

## Supporting Information

# Growth and Characterization of Tetraphenylphosphonium Bromide Crystal

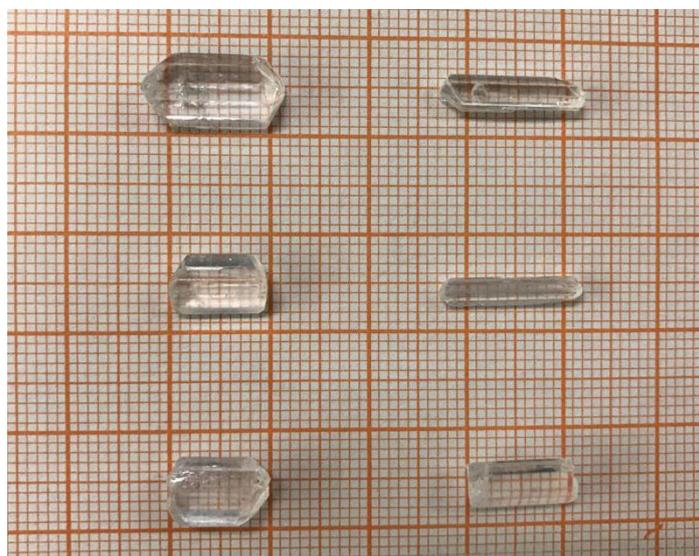
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**Table S1.** Crystallographic data and refinement details of TPPB obtained in this work and reported in literatures.

	TPPB (CH <sub>2</sub> Cl <sub>2</sub> )		TPPB (2H <sub>2</sub> O)	
Formula	C <sub>25</sub> H <sub>22</sub> BrCl <sub>2</sub> P	C <sub>25</sub> H <sub>22</sub> BrCl <sub>2</sub> P	C <sub>24</sub> H <sub>24</sub> BrO <sub>2</sub> P	C <sub>24</sub> H <sub>24</sub> BrO <sub>2</sub> P
M [g mol <sup>-1</sup> ]	504.21		455.30	
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>Pnma</i>	<i>Pnma</i>
<i>a</i> [Å]	10.3525(14)	10.2403(4)	16.2842(10)	16.255(4)
<i>b</i> [Å]	16.965(2)	16.8601(7)	10.8087(10)	10.810(4)
<i>c</i> [Å]	13.4858(17)	13.4077(5)	12.6638(12)	12.667(9)
$\alpha$ [°]	90	90	90	90
$\beta$ [°]	95.727(2)	95.781(1)	90	90
$\gamma$ [°]	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	2356.7(5)	2303.1	2229.0(3)	2225.8
<i>T</i> [K]	296	120	293(2)	295
<i>Z</i>	4	4	4	4
Reflections measured	14291		11236	
Independent reflections	5354		2125	
<i>R</i> <sub>int</sub>	0.0292		0.0292	
<i>R</i> <sub><i>I</i></sub> values ( <i>I</i> > 2σ( <i>I</i> ))	0.0380	0.0263	0.0314	0.039
<i>wR</i> ( <i>F</i> <sup>2</sup> ) values ( <i>I</i> > 2σ( <i>I</i> ))	0.0867	0.0263	0.0824	0.039
<i>R</i> <sub><i>I</i></sub> values (all data)	0.0628		0.0463	
<i>wR</i> ( <i>F</i> <sup>2</sup> ) values (all data)	0.0964		0.0899	
	This work	CCDC 270973	This work	CCDC 1280681



(a)

Figure S1 The bulk crystal of TPPS grown in our group.

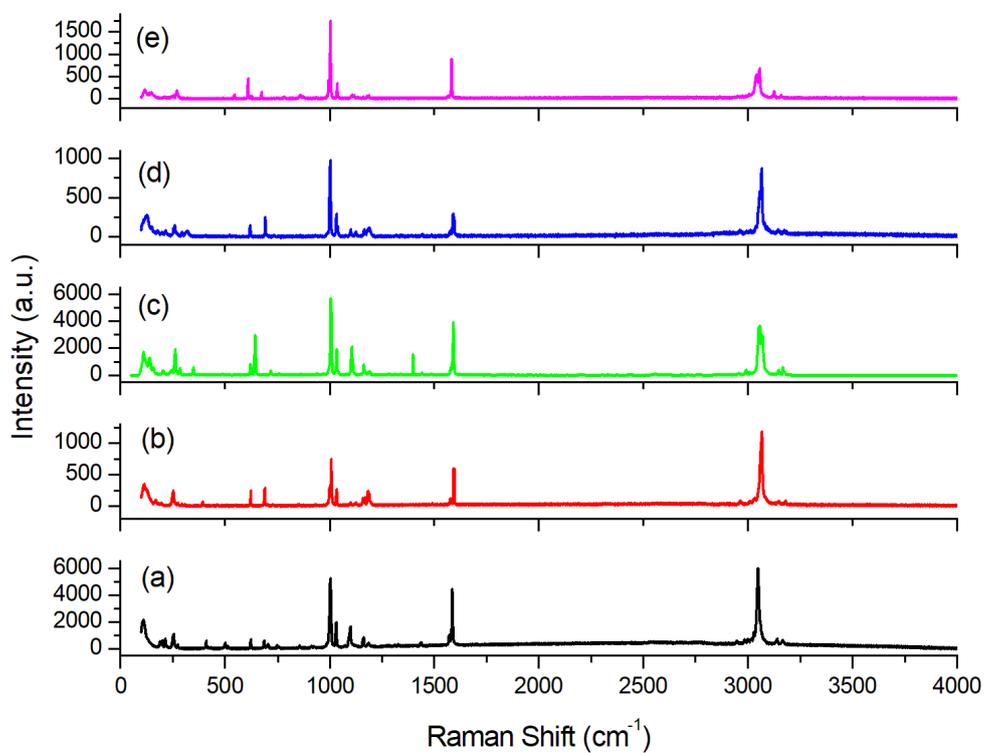


Figure S2. Spontaneous Raman scattering spectra of (a) triphenylphosphine (TPP) microcrystals, (b) triphenylphosphine oxide (TPPO) microcrystals, (c)

triphenylphosphine sulfide (TPPS) bulk crystal, (d) triphenylphosphine oxide zinc dichloride (TPPO)<sub>2</sub>ZnCl<sub>2</sub> (bulk crystal) and (e) sodium tetraphenylboron (NaBPh<sub>4</sub>) microcrystals.