Supporting Information

P≡B and As≡B Triple Bond in the Linear PB_2O^- and AsB_2O^- Species

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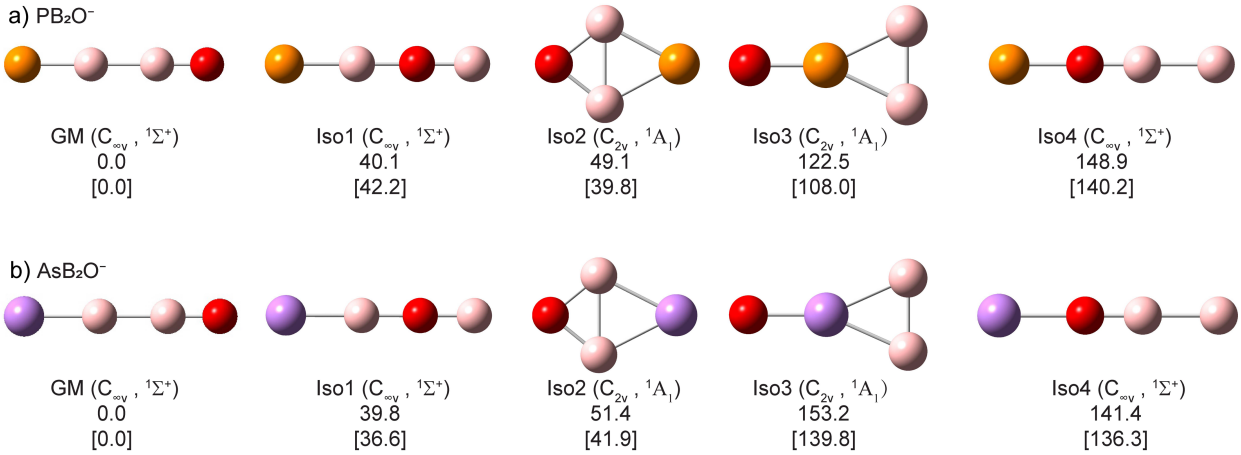

Figure S1. Global minimum and low-lying isomers of (a) PB_2O^- and (b) AsB_2O^- and their relative energies in kcal/mol at B3LYP/6-311+G* and TPSSh/Aug-cc-pVTZ/ (in brackets) levels.

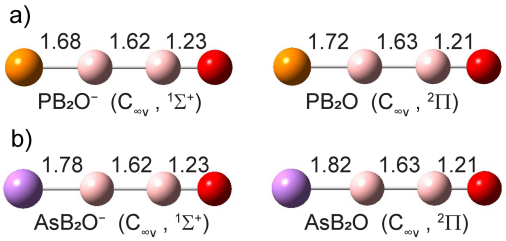

Figure S2. The optimized structures for (a) PB_2O^- and (b) AsB_2O^- and their corresponding neutrals at the TPSSh/Aug-cc-pVTZ level. The point group symmetries and electronic states are also given. The bond lengths are given in Å. The bond lengths are almost the same to those obtained with B3LYP.

