Building new discrete supramolecular assemblies through the interaction of iso-tellurazole N-Oxides with Lewis acids and bases

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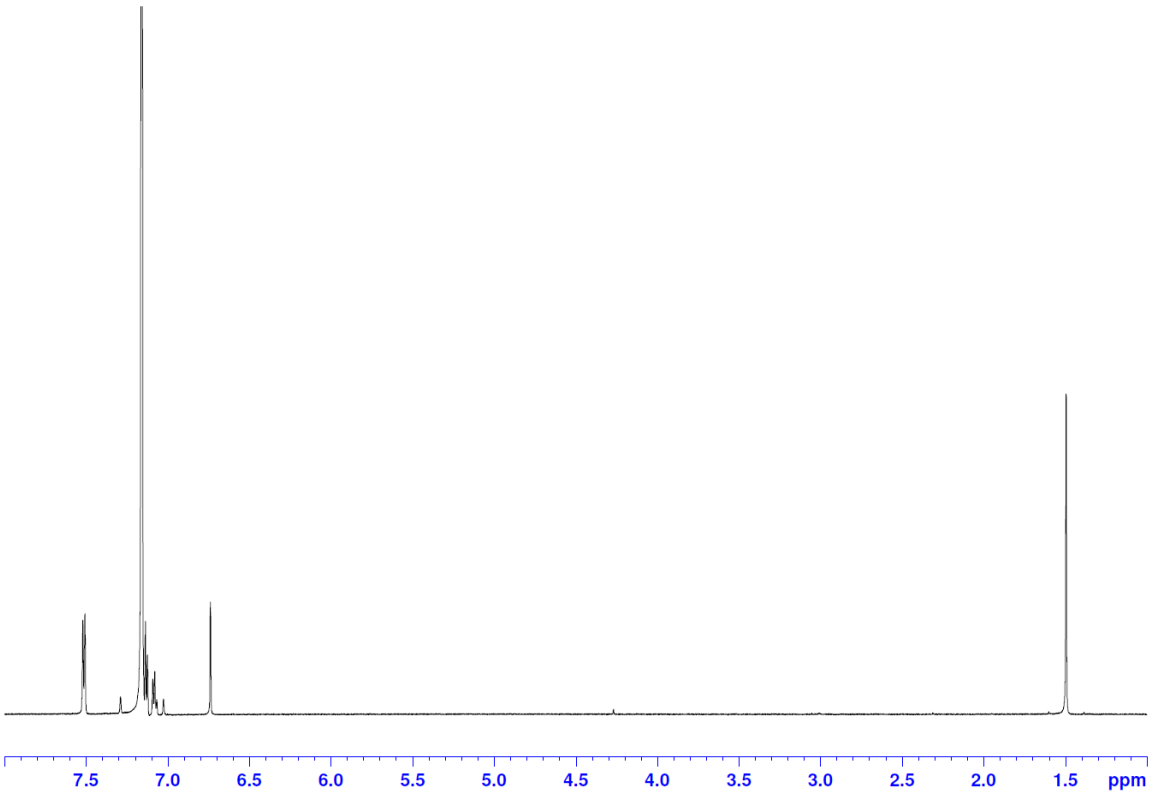
Electronic Supplementary Information

a)



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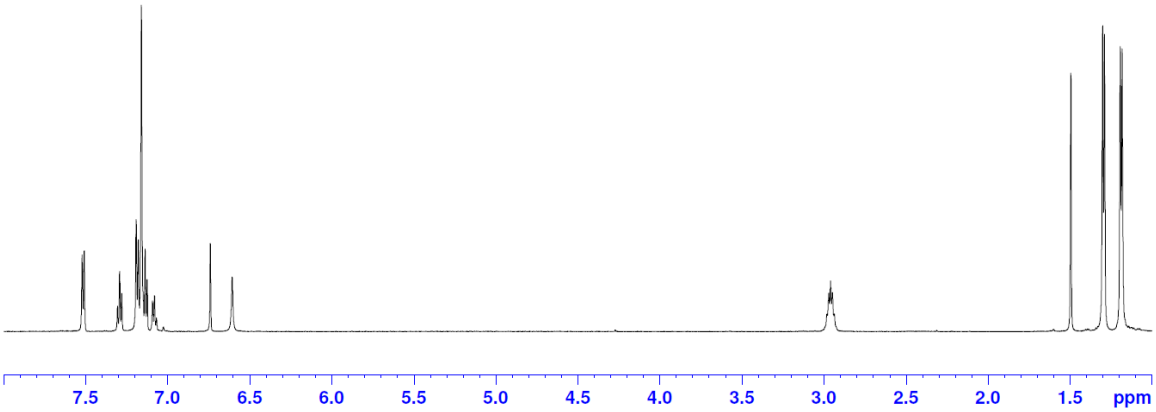
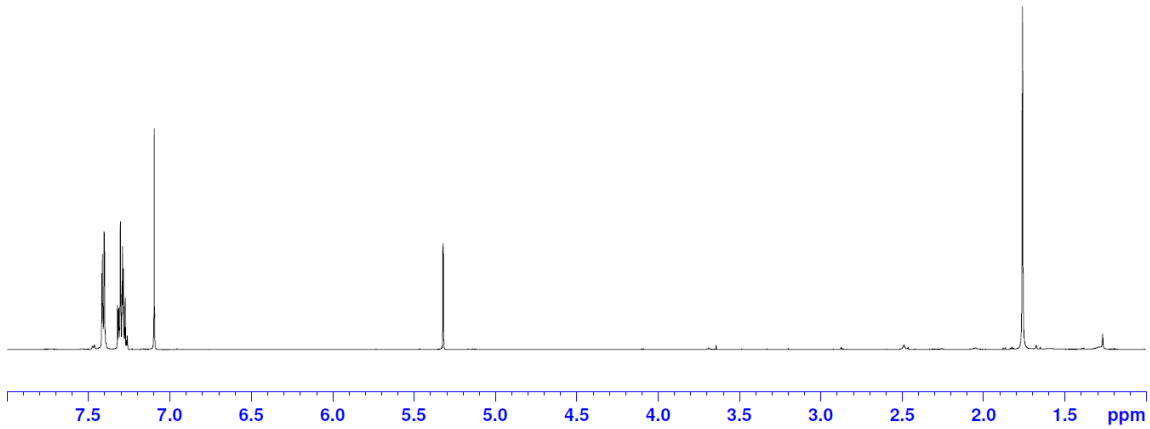


Figure S1. ^{1}H NMR spectra in C_6D_6 solution of a) compound **1**; b) **1** + **3** (1:1).

a)



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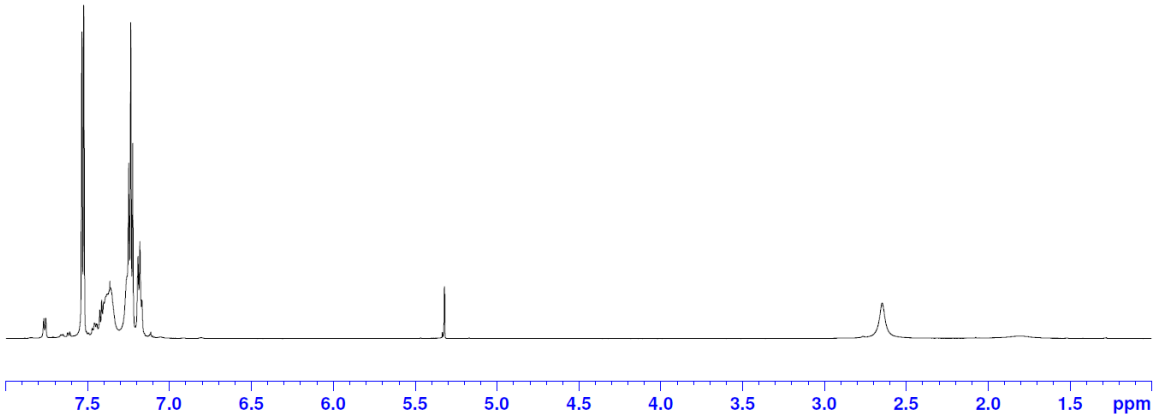


c)

