993986526	-0.6727429399
H	4.4737405937	-2.7067371636	-1.3062580710
C	3.3353854690	-3.7664192025	0.1776421544
H	4.0148805702	-4.6110212169	0.2078321865
H	0.6769554078	2.6486448922	-1.5437063649
H	2.1944180563	4.5841985569	-1.3914722196
H	0.4794568335	-2.6486448893	1.6159885815
H	2.0040652317	-4.5841985584	1.6539008529
Cl	0.0929333411	-0.0146354556	2.5035090874
Cl	0.4039585880	0.0146354594	-2.4724505708

Ph_2TeBr_2 (TB):

Te	-0.6883647745	0.0000000008	-0.5902456629
C	-0.6875735361	0.0166500491	1.5333483983
C	1.4104853703	-0.0166500499	-0.9134799934
C	-1.5925197873	0.8414378923	2.1880383519
C	1.9194337342	-0.8414378926	-1.9077225274
C	-1.6444605540	0.8207956415	3.5754858497
C	3.2827108678	-0.8207956434	-2.1707507757
C	4.1223551739	0.0056522696	-1.4375680304
H	5.1872480565	0.0145487545	-1.6420306656
C	3.6012260133	0.8216881787	-0.4420568303
H	4.2549932938	1.4682702776	0.1326194876
C	2.2381969774	0.8235840736	-0.1810129694
H	1.8304613660	1.4821649181	0.5764253707
C	0.1626087930	-0.8235840764	2.2396092920
H	0.8489664945	-1.4821649212	1.7210784126
C	0.1125913244	-0.8216881830	3.6265088207
H	0.7802901924	-1.4682702834	4.1849376408
C	-0.7917502021	-0.0056522734	4.2934305211
H	-0.8313383194	-0.0145487595	5.3770515810
H	1.2717626437	-1.5125470430	-2.4595095044
H	3.6859061276	-1.4593884103	-2.9486297767
H	-2.2366671681	1.5125470441	1.6321419054
H	-2.3517123452	1.4593884088	4.0926483591
Br	-0.7214286781	-2.6726401231	-0.5880897383
Br	-0.6912789538	2.6726401247	-0.6232513756

Ph_2TeI_2 (TB):

Te	0.0072372469	0.0000000001	0.0062099998
C	0.0091796888	0.0205445714	2.1304515756
C	2.1071253659	-0.0205445713	-0.3145327832
C	-0.9496983544	0.7839444257	2.7829505620
C	2.6064038837	-0.7839444255	-1.3613961891
C	-1.0088613804	0.7533233065	4.1699420903
C	3.9683149462	-0.7533233065	-1.6305504595
C	4.8159877317	0.0223350587	-0.8524277411
H	5.8796350534	0.0393823862	-1.0625640668
C	4.3046116507	0.7772259034	0.1949261758
H	4.9644769499	1.3853424120	0.8035608112
C	2.9431307149	0.7684628173	0.4639360050
H	2.5436675352	1.3810422026	1.2632252854
C	0.9056009936	-0.7684628173	2.8385105011
H	1.6349391206	-1.3810422027	3.3222740416
C	0.8465153984	-0.7772259035	4.2250549537
H	1.5483183336	-1.3853424123	4.7848146991
C	-0.1110098990	-0.0223350588	4.8895856364
H	-0.1571447044	-0.0393823864	5.9728097499
H	1.9525961174	-1.4160110084	-1.9513518646
H	4.3638304861	-1.3447176295	-2.4486044415
H	-1.6321189579	1.4160110087	2.2263408117
H	-1.7573461025	1.3447176296	4.6851269896
I	-0.0322647063	2.9181589137	-0.0957137987
I	-0.0995040534	-2.9181589134	-0.0173518312

$(8\text{-}Me_2NC_{10}H_6)_2Te$:

