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Supporting information for article:

1,3,5-Tri(iodoethynyl)-2,4,6-trifluorobenzene: halogen-bonded frameworks and NMR spectroscopic analysis

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Table S1 Masses of the reagents used in the cocrystallization process, and the melting points of the products.

compound	mass of **1** (mg)	mass of XB acceptor (mg)	mass of isolated product	melting point (ºC)
1a	158.1	41.5	59.6 mg	178-180
1b	146.5	60.0	165.0 mg	180-182
1c	30.0	10.7	11.0 mg	90[a]
1d	24.0	12.9	< 10 mg	140-150
1e	52.4	37.2	< 10 mg	142
1f	22.8	11.1	< 10 mg	n/a
1g	30.0	28.0	23.0 mg	168

[a] Sample decomposition.

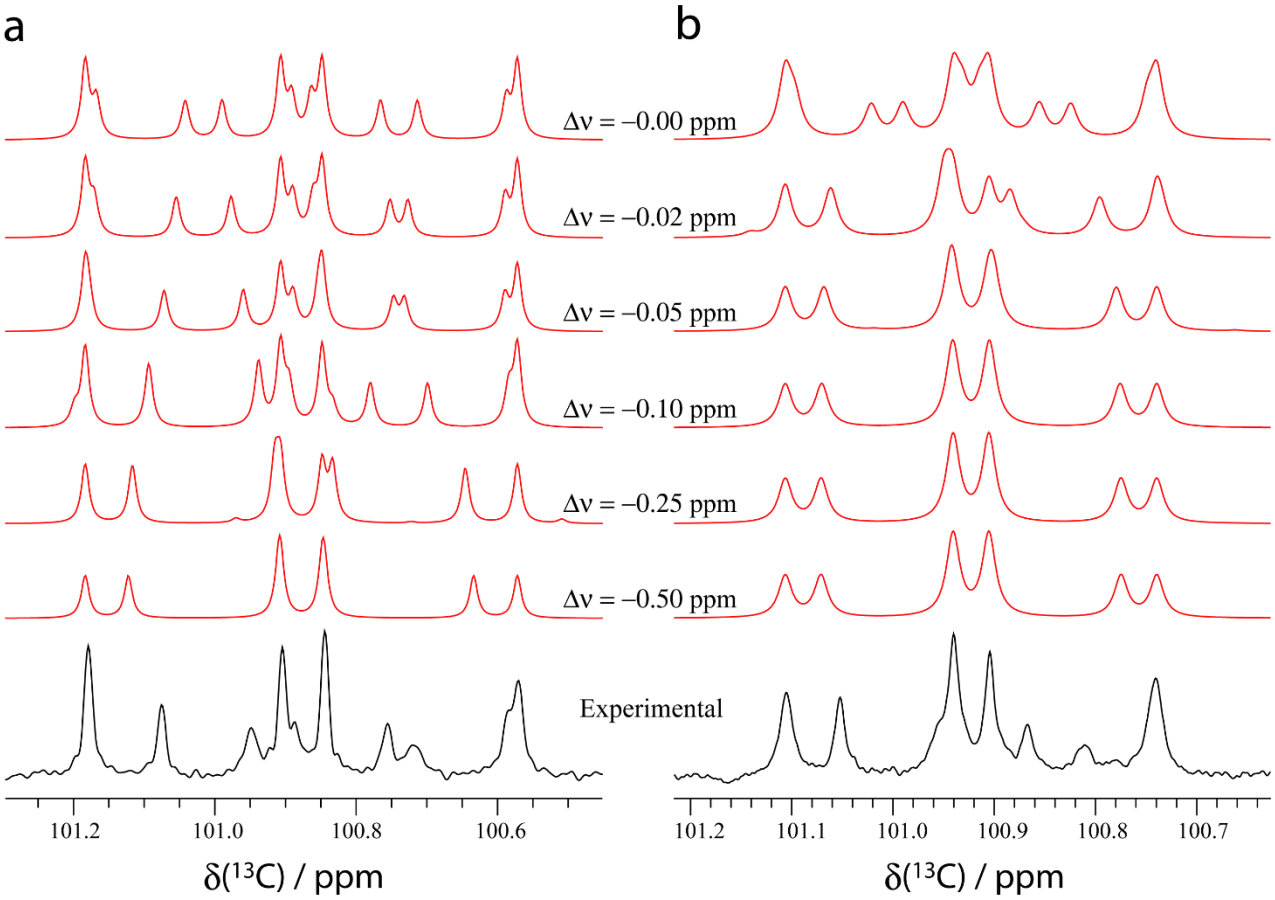

Figure S1 Experimental (black) and simulated (red) ^{13}C solution NMR spectra of the ipso carbon for (a) 300 MHz and (b) 500 MHz NMR spectrometers with incremented $\Delta\nu(^{19}F)$ isotope shifts ($^{2}\Delta^{19}F(^{13/12}C)$).

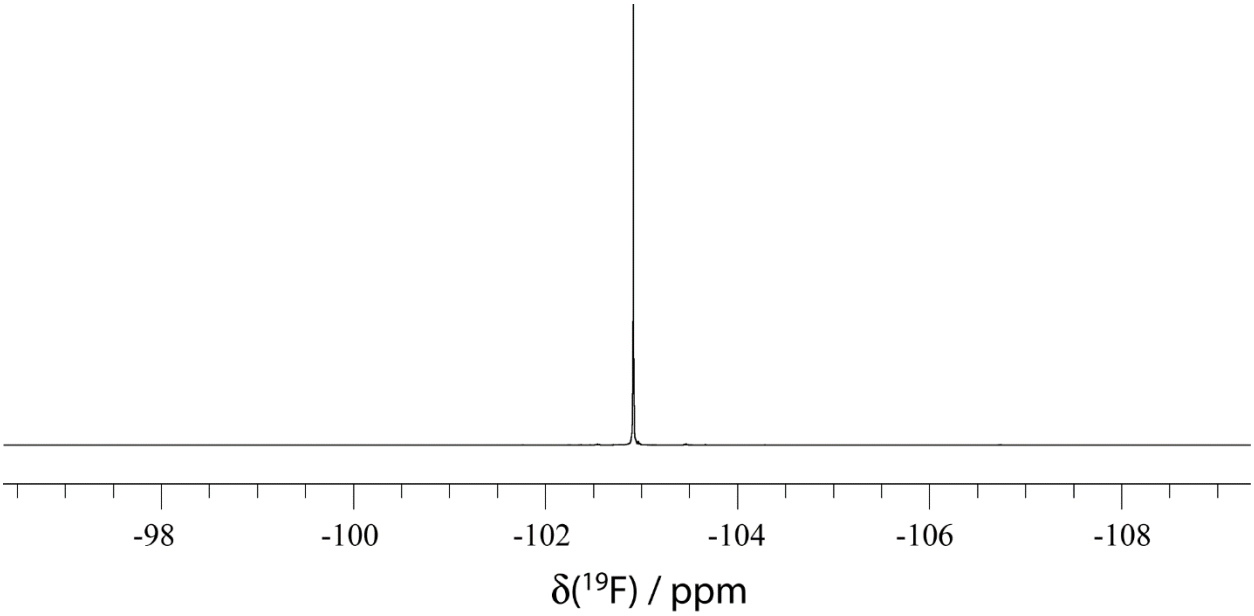

Figure S2 Experimental ^{19}F NMR spectrum of **1** in deuterated methanol.

