

1,2-Benzenedithiol and toluene-3,4-dithiol arsenic(III) complexes - synthesis, structure, spectroscopic characterization and toxicological studies

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Supplementary Materials

Legends

Tables S1-S4. Comparison of the experimentally obtained and calculated (DFT/B3LYP/6-31+G(d,p);LANL2DZ for I) bond lengths and angles for compounds **1-4** (MAD means the Mean Absolute Deviation).

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Figure S7. Experimental (black line) and TD-DFT simulated (red vertical lines) UV-vis absorption spectra of the studied complexes in CH_2Cl_2 solution.

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Figure S11 a) ^1H NMR and **b)** ^{13}C NMR spectra of $\text{AsI}(\text{MePhS}_2)$ (**3**).

Figure S12 a) ^1H NMR and **b)** ^{13}C NMR spectra of $\text{AsBr}(\text{MePhS}_2)$ (**4**).

Table S1. Comparison of the experimentally obtained and calculated (DFT/B3LYP/6-31+G(d,p);LANL2DZ for I) bond lengths and angles for compound **1** (MAD means the Mean Absolute Deviation).

AsI(PhS ₂) (1)		B3LYP 6-31G(d,p) LANL2DZ		B3LYP 6-31+G(d,p) LANL2DZ		B3LYP 6-31++G(d,p) LANL2DZ		B3LYP 6-311++G(d,p) LANL2DZ		B3LYP def2-TZVP ecp	
	exp	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc
As-I1	2.730	2.713	0.017	2.700	0.030	2.783	0.053	2.753	0.023	2.660	0.070
As-S1	2.218	2.251	0.033	2.252	0.034	2.353	0.135	2.334	0.116	2.245	0.027
As-S2	2.227	2.250	0.023	2.252	0.025	2.352	0.125	2.334	0.107	2.245	0.018
S1-C1	1.764	1.780	0.016	1.779	0.015	1.842	0.078	1.842	0.078	1.766	0.002
S2-C2	1.763	1.780	0.017	1.779	0.016	1.842	0.079	1.842	0.079	1.766	0.003
MAD			0.021		0.024		0.094		0.081		0.024
I1-As-S1	98.69	103.32	4.63	103.27	4.58	103.85	5.16	104.52	5.83	103.59	4.90
I1-As-S2	106.10	103.34	2.76	103.29	2.81	103.87	2.23	104.56	1.54	103.61	2.49
S1-As-S2	92.97	92.16	0.81	92.09	0.88	91.54	1.43	92.02	0.95	91.71	1.26
MAD			2.73		2.76		2.94		2.77		2.88

Table S2. Comparison of the experimentally obtained and calculated (DFT/B3LYP/6-31+G(d,p)) bond lengths and angles for compound **2** (MAD means the Mean Absolute Deviation). * Experimental data are given as mean values taken from 13 molecules of **2**.

AsBr(PhS ₂) (2)		B3LYP 6-31G(d,p)		B3LYP 6-31+G(d,p)		B3LYP 6-31++G(d,p)		B3LYP 6-311++G(d,p)		B3LYP def2-TZVP ecp	
	exp*	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc
As-Br1	2.467	2.395	0.072	2.421	0.046	2.422	0.045	2.442	0.025	2.433	0.034
As-S1	2.212	2.251	0.039	2.243	0.031	2.245	0.033	2.260	0.048	2.243	0.031
As-S2	2.210	2.251	0.041	2.246	0.036	2.245	0.035	2.260	0.050	2.243	0.033
S1-C1	1.759	1.784	0.025	1.778	0.019	1.778	0.019	1.780	0.021	1.767	0.008
S2-C2	1.759	1.784	0.025	1.779	0.020	1.778	0.019	1.780	0.021	1.767	0.008
MAD			0.040		0.030		0.030		0.033		0.023
Br1-As-S1	100.81	101.16	0.35	101.91	1.10	101.81	1.00	102.98	2.17	102.89	2.08
Br1-As-S2	100.83	101.17	0.34	101.57	0.74	101.79	0.96	102.98	2.15	102.89	2.06
S1-As-S2	93.20	92.49	0.71	93.1	0.10	93.24	0.04	91.85	1.35	91.85	1.35
MAD			0.47		0.65		0.67		1.89		1.83

Table S3. Comparison of the experimentally obtained and calculated (DFT/B3LYP/6-31+G(d,p);LANL2DZ for I) bond lengths and angles for compound **3** (MAD means the Mean Absolute Deviation).