Te	-0.0005367157	-0.0000000004	-0.0002580707
N	0.0000475824	-0.0004317124	2.8458704677
N	2.2228862279	0.0004317113	-1.7770074655
C	-0.6233455555	-0.4004740553	-2.0161296017
C	-1.9639965212	0.4004740547	0.7720465794
C	-1.3699568025	-0.2759962457	3.1182175713
C	1.5801407393	0.2759962449	-3.0171539069
C	0.2019924402	-0.0689646781	-3.1330587365
C	-2.3210439563	0.0689646775	2.1141459157
C	-0.3693787881	-0.0860713962	-4.4435972901
C	-3.7014621386	0.0860713958	2.4861970177
C	0.9657135390	-0.9392532586	3.3821596084
H	1.9379979558	-0.7483249954	2.9201372186
H	1.0952012819	-0.8575863689	4.4725347372
H	0.6644070707	-1.9581880983	3.1373268490
C	0.3571115829	1.3834406517	3.1432603894
H	0.3743067433	1.5783443730	4.2272975789
H	1.3463925081	1.5995089195	2.7323838524
H	-0.3613093743	2.0603992178	2.6805091612
C	3.2447617312	0.9392532573	-1.3576183403
H	4.1772894022	0.8575863675	-1.9373399459
H	2.8653828563	1.9581880971	-1.4400824961
H	3.4910074166	0.7483249939	-0.3096847841
C	2.6781331568	-1.3834406529	-1.6838103650
H	3.5355916131	-1.5783443743	-2.3472840248
H	2.9749410331	-1.5995089208	-0.6545381163
H	1.8680837481	-2.0603992188	-1.9560002378
C	-1.7870177974	-0.7740415525	4.3301979538
H	-1.0547720502	-1.0482814477	5.0807925884
C	-3.1551090793	-0.8761074560	4.6358728185
H	-3.4601144375	-1.2734845929	5.5978962799
C	-4.0884259356	-0.4139216598	3.7509242875
H	-5.1435863284	-0.4243486921	4.0046151429
C	-4.6578617934	0.6003320604	1.5835077857
H	-5.7002361206	0.6288553327	1.8837507845
C	-4.2646577415	1.0713840657	0.3615916775
H	-4.9895542381	1.5060868569	-0.3187283761
C	-2.9251091003	0.9506351271	-0.0470448129
H	-2.6630105406	1.2612560534	-1.0513678643
C	-1.8632693781	-0.9506351274	-2.2553721833
H	-2.4840654478	-1.2612560536	-1.4235232268
C	-2.3805443047	-1.0713840658	-3.5568332830
H	-3.3645761940	-1.5060868567	-3.6982247506
C	-1.6716564416	-0.6003320605	-4.6269577615
H	-2.0880311888	-0.6288553327	-5.6286174673
C	0.3768446749	0.4139216594	-5.5355801610
H	-0.0838750789	0.4243486919	-6.5181583071
C	1.6508518231	0.8761074553	-5.3591714225
H	2.2118162114	1.2734845922	-6.1981209824
C	2.2663710198	0.7740415516	-4.0997084428
H	3.3098821646	1.0482814466	-3.9964581130

$(8\text{-}Me_2NC_{10}H_6)_2Te\cdots Cl_2$ (MC):

Te	-0.0355449984	0.0197627103	0.0110062812
C	-0.0018151613	0.0122603564	2.1519390818
C	1.2402703565	-0.0103295719	2.8477430276
C	-1.1798894068	-0.0083131417	2.8611777372
C	-1.1829179865	-0.1470365278	4.2607225832
C	-0.0064929395	-0.3241807553	4.9342985005
C	1.2287181689	-0.2703355508	4.2516888235
C	2.4969116393	0.2127406071	2.2191994628
C	3.6638182816	-0.0080522815	2.9090195341
C	3.6405717292	-0.3816114274	4.2636674772
C	2.4515096463	-0.4685120353	4.9316051989
N	2.4796554643	0.7481365471	0.8961356842
C	3.5797951415	0.3403375449	0.0302131288
C	2.3337423884	2.2054815486	0.9114082171
H	-2.1303613021	0.0401260320	2.3438479878
H	-2.1284236295	-0.1572546832	4.7916390373
H	-0.0030707573	-0.5004887488	6.0049617721
H	4.6177400536	0.1370598664	2.4168060371
H	4.5756913606	-0.5567568534	4.7836186589
H	2.4272387031	-0.6968601456	5.9919334110
H	3.7080813636	-0.7394851020	0.0752233740
H	3.3365964198	0.6129171845	-0.9992297445
H	4.5249349777	0.8363855005	0.2930745302
H	1.4848406485	2.4931288542	1.5330577294
H	2.1586984131	2.5626271949	-0.1062870050
H	3.2352075385	2.6959499915	1.3054732399
C	-1.8963868913	-1.0275860490	-0.1713073786
C	-2.8493251211	-0.6754168842	-1.1694298384
C	-2.1938421216	-2.0175749878	0.7349598921
C	-3.4673159434	-2.6123094547	0.7695459588
C	-4.4530866042	-2.1672758052	-0.0671199508
C	-4.1767549657	-1.1907939888	-1.0495709048
C	-2.5501758550	0.1412318714	-2.2985591541
C	-3.5623209251	0.5833541179	-3.1167541248
C	-4.8921608858	0.1778010142	-2.9067726443
C	-5.1851867889	-0.7248855872	-1.9234403365
N	-1.1758503451	0.3924967769	-2.5793700234
C	-0.5660763198	-0.6907689278	-3.3556157772
C	-0.8673562614	1.6964693087	-3.1375107442
H	-1.4510391283	-2.3336338828	1.4576858774
H	-3.6683491480	-3.3977029533	1.4896063763
H	-5.4574988807	-2.5732204904	-0.0043339094
H	-3.3309997248	1.2144482669	-3.9669367119
H	-5.6716117351	0.5424116610	-3.5665937088
H	-6.1954099251	-1.1012167258	-1.8009546985
H	0.5165439202	-0.5514861238	-3.3887494756
H	-0.7678070066	-1.6515208301	-2.8828135798
H	-0.9516131025	-0.7152933700	-4.3855564015
H	0.2146355524	1.8486377658	-3.1059805675
H	-1.3445710508	2.4775179001	-2.5438812553
H	-1.1837852877	1.8065968221	-4.1854606522
Cl	1.2794475730	-2.1424691830	-0.4020099812
Cl	2.4959152763	-4.1325570654	-0.7630568935