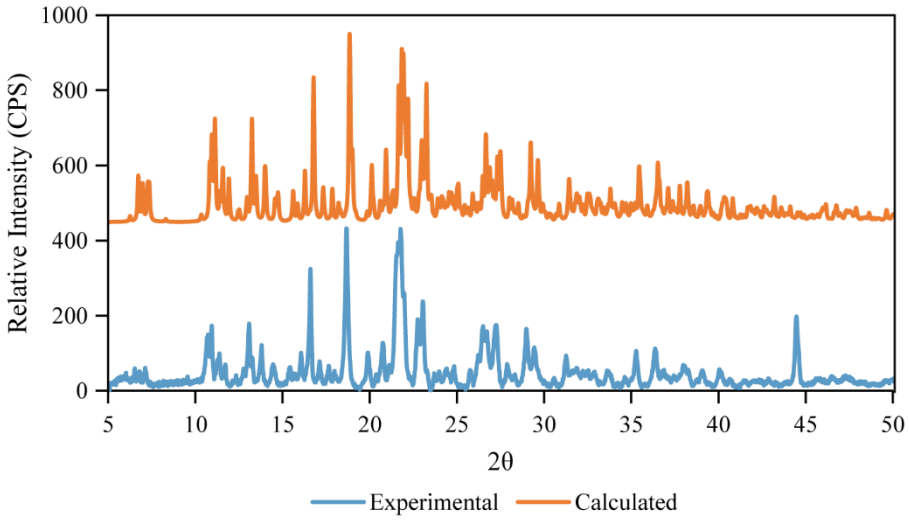

Figure S3 Powder X-ray diffractogram pattern for compound **1b**, with the calculated diffraction pattern overlaid.

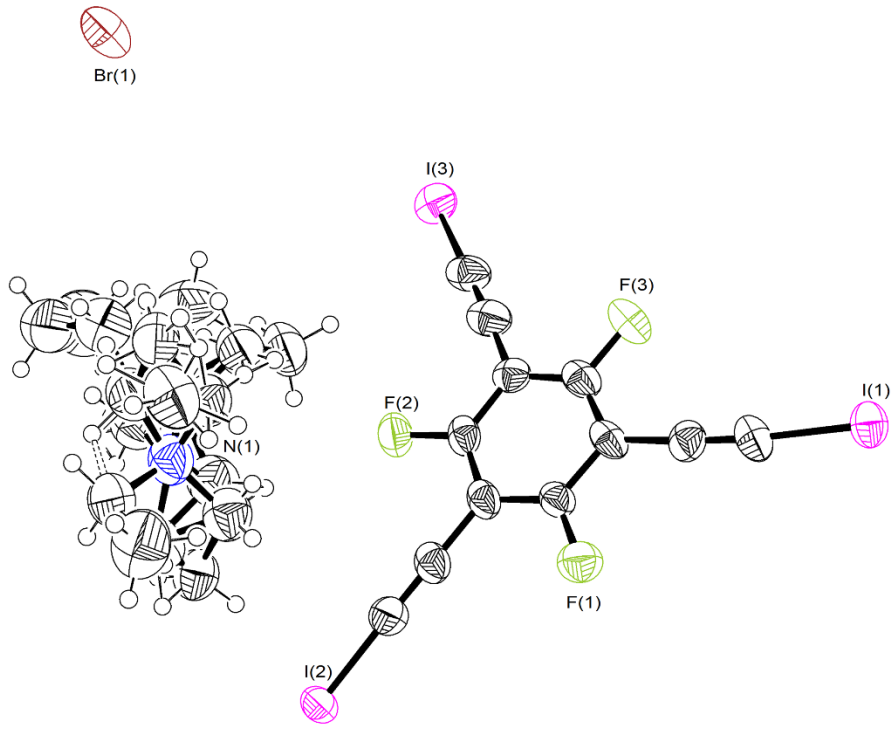

Figure S4 Thermal ellipsoid plot of compound **1a**.