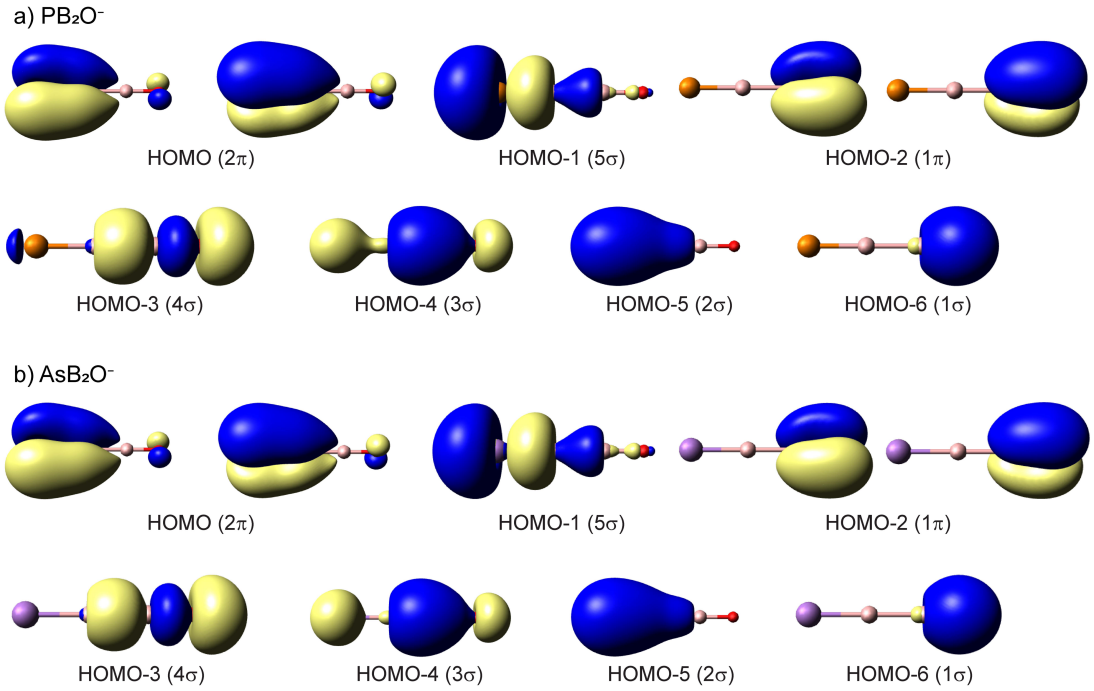

Figure S3. The occupied valence molecular orbitals of (a) PB_2O^- and (b) AsB_2O^-.

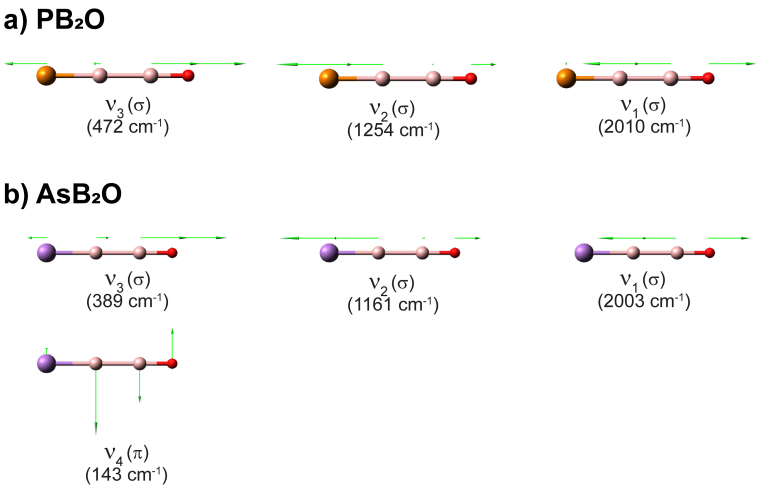

Figure S4. The observed vibrational modes for (a) PB_2O and (b) AsB_2O with their computed frequencies scaled by a factor of 0.97.

Table S1. The experimental EAs, and vibrational frequencies for EB_2O, compared with calculated values using two DFT functional.

	EA (eV)[a]			Frequency (cm^{-1})[b]		
	Exp.	B3LYP	TPSSh	Exp.[c]	B3LYP[d]	TPSSh[d]
PB_2O	3.592	3.52	3.43	2010 (ν_1)	2010(166.05)	1995(122.08)
				1260 (ν_2)	1254(29.32)	1253(27.61)
				470 (ν_3)	472(0.00)	473(0.02)
AsB_2O	3.432	3.39	3.32	2000 (ν_1)	2003(201.77)	1986(150.90)
				1165 (ν_2)	1161(15.70)	1164(15.55)
				400 (ν_3)	389(0.04)	390(0.07)
				135 (ν_4)	143(14.17)	141(13.91)

[a] Spin-orbital coupling is not considered in the computed EAs.

[b] Calculated frequencies using the B3LYP functional are scaled by a factor of 0.97. Calculated frequencies using the TPSSh functional are scaled by a factor of 0.98 . n_1 = B-O stretching, n_2 = B-B stretching, n_3 = E-B stretching, n_4 = *cis*-bending.

[c] The experimental uncertainty is estimated to be $\pm$10 cm^{-1}.

[d] The numbers in the parentheses represent the IR intensity.