(8-$Me_2NC_{10}H_6)_2Te\cdots Br_2$ (MC):

Te	0.0197486713	-0.0264544403	-0.0122715287
C	0.0025739134	-0.0137923154	2.1298155573
C	1.2244984844	0.0017851205	2.8619229616
C	-1.1937169513	-0.0527746769	2.8066236817
C	-1.2348262104	-0.1776684755	4.2068082919
C	-0.0754008169	-0.3201245454	4.9164062193
C	1.1769754960	-0.2422903482	4.2684461673
C	2.4950049274	0.2488383759	2.2698881446
C	3.6450594564	0.0659716896	2.9986318180
C	3.5895678931	-0.2921577146	4.3563457046
C	2.3826805666	-0.4019581628	4.9877892384
N	2.5078763945	0.7677593632	0.9410496074
C	3.6479322820	0.3861610523	0.1181290552
C	2.3131038012	2.2193450545	0.9314824385
H	-2.1295894317	-0.0279403631	2.2625199462
H	-2.1953984395	-0.2040489054	4.7094218502
H	-0.0981664866	-0.4851241890	5.9885762515
H	4.6101649430	0.2314564955	2.5353537341
H	4.5122537385	-0.4360476775	4.9072536071
H	2.3310139901	-0.6184140883	6.0496203933
H	3.8029995781	-0.6897317562	0.1763802161
H	3.4350642611	0.6454602467	-0.9214924759
H	4.5712507394	0.9071262232	0.4095571260
H	1.4315481862	2.4847678855	1.5163746709
H	2.1643442263	2.5586565034	-0.0963897473
H	3.1819303566	2.7453178575	1.3528888641
C	-1.8696832307	-1.0235209939	-0.2309329386
C	-2.8306238097	-0.5991668509	-1.1933312859
C	-2.1820171073	-2.0431082388	0.6371526169
C	-3.4719746904	-2.6014811816	0.6710265180
C	-4.4585033898	-2.0922365149	-0.1272548709
C	-4.1705523540	-1.0811179049	-1.0703835740
C	-2.5303967941	0.2613496105	-2.2897706734
C	-3.5459683093	0.7719593219	-3.0631446171
C	-4.8825894327	0.3949537784	-2.8448089431
C	-5.1821730476	-0.5461405954	-1.9002626270
N	-1.1577405743	0.4877590884	-2.5901831692
C	-0.5884666079	-0.5787636182	-3.4158324733
C	-0.8209421501	1.8040197122	-3.0980189939
H	-1.4366658191	-2.4110553981	1.3326774675
H	-3.6838160471	-3.4100558915	1.3618162616
H	-5.4733722169	-2.4710410813	-0.0631320267
H	-3.3133528641	1.4371907199	-3.8865839115
H	-5.6640106759	0.8131959946	-3.4695991457
H	-6.2001016255	-0.9000281952	-1.7745033875
H	0.4969684851	-0.4659544845	-3.4608215841
H	-0.8106508629	-1.5520236610	-2.9786752072
H	-0.9877932805	-0.5542605080	-4.4409337812
H	0.2647865149	1.9276944078	-3.0659866998
H	-1.2748741919	2.5719473827	-2.4701078724
H	-1.1404920603	1.9646132162	-4.1387652842
Br	1.4046889786	-2.4042286748	-0.4057114683
Br	2.6554092752	-4.6067251883	-0.7510838378

(8-$Me_2NC_{10}H_6)_2Te\cdots I_2$ (MC):