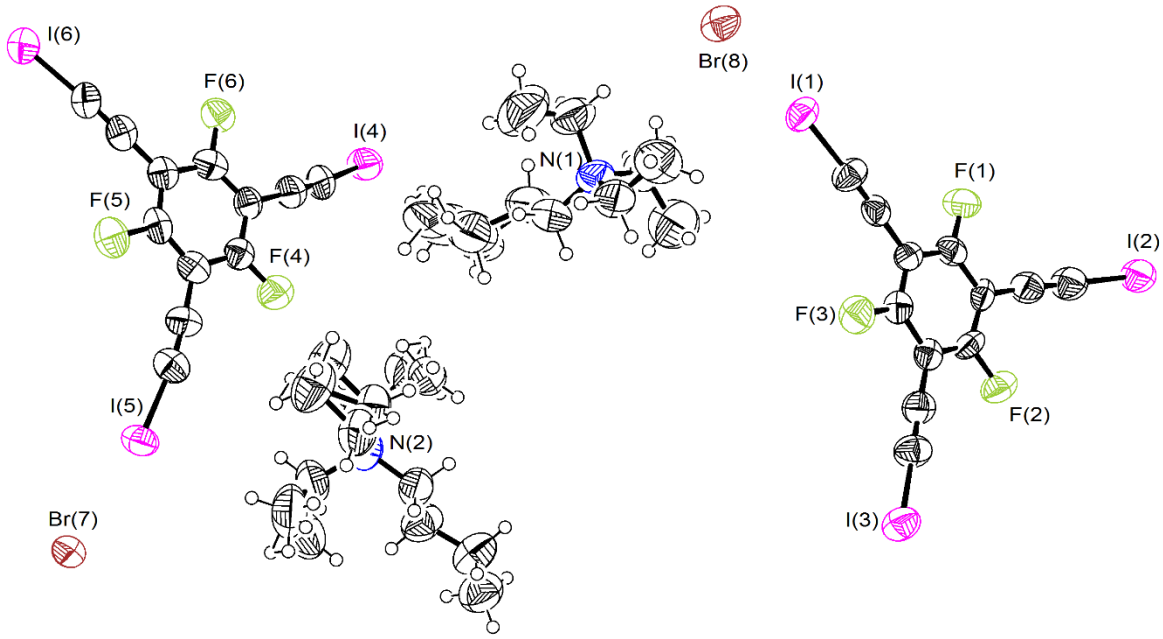

Figure S5 Thermal ellipsoid plot of compound **1b**.

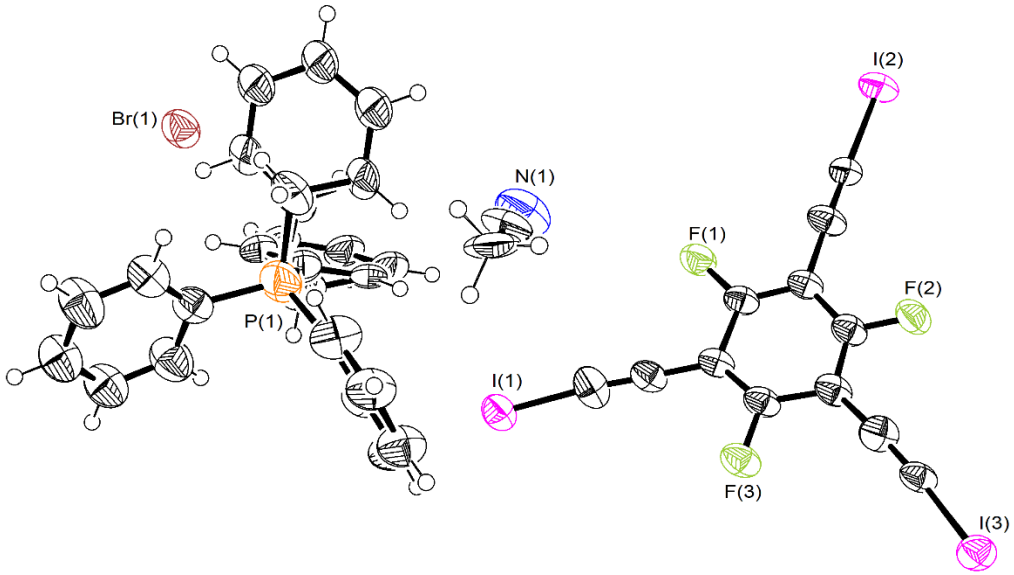

Figure S6 Thermal ellipsoid plot of compound **1c**.