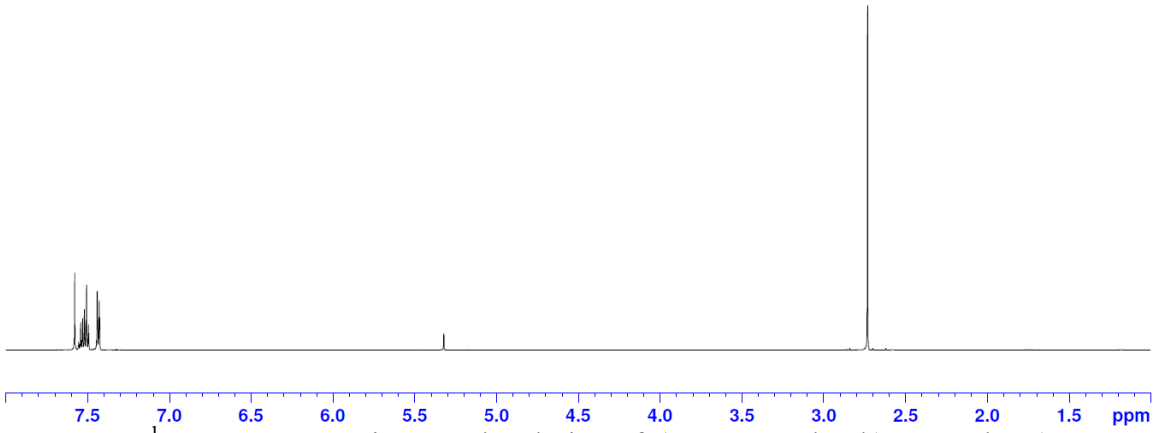
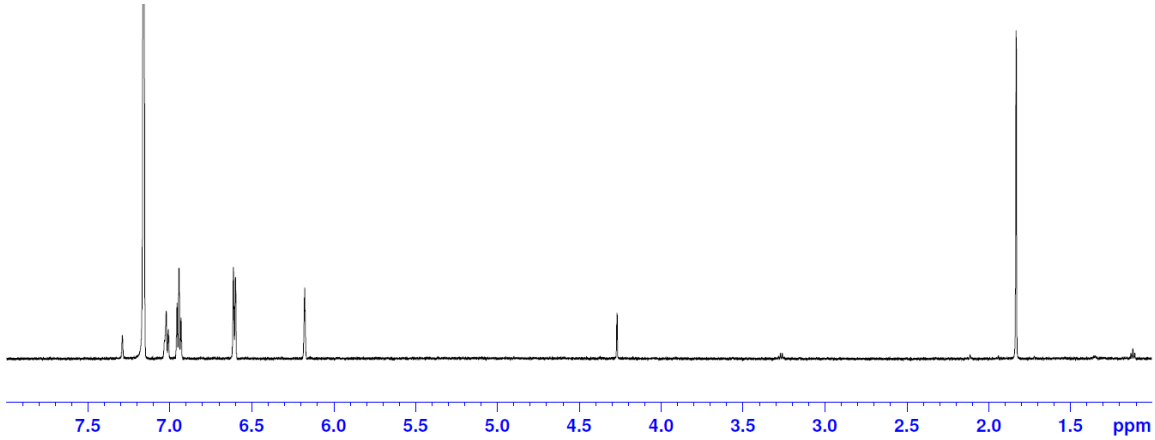


Figure S2. ^{1}H NMR spectra in CD_2Cl_2 solution of a) compound **1**; b) **1** + BPh_3; c) **1** + BF_3.

a)



b)

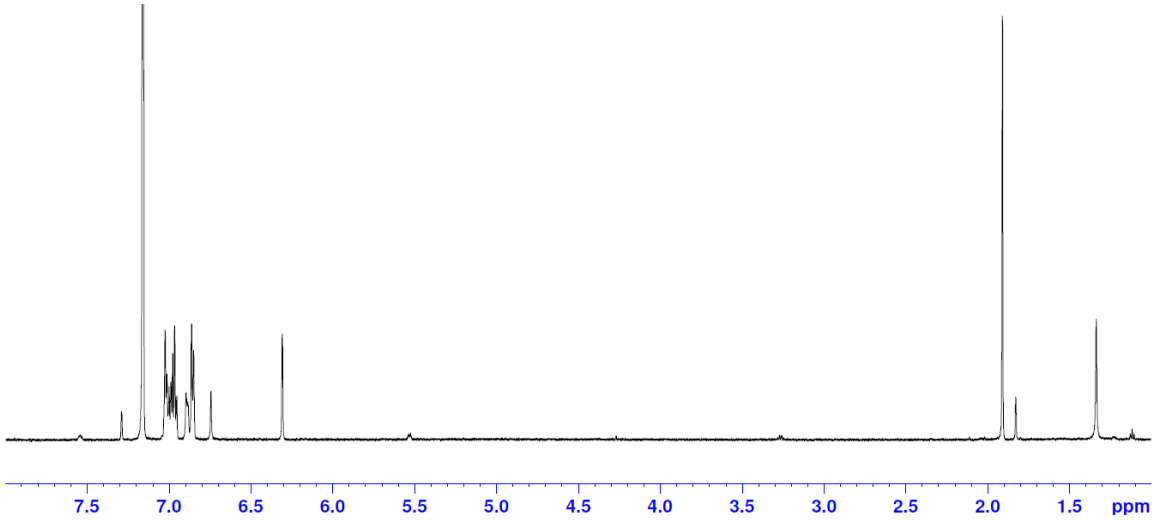


Figure S3. ^{1}H NMR spectra in C_6D_6 of a) **1**-BF_3; b) **1**-BF_3 + DMAP.

Single-Crystal X-ray Diffraction Experimental Details

All crystals were mounted on nylon loops (Hampton, California) or MiTeGen micromounts (Ithaca, New York) with Paratone-N oil. Data were collected at 100 K or 173.15 K using Mo-Kα radiation (λ = 0.71073 Å) with a Bruker APEX2 diffractometer. The CCD area detector was equipped with a low-temperature accessory (Oxford cryostream). A minimum of 50 frames from three different orientations were used for the determination of the precursory unit cell parameters and final cell advancement after integration in SAINT.[1] The absorption was corrected for each data set in SADABS.[2] Direct methods were used to solve all structures and then refined by the full-matrix least-squares techniques on F2 using SHELXL.[3] All non-hydrogen atoms were assigned anisotropic thermal parameters. Appropriate riding models were used to place hydrogen atoms in idealized positions.