AsI(MePhS ₂) (3)		B3LYP 6-31G(d,p) LANL2DZ		B3LYP 6-31+G(d,p) LANL2DZ		B3LYP 6-31++G(d,p) LANL2DZ		B3LYP 6-311++G(d,p) LANL2DZ		B3LYP def2-TZVP ecp	
	exp	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc
As-I1	2.699	2.716	0.017	2.704	0.005	2.787	0.088	2.757	0.058	2.663	0.036
As-S1	2.216	2.249	0.033	2.25	0.034	2.351	0.135	2.333	0.117	2.243	0.027
As-S2	2.212	2.250	0.038	2.252	0.040	2.352	0.140	2.334	0.122	2.245	0.033
S1-C1	1.752	1.779	0.027	1.779	0.027	1.841	0.089	1.841	0.089	1.766	0.014
S2-C2	1.762	1.780	0.018	1.779	0.017	1.842	0.080	1.842	0.080	1.766	0.004
MAD			0.027		0.025		0.106		0.093		0.023
I1-As-S1	103.32	103.42	0.10	103.40	0.08	103.97	0.65	104.63	1.31	103.74	0.42
I1-As-S2	101.31	103.29	1.98	103.22	1.91	103.82	2.51	104.49	3.18	103.53	2.22
S1-As-S2	93.29	92.20	1.09	92.15	1.14	91.58	1.71	92.08	1.21	91.75	1.54
MAD			1.06		1.04		1.62		1.90		1.39

Table S4. Comparison of the experimentally obtained and calculated (DFT/B3LYP/6-31+G(d,p)) bond lengths and angles for compound **4** (MAD means the Mean Absolute Deviation).

AsBr(MePhS ₂) (4)		B3LYP 6-31G(d,p)		B3LYP 6-31+G(d,p)		B3LYP 6-31++G(d,p)		B3LYP 6-311++G(d,p)		B3LYP def2-TZVP ecp	
	exp	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc	calc	exp-calc
As-Br1	2.469	2.397	0.072	2.423	0.046	2.424	0.045	2.445	0.024	2.435	0.034
As-S1	2.208	2.250	0.042	2.245	0.037	2.244	0.036	2.259	0.051	2.242	0.034
As-S2	2.205	2.251	0.046	2.242	0.037	2.244	0.039	2.260	0.055	2.244	0.039
S1-C1	1.757	1.784	0.027	1.779	0.022	1.778	0.021	1.780	0.023	1.767	0.010
S2-C2	1.761	1.784	0.023	1.779	0.018	1.779	0.018	1.780	0.019	1.767	0.006
MAD			0.042		0.032		0.032		0.034		0.025
Br1-As-S1	102.96	101.24	1.72	101.66	1.30	101.85	1.11	103.12	0.16	103.04	0.08
Br1-As-S2	100.86	101.12	0.26	101.76	0.90	101.79	0.93	102.94	2.08	102.84	1.98
S1-As-S2	93.38	92.53	0.85	93.22	0.16	93.32	0.06	91.88	1.50	91.88	1.50
MAD			0.94		0.79		0.70		1.25		1.19

Figure S1.