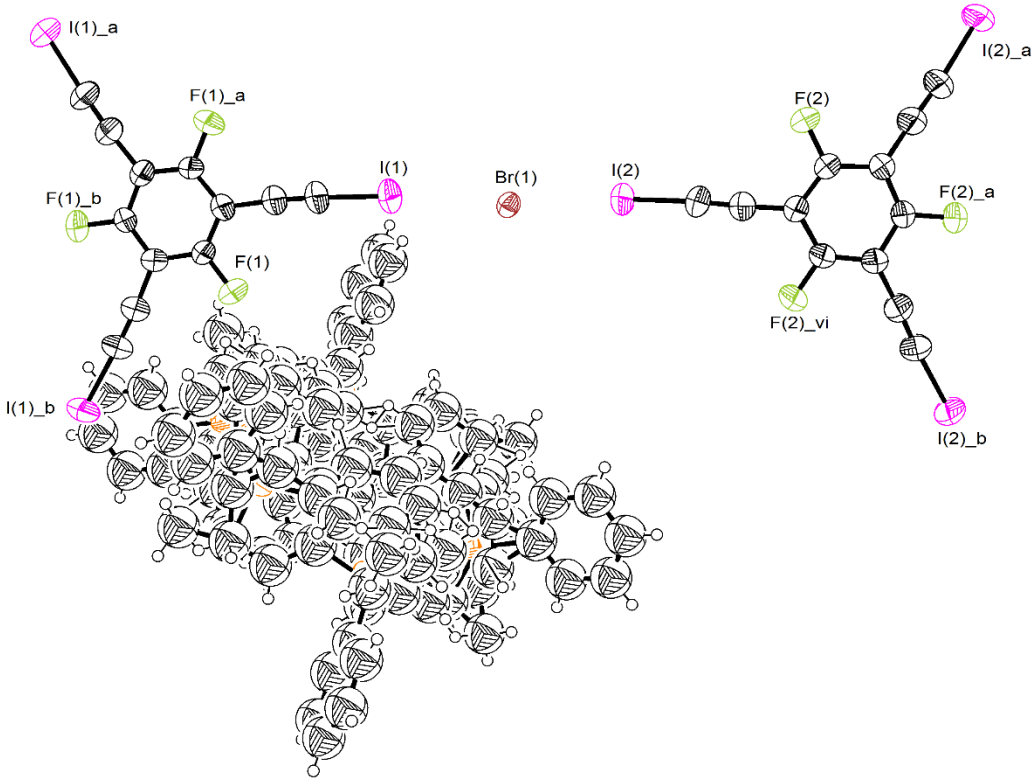

Figure S7 Thermal ellipsoid plot of compound **1d**.