References

1. Bruker, SAINT Bruker AXS Inc Madison Wisconsin USA 2012.

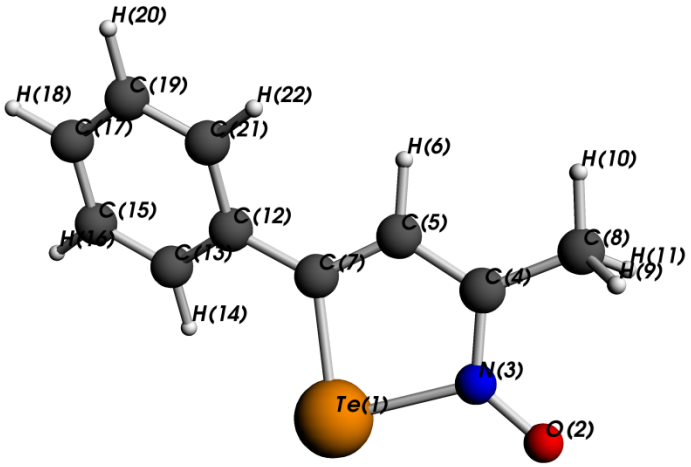
2. Bruker, SADABS, Bruker AXS Inc, Madison, Wisconsin, USA, 2001.

3. G. M. Sheldrick, *Acta Cryst C*, 2015, **71**, 3–8.

Table S1. Crystallographic and refinement parameters for all compounds

Crystal Composition	**1**-BPh_3	**1**-BF_3	CH_3CN-**2**-BF_3	BF_3-**1**-4,4'-bipy-**1**-BF_3	DMAP-**1**-BF_3•$CHCl_3$	**1**-**1**-BF_3	$[\mathbf{3}\text{-H}]^+_2[BF_3\text{-}\mathbf{1}\text{-O-}\mathbf{1}\text{-}BF_3]^{2-}$	Ph_3P-**2**-BF_3	**3**-**2**-BF_3
CCDC	1532984	1532991	1532996	1532977	1532985	1532987	1532988	1532990	1532989
Empirical formula	$C_{28}H_{24}BNOTe$	$C_{10}H_9BF_3NOTe$	$C_9H_8BF_3N_2OTe$	$C_{15}H_{13}BF_3N_2OTe$	$C_{18}H_{20}BCl_3F_3N_3OTe$	$C_{10}H_9B_{0.5}F_{1.5}NOTe$	$C_{44}H_{54}BF_3N_3O_{1.5}Te$	$C_{25}H_{20}BF_3NOPTe$	$C_{34}H_{41}BF_3N_3OTe$
Crystal system,	monoclinic	monoclinic	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	P21/n	P-1	C2/c	$P2_1$	$P2_1$	Pn	$P2_1/c$	$P2_1/n$
a [Å]	10.109(2)	8.027(2)	6.736(1)	24.509(2)	10.2886(2)	7.2898(8)	12.2007(6)	10.1170(7)	10.771(2)
b [Å]	9.698(2)	7.105(2)	8.218(1)	6.9948(4)	15.0565(3)	13.303(1)	20.912(1)	13.3307(9)	16.584(2)
c [Å]	23.678(5)	19.994(5)	11.478(2)	21.112(1)	14.7817(3)	11.561(1)	17.3413(8)	20.405(1)	19.770(3)
α [°]	90	90	109.16(3)	90	90	90	90	90	90
β [°]	101.817(4)	95.552(4)	92.23(3)	119.654(2)	91.1560(10)	104.610(2)	107.7730(10)	99.848(2)	102.005(3)
γ [°]	90	90	106.25(3)	90	90	90	90	90	90
V [$Å^3$]	2272.3(8)	1135.0(5)	570.3(2)	3145.4(3)	2289.37(8)	1084.9(2)	4213.2(3)	2711.4(3)	3454.2(8)
Z, ρ (calc.) [g. cm^{-3}]	4, 1.546	4, 2.075	2, 2.071	8, 1.827	4, 1.730	4, 1.963	4, 1.331	4, 1.413	4, 1.352
T [K]	100.15	99.15	100.15	100.15	100.15	100.15	100.15	100.15	99.95
μ [mm^{-1}]	1.330	2.641	2.631	1.926	1.689	2.733	0.757	1.192	0.907
2θ range [°]	3.514 to 59.136	6.088 to 60.87	3.796 to 75.164	6.13 to 54.2	3.96 to 61.996	6 to 52.778	5.24 to 52.774	3.666 to 52.756	2.106 to 55.07
Limiting indices	$-14 \le h \le 13$, $-13 \le k \le 13$, $-32 \le l \le 32$	$-10 \le h \le 11$, $-10 \le k \le 10$, $-27 \le l \le 26$	$-11 \le h \le 11$, $-14 \le k \le 13$, $0 \le l \le 19$	$-31 \le h \le 31$, $-8 \le k \le 8$, $-27 \le l \le 27$	$-14 \le h \le 14$, $-21 \le k \le 21$, $-21 \le l \le 21$	$-8 \le h \le 9$, $-16 \le k \le 16$, $-14 \le l \le 13$	$-15 \le h \le 15$, $-26 \le k \le 26$, $-21 \le l \le 21$	$-12 \le h \le 12$, $-16 \le k \le 16$, $-25 \le l \le 25$	$-13 \le h \le 13$, $-21 \le k \le 21$, $-25 \le l \le 25$
Refl. collected/ unique	37517/ 6340	14832/ 3303	5920/ 5920	38448/ 3467	85052/ 14583	7428/ 4406	57637/ 17086	28523	38007/ 7956
R(int.)	0.0587	0.0536	Merged in TWINABS	0.0398	0.0290	0.0331	0.0335	0.0574	0.0529
No. of parameters	290	155	176	209	547	271	984	298	397
R1* / wR2* (I>2σ(I))	0.0299/ 0.0609	0.0380/ 0.0841	0.0243/ 0.0555	0.0205/ 0.0511	0.0245/ 0.0597	0.0335/ 0.0561	0.0283/ 0.0652	0.0339/ 0.0796	0.1063/ 0.2678
R1* / wR2* for all data	0.0435/ 0.0655	0.0633/ 0.0908	0.0277/ 0.0567	0.0266/ 0.0523	0.0258/ 0.0605	0.0439/ 0.0583	0.0317/ 0.0670	0.0501/ 0.0838	0.1176/ 0.2753
Goodness-of-fit on F^2	1.035	1.036	1.054	1.070	1.028	0.967	1.016	0.964	1.116
Largest difference peak/hole [$e.Å^{-3}$]	0.91/-0.59	1.07/-1.42	1.60/-1.22	0.69/-0.35	1.58/-0.93	0.67/-0.47	0.77/-0.32	0.80/-0.48	4.51/-3.06
Flack parameter	-	-	-	-	-0.002(3)	0.01(2)	-0.011(4)	-	-

Table S2. Optimized Cartesian Coordinates of **1**



Atom	X	Y	Z (Angstrom)
1.Te	4.418143	3.621927	5.094559
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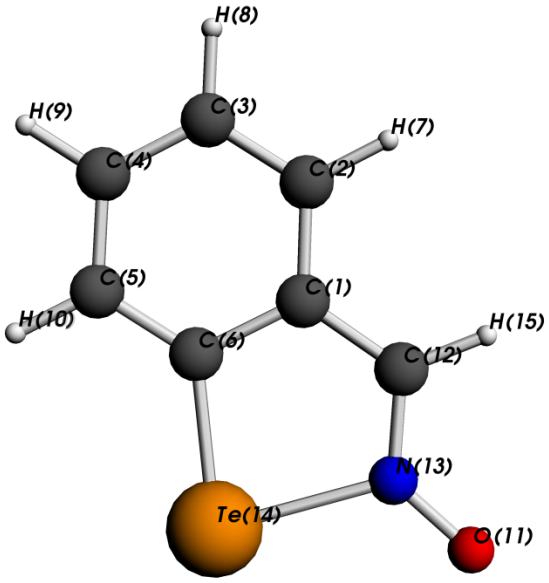
3.N	3.970347	3.309462	2.988728
4.C	2.691805	2.921702	2.845148
5.C	1.907086	2.786873	4.018240
6.H	0.877163	2.445331	3.908622
7.C	2.419714	3.030796	5.267149
8.C	2.218993	2.651863	1.451771
9.H	2.339636	3.546353	0.823461
10.H	1.166605	2.347864	1.455760
11.H	2.823706	1.860297	0.984756
12.C	1.720473	2.927049	6.542374
13.C	2.411689	2.666714	7.741052
14.H	3.494453	2.522825	7.710672
15.C	1.736819	2.551295	8.953486
16.H	2.297676	2.342636	9.864598
17.C	0.347731	2.691642	9.001091
18.H	-0.182527	2.601780	9.949163
19.C	-0.354739	2.956380	7.821743
20.H	-1.437360	3.083883	7.848589
21.C	0.319937	3.079317	6.610260
22.H	-0.237559	3.321610	5.705282