Te	0.0777456932	-0.1509599988	-0.0449791617
C	0.0390277279	-0.0911554059	2.0992700486
C	1.2520664129	-0.0144451196	2.8432148237
C	-1.1600471817	-0.1644756966	2.7686601277
C	-1.2082322924	-0.2696490799	4.1702607127
C	-0.0511933143	-0.3591315760	4.8919740284
C	1.2022983225	-0.2419415039	4.2523920857
C	2.5173635278	0.2801943135	2.2608234640
C	3.6674632667	0.1516409015	3.0014777552
C	3.6143718196	-0.1959712831	4.3620430898
C	2.4069035745	-0.3460210410	4.9838508187
N	2.5210719984	0.7908454356	0.9293757463
C	3.6887545404	0.4651952097	0.1232702730
C	2.2501906788	2.2297865078	0.9047444956
H	-2.0926043578	-0.1836464689	2.2190516287
H	-2.1718167322	-0.3236299362	4.6650017588
H	-0.0773600321	-0.5107390040	5.9660316380
H	4.6291040663	0.3545027682	2.5457892548
H	4.5369495702	-0.2978967726	4.9224599312
H	2.3535862978	-0.5523716688	6.0476273858
H	3.8959040200	-0.6021385435	0.1852176795
H	3.4775948878	0.7140820104	-0.9193702227
H	4.5833027080	1.0290863112	0.4251257464
H	1.3493606228	2.4531984803	1.4772019532
H	2.0954360131	2.5518622537	-0.1276775623
H	3.0861384362	2.8034466760	1.3307871037
C	-1.8012638229	-1.1720066795	-0.2638558943
C	-2.7646752033	-0.7620691689	-1.2302729771
C	-2.1116406208	-2.1810621422	0.6171427131
C	-3.4011582121	-2.7398871843	0.6616874260
C	-4.3901076419	-2.2405839882	-0.1395351565
C	-4.1045561510	-1.2413541065	-1.0963852968
C	-2.4676723571	0.0841988301	-2.3391210566
C	-3.4864790255	0.5892895967	-3.1122126053
C	-4.8226528560	0.2176597146	-2.8824239977
C	-5.1191958052	-0.7135466138	-1.9270571484
N	-1.0964858112	0.3011816301	-2.6501678491
C	-0.5289255077	-0.7872498184	-3.4467242559
C	-0.7596235932	1.6023088720	-3.1950057522
H	-1.3651090730	-2.5352382261	1.3186837122
H	-3.6110484511	-3.5392706294	1.3637353557
H	-5.4051260909	-2.6175793410	-0.0672053797
H	-3.2568289047	1.2447717831	-3.9441741870
H	-5.6065294358	0.6314750990	-3.5071273852
H	-6.1372064931	-1.0639935591	-1.7924606212
H	0.5564726528	-0.6756235728	-3.4960557809
H	-0.7514011092	-1.7479967277	-2.9827483969
H	-0.9293184967	-0.7915066487	-4.4718853347
H	0.3267874154	1.7221051138	-3.1773467475
H	-1.2041053743	2.3880219730	-2.5826097166
H	-1.0883745825	1.7372560764	-4.2366999520
I	1.6371219999	-2.7642018490	-0.4003709442
I	3.0422895349	-5.2479835879	-0.7290281088

(8-$Me_2NC_{10}H_6)_2TeCl^+$ (CI):