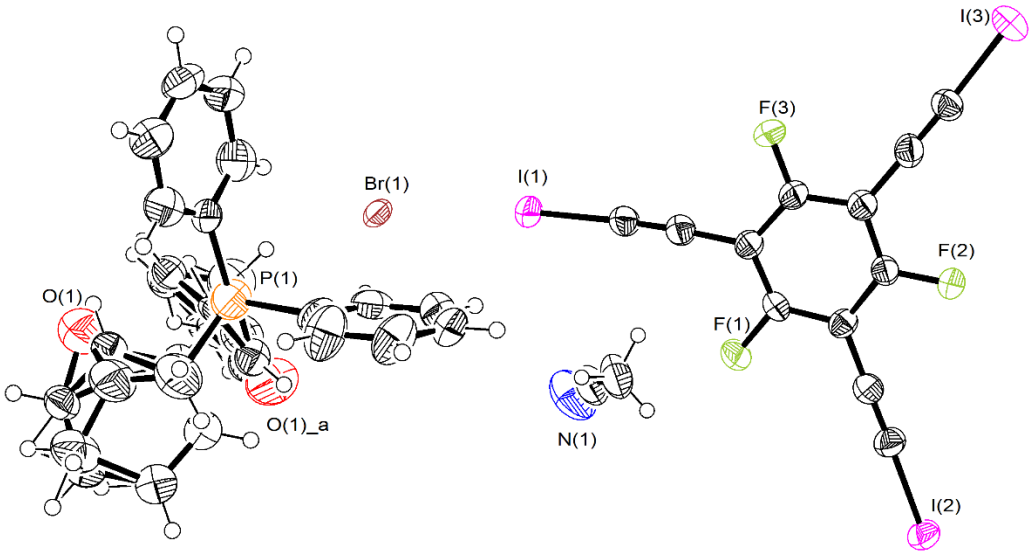

Figure S8 Thermal ellipsoid plot of compound **1e**.

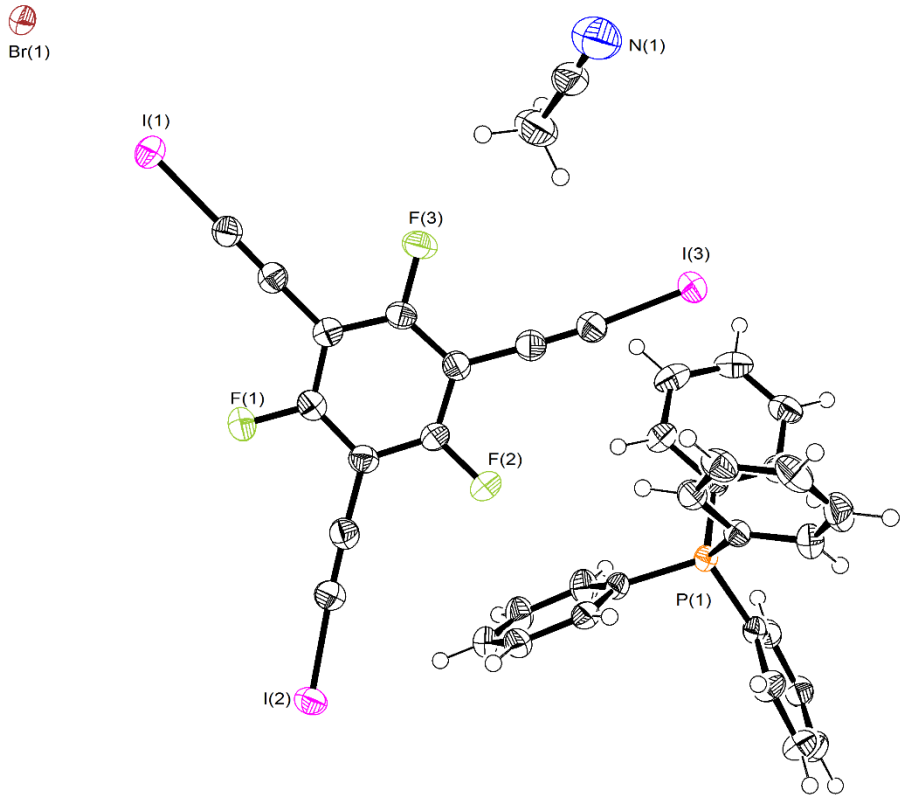

Figure S9 Thermal ellipsoid plot of compound **1f**.