Table S3. Optimized Cartesian Coordinates of **2**



Atom	X	Y	Z (Angstrom)
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3.C	-4.915857	-6.353082	0.000000
4.C	-3.699988	-7.052334	0.000000
5.C	-2.488146	-6.359998	0.000000
6.C	-2.497811	-4.964659	0.000000
7.H	-5.872448	-4.419102	0.000000
8.H	-5.857283	-6.901597	0.000000
9.H	-3.696025	-8.142001	0.000000
10.H	-1.546916	-6.909037	0.000000
11.O	-2.305413	-0.949017	0.000000
12.C	-3.668484	-2.812676	0.000000
13.N	-2.502871	-2.179840	0.000000
14.Te	-0.865454	-3.657946	0.000000
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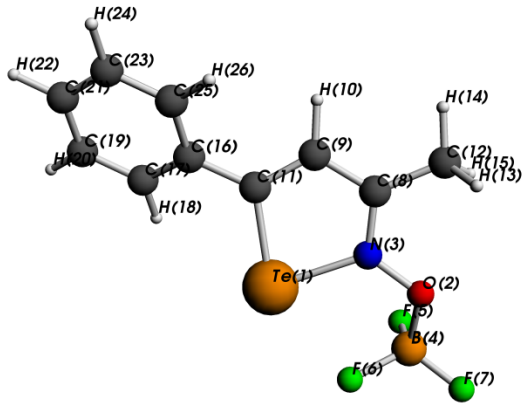
Table S4. Optimized Cartesian Coordinates of **1**-BF_3



Atom	X	Y	Z (Angstrom)
1.Te	4.428669	3.535234	5.056705
2.O	4.763956	3.348955	2.027406
3.N	3.931056	3.184583	3.056659
4.B	6.252341	3.042850	2.347763
5.F	6.397787	1.690801	2.587097
6.F	6.527360	3.779971	3.555837
7.F	6.953149	3.524559	1.279928
8.C	2.655466	2.876117	2.845192
9.C	1.843713	2.799992	4.006767
10.H	0.803446	2.491013	3.904887
11.C	2.405543	3.036561	5.237242
12.C	2.191473	2.623129	1.448357
13.H	2.301526	3.531198	0.838410
14.H	1.142226	2.310174	1.447233
15.H	2.811865	1.848798	0.976749
16.C	1.724184	2.955999	6.527742
17.C	2.397746	2.513395	7.681644
18.H	3.439329	2.193516	7.605309
19.C	1.738814	2.427533	8.905403
20.H	2.276185	2.070758	9.783824
21.C	0.392003	2.785003	9.003554
22.H	-0.124317	2.718159	9.961235
23.C	-0.288560	3.231877	7.867741
24.H	-1.336614	3.523531	7.938731
25.C	0.368575	3.319455	6.643010
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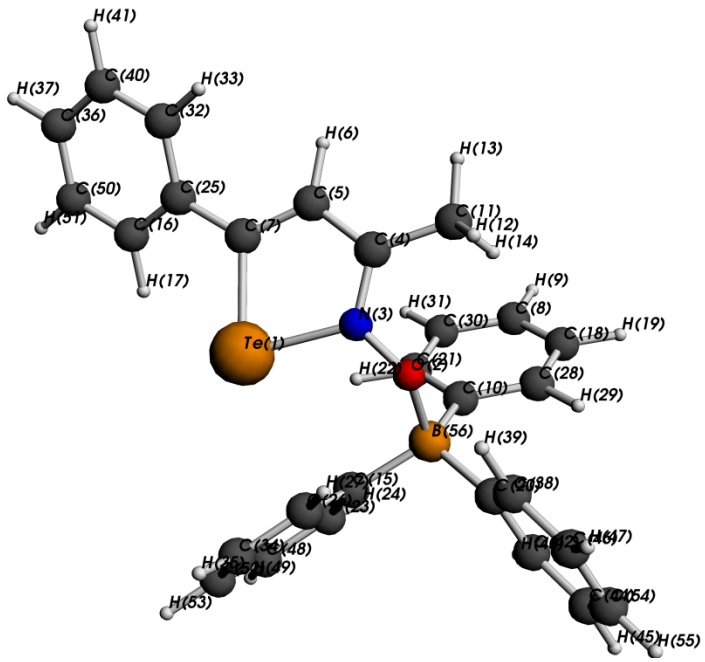
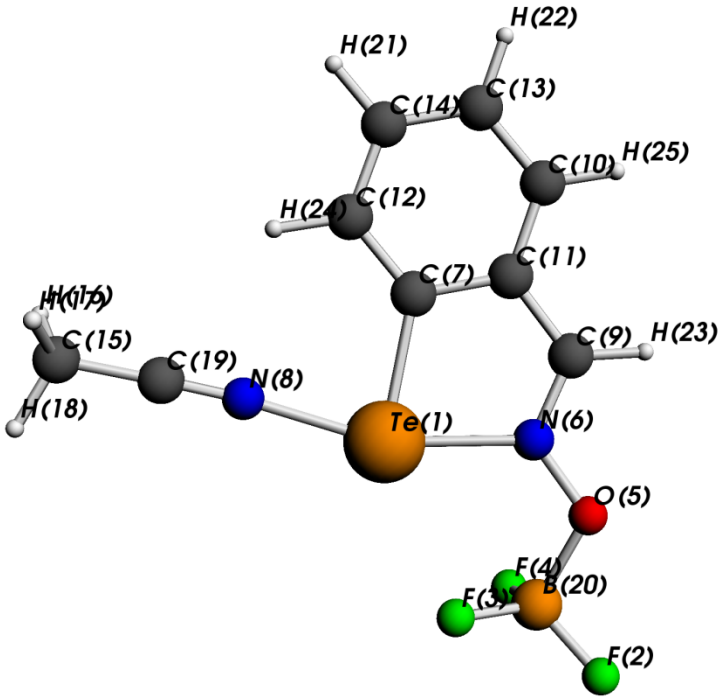
Table S5. Optimized Cartesian Coordinates of **1**-BPh_3