Te	-0.0118220481	-1.0608675528	0.3293194958
N	-1.0754692504	0.7846216273	1.6873001966
N	2.7073183179	-1.0412593971	0.9093377757
C	-1.9862584796	-0.8693335549	-0.4583563822
C	0.8917946576	0.4382554174	-0.8542207138
C	-2.3533440734	1.0691930226	1.0612740690
C	-0.2155127641	1.9705351010	1.8306845842
C	-1.2823998976	0.1299869257	2.9962748926
C	2.7769509550	-0.9641277577	2.3689747460
C	3.1450963092	0.1588717995	0.2472106719
C	3.4317298118	-2.2247489524	0.4241823953
C	-2.7934919377	0.1808461690	0.0541667896
C	-2.4759906009	-1.7244694797	-1.4127972184
C	2.2476147733	0.8145775763	-0.6376742892
C	0.1101973900	1.0765439329	-1.7850236170
C	-3.1417531486	2.1139553663	1.4712992402
C	4.4193190273	0.6408071959	0.4225565341
C	-4.1007587873	0.3641628178	-0.4873202764
C	-3.7821997677	-1.5630498445	-1.9128528852
C	2.7383180549	1.9373057035	-1.3789841307
C	0.6234981843	2.1442467978	-2.5404556978
C	-4.4155660016	2.3089513398	0.9106615720
C	4.8788755491	1.7688518013	-0.2741288466
C	-4.8900528954	1.4442547425	-0.0369422855
C	-4.5686462782	-0.5362506516	-1.4704643476
C	1.9024221843	2.5736071505	-2.3237622637
C	4.0572370194	2.3941644267	-1.1693452150
H	-1.8591081428	-2.5238900694	-1.8030977359
H	3.3780413644	-2.2735902703	-0.6617993578
H	0.7740205208	1.6604684261	2.1683505903
H	-0.6194162439	2.6702741445	2.5684464315
H	-0.1213837010	2.4735351474	0.8704581783
H	-0.3179803369	-0.1592232092	3.4174027866
H	-1.8997573766	-0.7604171923	2.8699595732
H	-1.7858655808	0.8071372579	3.6925144931
H	2.2779596957	-1.8362268040	2.7988084511
H	2.2787100149	-0.0603554951	2.7240235524
H	3.8085736930	-0.9488599633	2.7416911079
H	2.9724331068	-3.1251750187	0.8353061488
H	4.4863875835	-2.2016098056	0.7269178506
H	-0.9145002604	0.7653447413	-1.9466592890
H	-2.7999966908	2.7924587028	2.2443478846
H	5.0949149633	0.1279111848	1.0983139361
H	-4.1493025030	-2.2528880643	-2.6636235825
H	-0.0054150307	2.6258104865	-3.2797793625
H	-5.0227093445	3.1405204029	1.2480611240
H	5.8903660916	2.1231742426	-0.1140813445
H	-5.8799930484	1.5796226700	-0.4586207679
H	-5.5668723299	-0.3966127331	-1.8712709806
H	2.3021581974	3.4118255830	-2.8844675938
H	4.4078472887	3.2488076010	-1.7374594146
Cl	0.5512302868	-2.8453369007	-1.1567949560

(8-$Me_2NC_{10}H_6)_2TeBr^+$ (CI):

Te	0.0082388441	-0.0017143592	0.0042778195
N	-0.0067920886	0.0013961622	2.5424555465
N	2.7218213974	-0.0000581392	-0.6760780544
C	-2.0216855133	0.3991203436	0.5433579209
C	0.7047807928	1.9923675435	0.0965241866
C	-1.3332415954	0.4330404267	2.9397498969
C	1.0710195578	0.8146714311	3.1271975857
C	0.1836047512	-1.4287808097	2.8598457404
C	3.3250300206	-1.0411643215	0.1562510689
C	3.1103072667	1.3347825156	-0.3060244673
C	2.9891401787	-0.2644503731	-2.0968172249
C	-2.3113212056	0.5500029095	1.9267039205
C	-3.0211040390	0.4899622185	-0.3914016228
C	2.0962006260	2.2815839562	0.0030863595
C	-0.2197707056	2.9812300566	0.3266941770
C	-1.6518746492	0.6519569035	4.2558998544
C	4.4316152922	1.7106447277	-0.3028584314
C	-3.6515302988	0.8524487805	2.3141120811
C	-4.3477768429	0.7505728104	0.0010587101
C	2.4964323119	3.6363927043	0.2389937962
C	0.1866562418	4.3148931918	0.5002387710
C	-2.9663707312	0.9797884908	4.6275040856
C	4.8189743283	3.0300062029	-0.0245946712
C	-3.9470278707	1.0645290788	3.6779563236
C	-4.6516587182	0.9395138618	1.3199507161
C	1.5167931129	4.6261882500	0.4769485119
C	3.8660831914	3.9774520539	0.2239389828
H	-2.7982163395	0.3753691113	-1.4449227880
H	2.5450726736	0.5177345898	-2.7097796521
H	2.0212711045	0.5418017467	2.6673131654
H	1.1568713227	0.6484648974	4.2052851115
H	0.8771730660	1.8687595253	2.9395827035
H	1.1486460888	-1.7632458600	2.4762196613
H	-0.6088377530	-2.0180519083	2.3965230391
H	0.1540125657	-1.5936719432	3.9410006549
H	2.8642738401	-2.0033158416	-0.0806176052
H	3.1632624940	-0.8219804606	1.2128460568
H	4.4056771858	-1.1395492946	-0.0060228057
H	2.5447526702	-1.2205235541	-2.3780500824
H	4.0667783180	-0.3057315475	-2.3015008260
H	-1.2758869554	2.7459773936	0.3809770418
H	-0.8956991733	0.5576659155	5.0266275639
H	5.1946458820	0.9783967190	-0.5429081159
H	-5.1201364538	0.8137484486	-0.7564048050
H	-0.5597672784	5.0825792553	0.6663201239
H	-3.1973548995	1.1489542018	5.6724689991
H	5.8698947931	3.2942053132	-0.0325408416
H	-4.9674821158	1.2990933080	3.9603900864
H	-5.6691818475	1.1610273326	1.6235871595
H	1.8436119722	5.6484121170	0.6352052213
H	4.1467416649	5.0084482304	0.4095243627
Br	-0.4492238389	0.0320537498	-2.5120499542