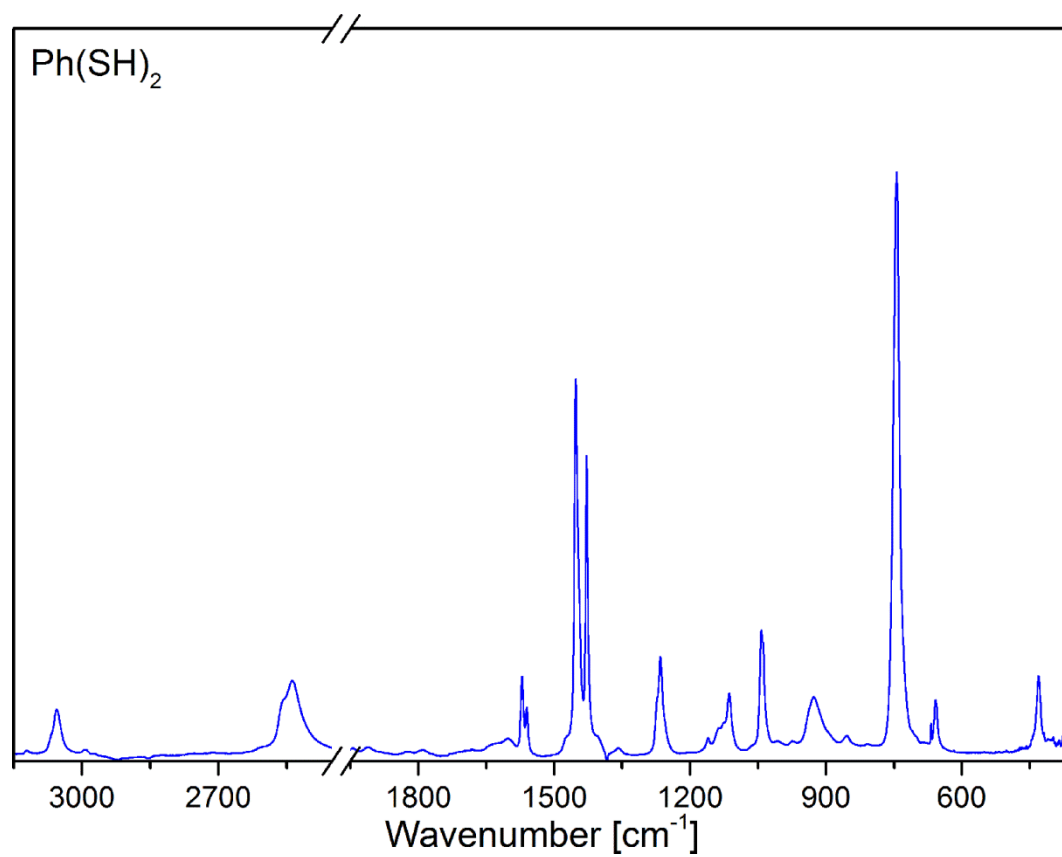


Figure S2.