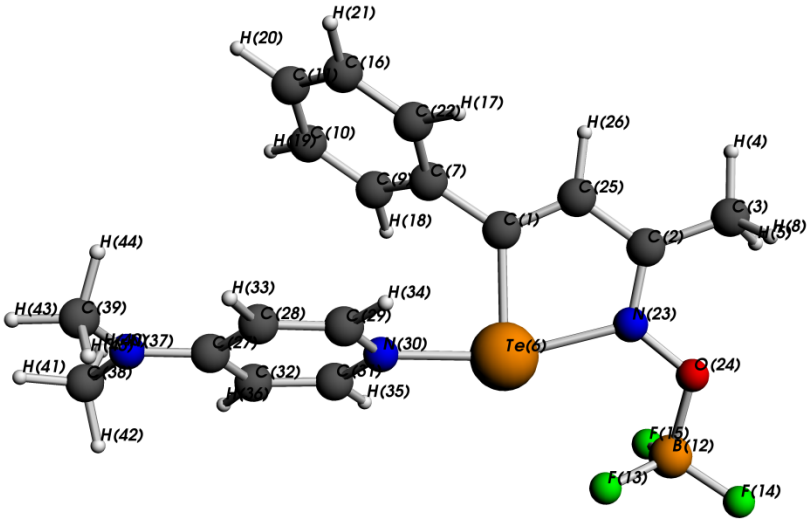
Atom	X	Y	Z(Angstrom)	Atom	X	Y	Z(Angstrom)
1.Te	5.155668	4.740853	4.698724	29.H	7.034418	5.907113	10.305971
2.O	6.013085	6.553385	7.028161	30.C	7.497631	2.493878	8.540088
3.N	6.429730	5.823499	6.000130	31.H	7.623124	1.534265	8.035647
4.C	7.718787	5.761518	5.686198	32.C	8.225655	3.789073	1.732668
5.C	8.036244	4.997096	4.532852	33.H	8.887059	4.640209	1.895399
6.H	9.083481	4.876100	4.256335	34.C	1.975400	5.661259	5.993454
7.C	7.031466	4.370206	3.840599	35.H	1.445504	6.355313	5.339663
8.C	8.327912	2.836439	9.609016	36.C	7.518311	1.921686	0.364635
9.H	9.102448	2.147340	9.949523	37.H	7.644640	1.299529	-0.521300
10.C	6.298232	4.632192	8.727561	38.C	4.905674	8.243941	8.981910
11.C	8.715498	6.451448	6.558036	39.H	5.305449	8.588049	8.026419
12.H	8.481892	7.521574	6.640211	40.C	8.387046	2.990038	0.603626
13.H	9.725889	6.323251	6.156353	41.H	9.189277	3.209588	-0.101013
14.H	8.665133	6.033625	7.574659	42.C	4.311915	6.478036	10.491432
15.C	3.899321	5.181401	7.457218	43.H	4.242877	5.414269	10.731408
16.C	6.324333	2.454535	2.398184	44.C	3.882123	7.414334	11.432650
17.H	5.535477	2.220396	3.116259	45.H	3.479751	7.078098	12.389948
18.C	8.151632	4.071453	10.239604	46.C	4.480816	9.192492	9.919069
19.H	8.791298	4.352371	11.078207	47.H	4.551970	10.256639	9.686204
20.C	4.834893	6.865151	9.242890	48.C	2.131325	3.522207	7.103776
21.C	6.503057	3.380295	8.114262	49.H	1.715808	2.535558	7.315165
22.H	5.871940	3.081605	7.275031	50.C	6.484483	1.658915	1.266720
23.C	3.326020	3.916156	7.704768	51.H	5.804680	0.825022	1.093163
24.H	3.832319	3.230162	8.384931	52.C	1.457627	4.387682	6.231195
25.C	7.192705	3.532107	2.654891	53.H	0.523994	4.075735	5.761196
26.C	3.176322	6.047808	6.600190	54.C	3.965113	8.781612	11.149758
27.H	3.557241	7.058354	6.439763	55.H	3.629363	9.517776	11.881880
28.C	7.155336	4.946853	9.801249	56.B	5.248353	5.734058	8.172654

Table S6. Optimized Cartesian Coordinates of CH_3CN-**2**-BF_3



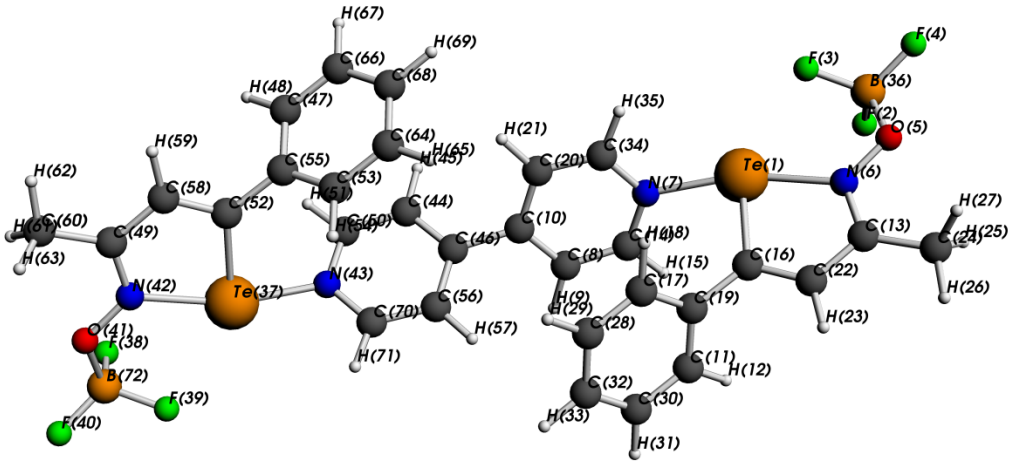
Atom	X	Y	Z (Angstrom)
1.Te	1.451741	-1.214053	8.378876
2.F	1.784915	3.355422	8.830236
3.F	1.494461	1.170336	9.573546
4.F	3.498343	1.806756	8.629499
5.O	1.549872	1.677612	7.247455
6.N	1.558208	0.379706	6.949071
7.C	1.439492	-2.268679	6.542329
8.N	1.319540	-3.717146	9.509866
9.C	1.544826	0.004409	5.695382
10.C	1.476468	-1.917754	4.115909
11.C	1.482734	-1.393865	5.424780
12.C	1.399441	-3.650762	6.327224
13.C	1.429586	-3.289233	3.919635
14.C	1.392156	-4.152056	5.026863
15.C	1.228904	-5.987910	10.794439
16.H	2.052463	-6.637667	10.471642
17.H	0.274862	-6.499276	10.612977
18.H	1.329354	-5.793844	11.870258
19.C	1.271944	-4.732682	10.067503
20.B	2.135766	2.045506	8.642408
21.H	1.356047	-5.230700	4.870623
22.H	1.422992	-3.696797	2.909438
23.H	1.585254	0.779100	4.931095
24.H	1.368647	-4.336506	7.169821
25.H	1.509233	-1.233735	3.267140