$(8\text{-}Me_2NC_{10}H_6)_2TeI^+$ (CI):

Te	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	2.1451527500
C	1.2610889638	0.0000000000	2.8036701391
C	-1.1619275408	-0.0100279761	2.8734009898
C	-1.1320808835	0.0014425279	4.2804691597
C	0.0623179004	0.0521845463	4.9412458985
C	1.2831478993	0.0601015962	4.2303440741
C	2.4975735835	-0.0394982135	2.1193749308
C	3.6840905549	0.0411559001	2.8041464142
C	3.6973131270	0.1403865530	4.2049972550
C	2.5217259715	0.1328805475	4.9031882558
N	2.4650892211	-0.2441401168	0.6863045750
C	3.3692804279	0.6479405368	-0.0532479723
C	2.7373772819	-1.6581417425	0.3617519134
H	-2.1231990579	-0.0103324738	2.3738290615
H	-2.0664304352	-0.0116461439	4.8292053418
H	0.0910801874	0.0876934581	6.0249952138
H	4.6274155703	0.0101918643	2.2715232244
H	4.6455186029	0.2035436795	4.7254665280
H	2.5242859569	0.1855895674	5.9864002840
H	3.1992656448	1.6782040559	0.2531989427
H	4.4186551046	0.3881946392	0.1188828744
H	3.1727373168	0.5596242402	-1.1218660414
H	2.0406694958	-2.3013716150	0.9009281115
H	3.7573660237	-1.9329293287	0.6479537192
H	2.6145870107	-1.8179134947	-0.7106973464
C	0.3984817705	2.0618334100	-0.2586726293
C	0.7773302127	2.5797876117	-1.5304843477
C	0.3657707501	2.8566722773	0.8603117737
C	0.7323185315	4.2107515750	0.7885852345
C	1.1633704981	4.7325117727	-0.3980447392
C	1.2067531030	3.9461772902	-1.5711260151
C	0.7650135186	1.8521849998	-2.7519728490
C	1.2280236983	2.4337659814	-3.9074514273
C	1.6949478446	3.7567348341	-3.9284447995
C	1.6650031104	4.5030405647	-2.7843421530
N	0.1996738352	0.5289193016	-2.7650900240
C	-1.0777316507	0.5024439303	-3.4907580906
C	1.0987055139	-0.4974011016	-3.2928412031
H	0.0592780248	2.4473628341	1.8153097881
H	0.6858302253	4.8243737687	1.6803845758
H	1.4762804053	5.7693341819	-0.4603418734
H	1.2095387396	1.8681014068	-4.8324844589
H	2.0514488308	4.1857848303	-4.8574775508
H	1.9901484763	5.5376186719	-2.7906470431
H	-1.7417759861	1.2725325615	-3.1020967972
H	-1.5536395404	-0.4696126663	-3.3517218435
H	-0.9322419063	0.6709766193	-4.5658234189
H	2.0635786989	-0.4533234444	-2.7862446988
H	0.6572529211	-1.4827539738	-3.1249233777
H	1.2773451657	-0.3909879415	-4.3702467438
I	-2.7619520543	0.2035477348	-0.2712789419

$(8\text{-}Me_2NC_{10}H_6)_2TeCl_2$ (TB):