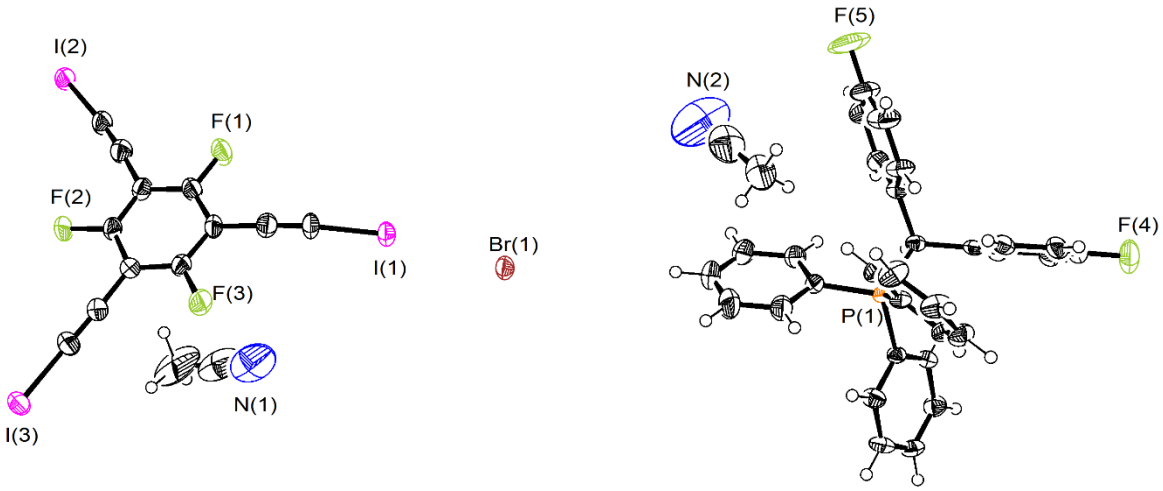

Figure S10 Thermal ellipsoid plot of compound **1g**.

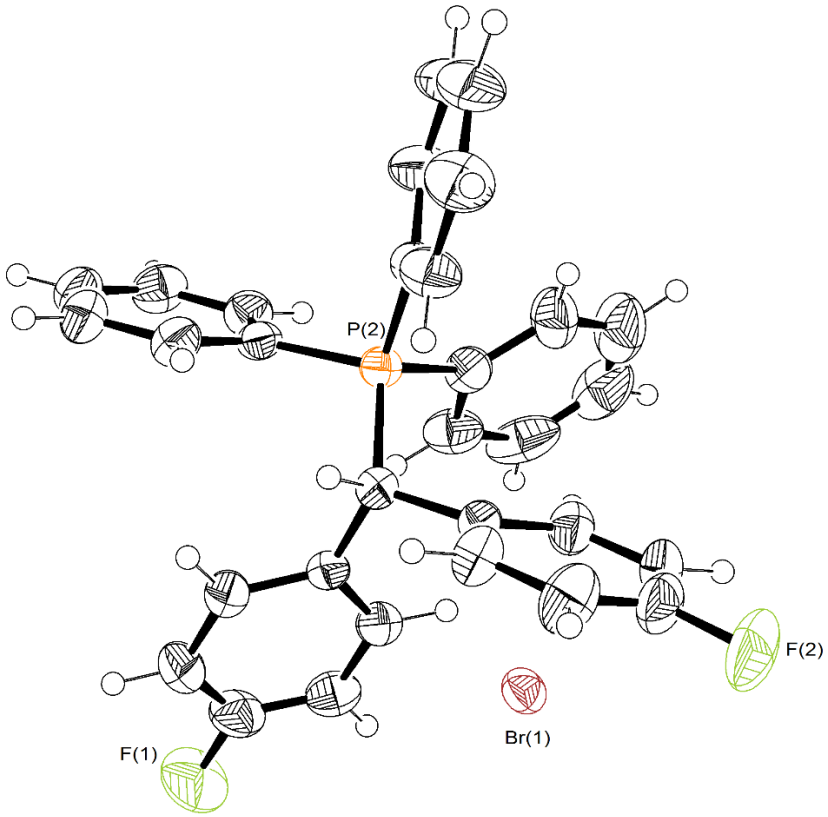

Figure S11 Thermal ellipsoid plot of compound **g**.