Table S7. Optimized Cartesian Coordinates of DMAP-**1**-BF_3



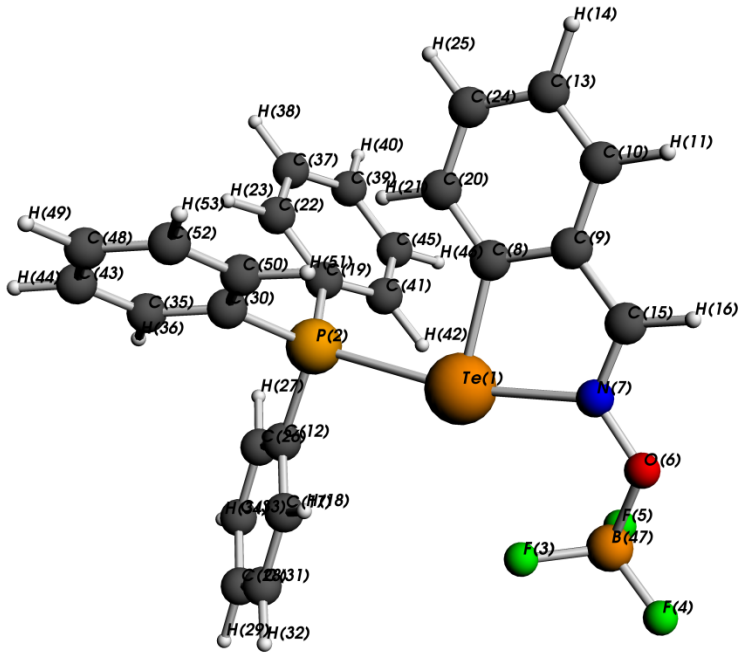
Atom	X	Y	Z (Angstrom)
1.C	4.347629	7.709745	-1.029249
2.C	5.737334	9.632026	-1.559823
3.C	6.318486	10.980208	-1.280990
4.H	5.885218	11.407822	-0.370166
5.H	6.138051	11.652391	-2.131256
6.Te	5.163839	6.989114	-2.837851
7.C	3.361847	6.991530	-0.208777
8.H	7.410162	10.911330	-1.166493
9.C	2.104805	6.629114	-0.722253
10.C	1.171157	5.971637	0.075599
11.C	1.474705	5.658924	1.404076
12.B	6.862623	9.034768	-4.968299
13.F	6.914806	7.613221	-4.910905
14.F	7.977386	9.574315	-5.568790
15.F	5.662539	9.439571	-5.543383
16.C	2.717390	6.018944	1.929229
17.H	4.627887	6.952163	1.535915
18.H	1.863902	6.884634	-1.754359
19.H	0.198087	5.708062	-0.339670
20.H	0.743185	5.143687	2.027297
21.H	2.962234	5.784763	2.965743
22.C	3.652594	6.679550	1.130773
23.N	6.032922	8.994066	-2.676086
24.O	6.922054	9.549708	-3.510870
25.C	4.832926	8.943854	-0.695534
26.H	4.485458	9.446378	0.208209
27.C	2.726689	2.390355	-1.896971
28.C	3.761736	2.871921	-1.053237
29.C	4.369665	4.078798	-1.337039
30.N	4.030511	4.850510	-2.387226
31.C	3.063253	4.399205	-3.206951
32.C	2.398690	3.202805	-3.014812
33.H	4.091303	2.314526	-0.180074
34.H	5.163880	4.463259	-0.697045
35.H	2.813791	5.041307	-4.053018
36.H	1.629830	2.910930	-3.726055
37.N	2.085438	1.212025	-1.648109
38.C	1.061499	0.729896	-2.561773
39.C	2.448877	0.415020	-0.486467
40.H	0.216569	1.433219	-2.628242
41.H	0.678130	-0.227482	-2.197782
42.H	1.464157	0.574445	-3.575141
43.H	1.796829	-0.461431	-0.434876
44.H	2.324953	0.988330	0.445108
45.H	3.491926	0.064447	-0.542449

Table S8. Optimized Cartesian Coordinates of BF_3-**1**-4,4′-bipy-**1**-BF_3



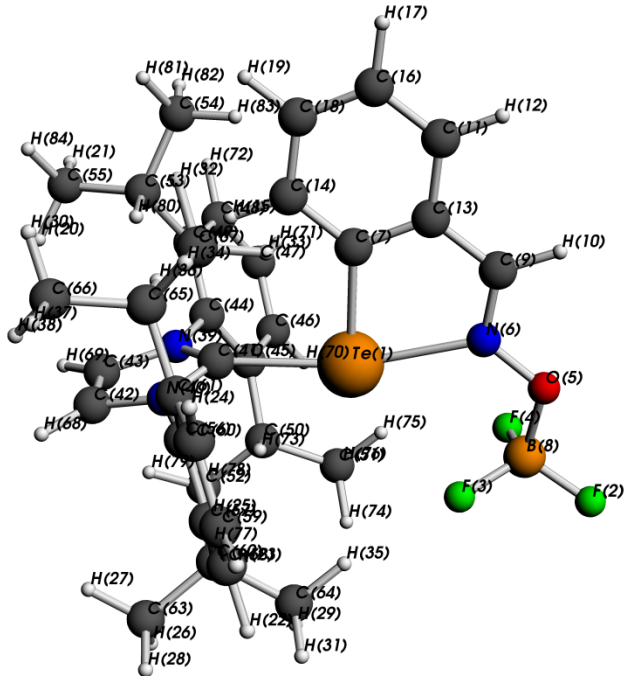
Atom	X	Y	Z(Angstrom)	Atom	X	Y	Z(Angstrom)
1.Te	4.890790	3.503868	-3.087786	37.Te	-4.890790	-3.503868	-3.087786
2.F	7.147220	5.658256	-4.909000	38.F	-7.147220	-5.658256	-4.909000
3.F	5.362498	6.143836	-3.537960	39.F	-5.362498	-6.143836	-3.537960
4.F	7.273943	7.468687	-3.464582	40.F	-7.273943	-7.468687	-3.464582
5.O	7.384496	5.343938	-2.551486	41.O	-7.384496	-5.343938	-2.551486
6.N	6.847015	4.127046	-2.408107	42.N	-6.847015	-4.127046	-2.408107
7.N	2.781935	2.159456	-3.700174	43.N	-2.781935	-2.159456	-3.700174
8.C	1.811725	0.102853	-4.451061	44.C	-1.811725	-0.102853	-4.451061
9.H	1.943977	-0.857768	-4.947451	45.H	-1.943977	0.857768	-4.947451
10.C	0.573939	0.466472	-3.909414	46.C	-0.573939	-0.466472	-3.909414
11.C	5.304322	-0.664484	-2.570032	47.C	-5.304322	0.664484	-2.570032
12.H	6.208282	-0.626938	-3.179133	48.H	-6.208282	0.626938	-3.179133
13.C	7.539759	3.195884	-1.777832	49.C	-7.539759	-3.195884	-1.777832
14.C	2.879253	0.987111	-4.345519	50.C	-2.879253	-0.987111	-4.345519
15.H	3.857008	0.743806	-4.760676	51.H	-3.857008	-0.743806	-4.760676
16.C	5.601491	1.771265	-2.108966	52.C	-5.601491	-1.771265	-2.108966
17.C	3.683748	0.455592	-1.171314	53.C	-3.683748	-0.455592	-1.171314
18.H	3.335652	1.361442	-0.673779	54.H	-3.335652	-1.361442	-0.673779
19.C	4.849519	0.514548	-1.954322	55.C	-4.849519	-0.514548	-1.954322
20.C	0.458555	1.728455	-3.310503	56.C	-0.458555	-1.728455	-3.310503
21.H	-0.490205	2.051843	-2.881152	57.H	0.490205	-2.051843	-2.881152
22.C	6.867125	1.946356	-1.623461	58.C	-6.867125	-1.946356	-1.623461
23.H	7.366745	1.143529	-1.079485	59.H	-7.366745	-1.143529	-1.079485
24.C	8.912969	3.493717	-1.271313	60.C	-8.912969	-3.493717	-1.271313
25.H	9.544113	3.869074	-2.088882	61.H	-9.544113	-3.869074	-2.088882
26.H	9.366131	2.598129	-0.833016	62.H	-9.366131	-2.598129	-0.833016
27.H	8.877646	4.291166	-0.514963	63.H	-8.877646	-4.291166	-0.514963
28.C	2.989887	-0.743620	-1.015776	64.C	-2.989887	0.743620	-1.015776
29.H	2.096035	-0.772205	-0.391635	65.H	-2.096035	0.772205	-0.391635
30.C	4.606205	-1.863967	-2.418360	66.C	-4.606205	1.863967	-2.418360
31.H	4.974812	-2.768049	-2.903524	67.H	-4.974812	2.768049	-2.903524
32.C	3.444507	-1.907257	-1.644089	68.C	-3.444507	1.907257	-1.644089
33.H	2.906884	-2.847637	-1.515438	69.H	-2.906884	2.847637	-1.515438
34.C	1.590354	2.528912	-3.206453	70.C	-1.590354	-2.528912	-3.206453
35.H	1.559009	3.490103	-2.690903	71.H	-1.559009	-3.490103	-2.690903
36.B	6.781595	6.208068	-3.687674	72.B	-6.781595	-6.208068	-3.687674