Te	0.0019986105	0.0000000007	0.0001209573
N	-1.1649622559	2.4619045138	-0.7681283863
N	-1.2490955783	-2.4619045108	0.6220277477
C	1.4411966827	-1.6011506628	0.0355264698
C	1.4349621735	1.6011506624	0.1385408779
C	-0.0127300144	3.2163707445	-1.1282999724
C	-0.1487098681	-3.2163707430	1.1185295062
C	1.1559132758	-2.8228945968	0.7037097149
C	1.2323437658	2.8228945966	-0.5591705607
C	2.2394538248	-3.7165186516	0.9622573007
C	2.3391565674	3.7165186501	-0.6851562757
C	-2.2046200982	2.3603386969	-1.7784444591
H	-2.9187251108	1.5917809996	-1.4718973307
H	-2.7651734985	3.2980065735	-1.9100117694
H	-1.7640016221	2.0606508913	-2.7282269238
C	-1.7113752875	2.8776502609	0.5254451450
H	-2.1754767550	3.8729404928	0.4666304777
H	-2.4676279720	2.1578880866	0.8477615829
H	-0.9238768273	2.9038448765	1.2787331225
C	-2.4030091001	-2.3603386926	1.4995871931
H	-2.9753381308	-3.2980065684	1.5625915866
H	-2.0801501925	-2.0606508874	2.4955758967
H	-3.0749324810	-1.5917809943	1.1091565594
C	-1.6355157314	-2.8776502573	-0.7280015660
H	-2.1033228572	-3.8729404886	-0.7255867241
H	-2.3473773815	-2.1578880821	-1.1391694135
H	-0.7629186722	-2.9038448740	-1.3808192848
C	-0.0814287366	4.3281918707	-1.9319420782
H	-1.0264607364	4.6113700224	-2.3797197926
C	1.0474107712	5.1382124586	-2.1469053594
H	0.9644707193	6.0085772920	-2.7883839510
C	2.2206176587	4.8628030363	-1.5035809999
H	3.0794496877	5.5169491003	-1.6118666285
C	3.5342045655	3.4410702974	0.0150086372
H	4.3603783061	4.1394276185	-0.0720772521
C	3.6433047999	2.3276835856	0.8002504650
H	4.5485482614	2.1375244108	1.3660913884
C	2.5962145854	1.3897300412	0.8378277097
H	2.7259217202	0.4825690961	1.4145232802
C	2.6783072131	-1.3897300432	-0.5186095907
H	2.8766170203	-0.4825690984	-1.0754533234
C	3.7132231227	-2.3276835889	-0.3550277327
H	4.6800997078	-2.1375244154	-0.8075665098
C	3.5102191710	-3.4410703005	0.4113253095
H	4.3198602974	-4.1394276227	0.5974119738
C	2.0230782388	-4.8628030377	1.7604127419
H	2.8625826030	-5.5169491027	1.9714829964
C	0.7808495495	-5.1382124584	2.2575530811
H	0.6211526618	-6.0085772916	2.8843470983
C	-0.3138262599	-4.3281918690	1.9080209413
H	-1.3059625744	-4.6113700195	2.2385597382
Cl	0.0069892265	0.0047119483	2.5238580782
Cl	0.3113150205	-0.0047119471	-2.5045940604

$(8\text{-}Me_2NC_{10}H_6)_2TeBr_2$ (TB):

Te	-0.0332204685	0.0000000000	-0.0157203584
N	0.0029094895	0.0235224916	2.8140680913
N	2.1778729648	-0.0235224919	-1.7820934427
C	-0.6678236866	-0.4631172109	-2.0231591702
C	-1.9878971470	0.4631172112	0.7664374966
C	-1.3720220951	-0.1985679235	3.1123509025
C	1.5367093330	0.1985679234	-3.0344187578
C	0.1585821334	-0.1467812737	-3.1366762822
C	-2.3249369276	0.1467812739	2.1115289895
C	-0.4248268417	-0.1924764250	-4.4395711029
C	-3.7023512288	0.1924764254	2.4865367078
C	0.9470593965	-0.8907621424	3.4360339557
H	1.9240181390	-0.7627464116	2.9629786316
H	1.0746178052	-0.7034709626	4.5127619383
H	0.6216423563	-1.9182224562	3.2798527485
C	0.3900719321	1.4192522671	3.0390870972
H	0.4028178431	1.6640220004	4.1111388907
H	1.3883782738	1.5899198804	2.6293407224
H	-0.3033750767	2.0919112874	2.5347506866
C	3.2574853375	0.8907621418	-1.4463886489
H	4.1709665566	0.7034709618	-2.0304831264
H	2.9303751295	1.9182224557	-1.5989918308
H	3.5111565477	0.7627464108	-0.3909832096
C	2.5973647248	-1.4192522675	-1.6253931781
H	3.4344297315	-1.6640220010	-2.2953033817
H	2.9135267820	-1.5899198810	-0.5936232438
H	1.7676770171	-2.0919112876	-1.8418239450
C	-1.7941626555	-0.6536467818	4.3376631352
H	-1.0648376497	-0.9334162633	5.0883177362
C	-3.1618986356	-0.7179823099	4.6557936950
H	-3.4660850802	-1.0851523500	5.6296883844
C	-4.0934011942	-0.2644654125	3.7656664465
H	-5.1469788340	-0.2497301507	4.0243327836
C	-4.6529661008	0.6985994993	1.5733141772
H	-5.6929946132	0.7474138226	1.8794521917
C	-4.2698187367	1.1354941621	0.3362790709
H	-4.9951203887	1.5595233332	-0.3491820598
C	-2.9336699858	0.9898607787	-0.0765186008
H	-2.6619305636	1.2873240904	-1.0813721213
C	-1.9193497487	-0.9898607781	-2.2199935194
H	-2.5240661425	-1.2873240898	-1.3727090369
C	-2.4473713265	-1.1354941613	-3.5149408604
H	-3.4373153204	-1.5595233322	-3.6411563000
C	-1.7337579055	-0.6985994986	-4.5955951262
H	-2.1564921456	-0.7474138216	-5.5939315188
C	0.3163261226	0.2644654130	-5.5530275445
H	-0.1517076606	0.2497301513	-6.5317402168
C	1.5952796208	0.7179823100	-5.3971382091
H	2.1554825528	1.0851523501	-6.2498825635
C	2.2165330423	0.6536467817	-4.1377919698
H	3.2594401713	0.9334162630	-4.0498032518
Br	-0.4604272034	-2.6123691413	0.5458103473
Br	0.1301100317	2.6123691413	-0.7021207338