Table S9. Optimized Cartesian Coordinates of Ph_3P-**2**-BF_3



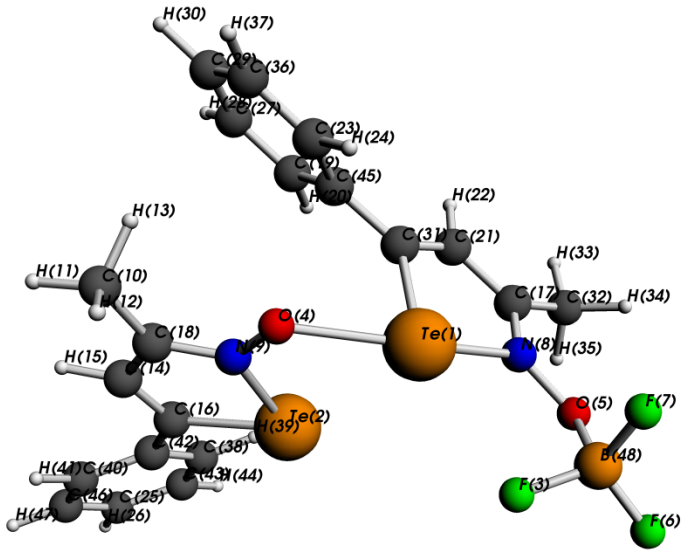
Atom	X	Y	Z(Angstrom)	Atom	X	Y	Z(Angstrom)
1.Te	3.387506	9.734083	12.614352	27.H	2.257893	7.556802	17.125943
2.P	3.762061	7.862106	14.562340	28.C	-0.624363	6.759261	15.491049
3.F	0.977335	10.222172	11.114860	29.H	-1.667667	6.514633	15.692825
4.F	0.241693	12.058721	9.897159	30.C	4.606179	6.305970	14.134311
5.F	0.995483	12.313487	12.076325	31.C	-0.164941	6.825509	14.172878
6.O	2.517428	11.862978	10.285297	32.H	-0.844952	6.638194	13.342520
7.N	3.517512	11.362308	11.001724	33.C	0.250153	7.016182	16.549689
8.C	5.469904	10.178486	12.509175	34.H	-0.105186	6.967399	17.579117
9.C	5.793170	11.146295	11.523302	35.C	4.443766	5.151889	14.918030
10.C	7.136453	11.520629	11.330328	36.H	3.805672	5.178139	15.802294
11.H	7.371750	12.264825	10.568290	37.C	6.133433	8.406272	17.894611
12.C	2.047308	7.410047	14.975069	38.H	6.953736	7.894834	18.398341
13.C	8.144948	10.954178	12.100059	39.C	5.658547	9.624308	18.383991
14.H	9.182232	11.248759	11.943776	40.H	6.108531	10.068509	19.272290
15.C	4.735417	11.737129	10.749911	41.C	4.044347	9.722302	16.584470
16.H	4.916242	12.484219	9.974661	42.H	3.244989	10.247341	16.059481
17.C	1.165783	7.148229	13.911617	43.C	5.085427	3.969022	14.553320
18.H	1.514074	7.201729	12.879232	44.H	4.953831	3.073620	15.160918
19.C	4.509044	8.486898	16.099063	45.C	4.612044	10.280518	17.727415
20.C	6.492839	9.628896	13.286383	46.H	4.245083	11.237209	18.098450
21.H	6.274529	8.904382	14.068229	47.B	1.095709	11.613814	10.878511
22.C	5.562469	7.835084	16.755054	48.C	5.883008	3.928839	13.404775
23.H	5.940533	6.886055	16.375074	49.H	6.376812	2.999677	13.118303
24.C	7.819874	10.009778	13.081183	50.C	5.398300	6.259990	12.977970
25.H	8.602362	9.566925	13.697476	51.H	5.504221	7.148283	12.354363
26.C	1.582845	7.344483	16.296714	52.C	6.037094	5.072059	12.617659
				53.H	6.647221	5.040883	11.715271

Table S10. Optimized Cartesian Coordinates of **3**-**2**-BF_3



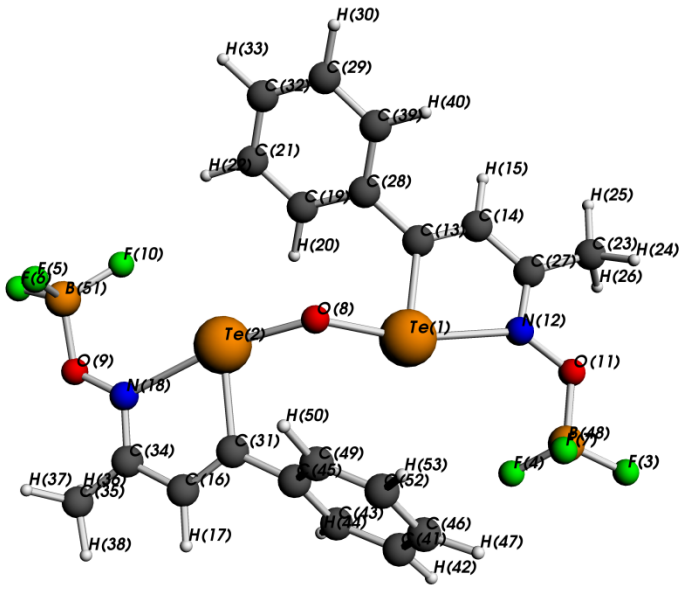
Atom	X	Y	Z(Angstrom)	Atom	X	Y	Z(Angstrom)
1.Te	1.372851	-1.144124	8.395315	43.C	2.189009	-4.644118	11.127574
2.F	1.113523	3.694792	8.304942	44.C	3.939648	-3.373722	9.876635
3.F	0.788373	1.628651	9.306149	45.C	4.457880	-2.193763	10.448182
4.F	2.865194	2.186344	8.494759	46.C	5.798685	-1.897993	10.178218
5.O	1.086351	1.841223	6.928015	47.C	6.580964	-2.739886	9.392202
6.N	1.216844	0.521843	6.763076	48.C	6.037919	-3.899368	8.849031
7.C	1.411580	-2.201212	6.559737	49.C	4.698983	-4.243084	9.076161
8.B	1.489512	2.367267	8.321739	50.C	3.636457	-1.298180	11.364825
9.C	1.158720	0.039232	5.559123	51.C	3.926691	0.196210	11.185035
10.H	1.037897	0.712523	4.707391	52.C	3.811233	-1.724042	12.835044
11.C	1.251171	-1.988744	4.132731	53.C	4.126405	-5.527437	8.494658
12.H	1.138745	-1.353444	3.253068	54.C	4.453002	-5.695043	7.004045
13.C	1.267908	-1.387328	5.405935	55.C	4.604312	-6.753305	9.294167
14.C	1.558691	-3.581487	6.404750	56.C	-0.961934	-3.239196	10.135489
15.H	1.690433	-4.214417	7.280636	57.C	-1.385366	-2.222371	11.011049
16.C	1.380800	-3.365596	3.995176	58.C	-2.723603	-1.822233	10.919071
17.H	1.365952	-3.820324	3.005010	59.C	-3.586810	-2.407998	9.998632
18.C	1.540644	-4.161277	5.136418	60.C	-3.130474	-3.406357	9.142953
19.H	1.653380	-5.241497	5.038665	61.C	-1.802672	-3.847645	9.190055
20.H	4.334957	-6.680270	10.356965	62.C	-0.462239	-1.579917	12.036381
21.H	5.698475	-6.849888	9.234192	63.C	-0.778161	-2.094918	13.452342
22.H	-3.088706	-1.030892	11.573004	64.C	-0.500084	-0.044772	11.988964
23.H	-4.623303	-2.076175	9.940300	65.C	-1.314530	-4.957852	8.274473
24.H	-3.815248	-3.846930	8.419377	66.C	-1.683279	-6.338691	8.846858
25.H	0.568985	-1.882048	11.806256	67.C	-1.823571	-4.807624	6.835630
26.H	-0.076903	-1.660150	14.179363	68.H	0.128102	-5.170460	11.796264
27.H	-0.701759	-3.190263	13.515166	69.H	2.917325	-5.216509	11.686206
28.H	-1.798233	-1.810994	13.751271	70.H	6.233965	-0.987486	10.587404
29.H	0.251089	0.364213	12.680165	71.H	7.622470	-2.485199	9.196635
30.H	-1.293053	-7.138321	8.200202	72.H	6.659789	-4.547044	8.230968
31.H	-1.479738	0.343234	12.304208	73.H	2.576806	-1.441294	11.114275
32.H	-1.355615	-5.566215	6.192781	74.H	3.215348	0.782691	11.782854
33.H	-1.575714	-3.819110	6.427800	75.H	3.815465	0.515770	10.140678
34.H	-2.912072	-4.949183	6.772886	76.H	4.937541	0.458769	11.529989
35.H	-0.282171	0.344043	10.986010	77.H	3.170239	-1.109447	13.484152
36.H	-0.219043	-4.896863	8.234985	78.H	4.854812	-1.587833	13.156388
37.H	-2.775854	-6.452514	8.909574	79.H	3.543091	-2.779045	12.991198
38.H	-1.272202	-6.483979	9.856088	80.H	3.031795	-5.480988	8.585497
39.N	2.564955	-3.723193	10.162627	81.H	3.924307	-6.570919	6.600708
40.N	0.409712	-3.689206	10.247956	82.H	5.528022	-5.859672	6.843861
41.C	1.472264	-3.132696	9.604006	83.H	4.150856	-4.812607	6.426275
42.C	0.829215	-4.623323	11.180125	84.H	4.157902	-7.673870	8.890574

Table S11. Optimized Cartesian Coordinates of **1**-**1**-BF_3



Atom	X	Y	Z(Angstrom)	Atom	X	Y	Z(Angstrom)
1.Te	4.813072	6.962211	4.902646	25.C	-1.498885	2.289159	9.107187
2.Te	2.725729	5.090559	6.536399	26.H	-2.314228	1.590321	9.293499
3.F	6.075662	4.837384	3.685289	27.C	1.017261	10.216323	7.157102
4.O	4.728803	7.331448	7.172839	28.H	-0.027166	10.257390	7.466422
5.O	4.495606	5.578836	2.059851	29.C	1.954818	11.076466	7.733416
6.F	6.182190	4.099323	1.480317	30.H	1.644256	11.799786	8.487636
7.F	6.785287	6.272586	2.031767	31.C	3.143480	8.268554	4.733376
8.N	4.034120	6.515033	2.894071	32.C	2.241702	6.886971	1.281984
9.N	3.727276	6.630165	7.660687	33.H	1.382411	7.552700	1.149669
10.C	3.867560	7.872432	9.747291	34.H	2.948647	7.021042	0.451222
11.H	3.378286	7.894415	10.726901	35.H	1.905142	5.841063	1.233407
12.H	4.944896	7.700255	9.879846	36.C	3.294320	11.003234	7.339102
13.H	3.755564	8.851937	9.259287	37.H	4.031641	11.673859	7.780242
14.C	2.194700	5.953999	9.273024	38.C	-0.222219	3.661384	7.579910
15.H	1.752631	6.088358	10.260911	39.H	-0.068034	4.055966	6.573395
16.C	1.705801	5.034888	8.387103	40.C	0.370628	3.594154	9.920766
17.C	2.923978	7.152774	2.583811	41.H	1.029474	3.886713	10.738455
18.C	3.267455	6.808150	8.888702	42.C	0.613673	4.095400	8.626597
19.C	1.413826	9.295424	6.188240	43.C	-1.264609	2.768950	7.816383
20.H	0.687372	8.608159	5.753693	44.H	-1.900927	2.451767	6.990393
21.C	2.469129	8.095205	3.561413	45.C	2.757962	9.217026	5.778888
22.H	1.596606	8.706721	3.327481	46.C	-0.676031	2.706716	10.157018
23.C	3.694633	10.076663	6.379993	47.H	-0.842650	2.327240	11.165303
24.H	4.739251	10.024051	6.074493	48.B	5.976888	5.176794	2.303007

Table S12. Optimized Cartesian Coordinates of $[BF_3\text{-}\mathbf{1}\text{-}O\text{-}\mathbf{1}\text{-}BF_3]^{2-}$



Atom	X	Y	Z(Angstrom)	Atom	X	Y	Z(Angstrom)
1.Te	4.340253	13.390616	11.791647	27.C	5.870698	10.637463	11.276677
2.Te	3.975141	16.893417	10.751218	28.C	7.241010	14.160486	10.826923
3.F	1.910300	8.722535	12.361894	29.C	9.413312	15.238276	11.103626
4.F	1.723975	10.773185	11.298736	30.H	10.396707	15.260259	11.579390
5.F	5.043329	20.482454	9.469774	31.C	1.907006	16.649773	11.102565
6.F	4.900263	20.451669	7.159179	32.C	9.045121	16.246907	10.207975
7.F	2.345688	10.677867	13.522566	33.H	9.734026	17.063188	9.982152
8.O	4.578479	15.415968	12.042155	34.C	1.520709	18.365684	9.391685
9.O	3.249251	19.362031	8.331891	35.C	0.592249	19.158612	8.516201
10.F	5.514509	18.537011	8.319068	36.H	0.750208	18.904926	7.456588
11.O	3.863688	9.818095	11.865204	37.H	0.805578	20.233996	8.607102
12.N	4.631840	10.921853	11.618534	38.H	-0.455181	18.964724	8.782016
13.C	6.322598	13.054206	11.134732	39.C	8.518629	14.212309	11.415657
14.C	6.731692	11.749298	11.021305	40.H	8.792107	13.443140	12.140176
15.H	7.744924	11.537862	10.670050	41.C	0.231899	13.566347	12.503847
16.C	1.051764	17.411221	10.350560	42.H	-0.342027	12.719131	12.129449
17.H	-0.027094	17.309479	10.491679	43.C	0.610304	14.587155	11.631768
18.N	2.826027	18.502140	9.307485	44.H	0.319482	14.547769	10.581155
19.C	6.897404	15.175029	9.916953	45.C	1.445538	15.635173	12.059913
20.H	5.919855	15.142066	9.436215	46.C	0.666405	13.581382	13.830191
21.C	7.778716	16.212066	9.615561	47.H	0.427850	12.747911	14.490492
22.H	7.456757	17.001144	8.934477	48.B	2.424575	10.038119	12.270363
23.C	6.340133	9.215149	11.150656	49.C	1.873170	15.638464	13.399684
24.H	6.231877	8.687008	12.110247	50.H	2.553743	16.422374	13.729641
25.H	7.389103	9.177908	10.828040	51.B	4.719588	19.705360	8.342317
26.H	5.713425	8.667266	10.431009	52.C	1.476369	14.629564	14.275878
				53.H	1.844425	14.635072	15.303125