$(8\text{-}Me_2NC_{10}H_6)_2TeI_2$ (TB):

Te	-0.0308028702	-0.0000000009	-0.0150599471
N	0.0003750805	0.0324274342	2.8236859876
N	2.2286373060	-0.0324274412	-1.7338911303
C	-0.6240720426	-0.4261063740	-2.0469834351
C	-1.9987243059	0.4261063781	0.7646621767
C	-1.3723365656	-0.2169857208	3.1162783114
C	1.6164856295	0.2169857184	-2.9969104705
C	0.2365459867	-0.1088613634	-3.1352548785
C	-2.3290156115	0.1088613663	2.1122176596
C	-0.3151608832	-0.1329766738	-4.4528600250
C	-3.7076828706	0.1329766811	2.4860363069
C	0.9600512595	-0.8612192847	3.4537151070
C	0.3543587036	1.4346798191	3.0698336875
C	3.3152380741	0.8612192731	-1.3634672663
C	2.6402946508	-1.4346798278	-1.6057064155
C	-1.7892605377	-0.6754697475	4.3422344609
C	-3.1558903561	-0.7629035930	4.6585023383
C	-4.0930977610	-0.3273308067	3.7656220175
C	-4.6670307319	0.6214164632	1.5724513906
C	-4.2916505803	1.0628765199	0.3348036296
C	-2.9537149295	0.9374182993	-0.0777526951
C	-1.8754065150	-0.9374182901	-2.2832712911
C	-2.3715266304	-1.0628765065	-3.5925227409
C	-1.6253376233	-0.6214164507	-4.6488769451
C	0.4579619629	0.3273308132	-5.5428899760
C	1.7382012524	0.7629035944	-5.3516300665
C	2.3279333702	0.6754697444	-4.0788698929
H	1.9381992718	-0.7067867337	2.9913651945
H	1.0714741160	-0.6730316888	4.5319808137
H	0.6627536713	-1.8963441389	3.2913838789
H	0.3451950321	1.6650205108	4.1452693123
H	1.3550202413	1.6311673514	2.6786730017
H	-0.3450866353	2.0986611390	2.5628399465
H	4.2346189424	0.6730316748	-1.9377588343
H	3.0045414586	1.8963441287	-1.4983927784
H	3.5510957247	0.7067867194	-0.3075732643
H	3.4833829777	-1.6650205214	-2.2734247905
H	2.9461605227	-1.6311673630	-0.5757664840
H	1.8106140480	-2.0986611442	-1.8463234085
H	-1.0567590816	-0.9411558055	5.0948450173
H	-3.4552963939	-1.1329862872	5.6327385830
H	-5.1472652489	-0.3294000148	4.0221742407
H	-5.7073990179	0.6540318953	1.8794252801
H	-5.0231995673	1.4757125146	-0.3507952442
H	-2.6874499430	1.2400907077	-1.0825953318
H	-2.5048833794	-1.2400906976	-1.4560079442
H	-3.3618761789	-1.4757124973	-3.7487837771
H	-2.0220285294	-0.6540318795	-5.6584488666
H	0.0130042205	0.3294000247	-6.5323851723
H	2.3231702355	1.1329862879	-6.1862506541
H	3.3717524112	0.9411557984	-3.9630128926
I	-0.4389415583	-2.8765424947	0.5413293695
I	0.1576291961	2.8765424935	-0.6788668571