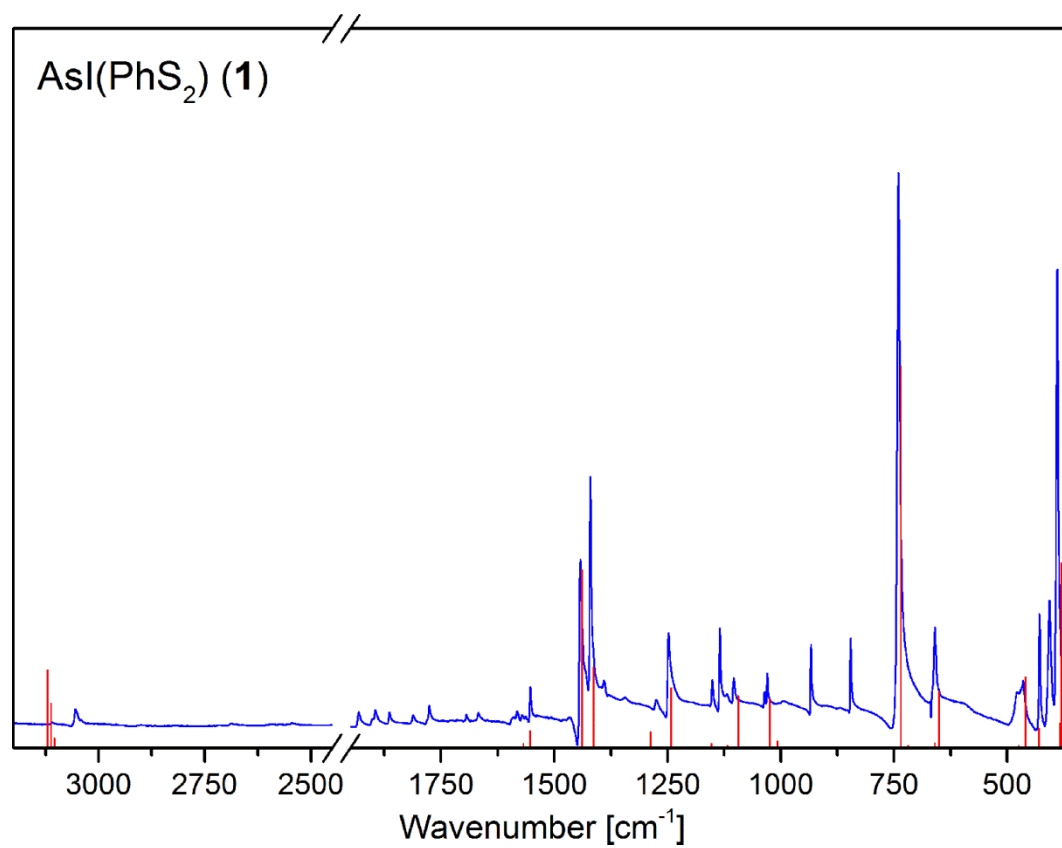


Figure S3.

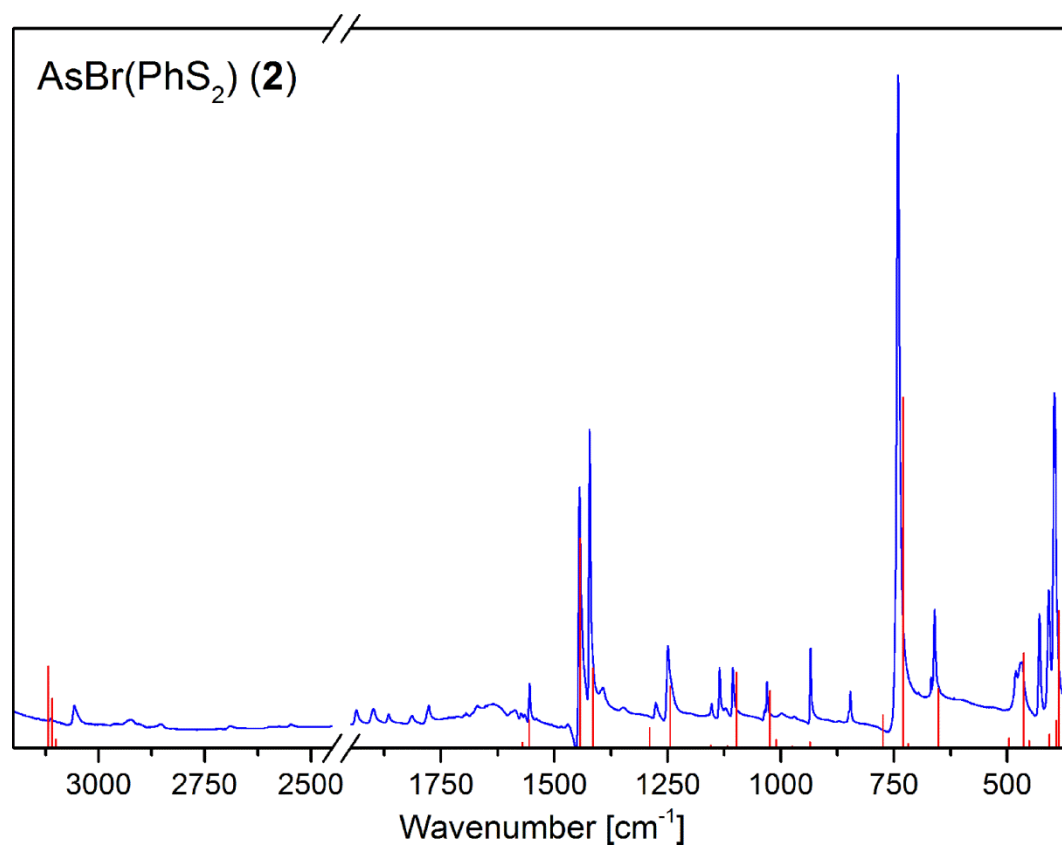


Figure S4.

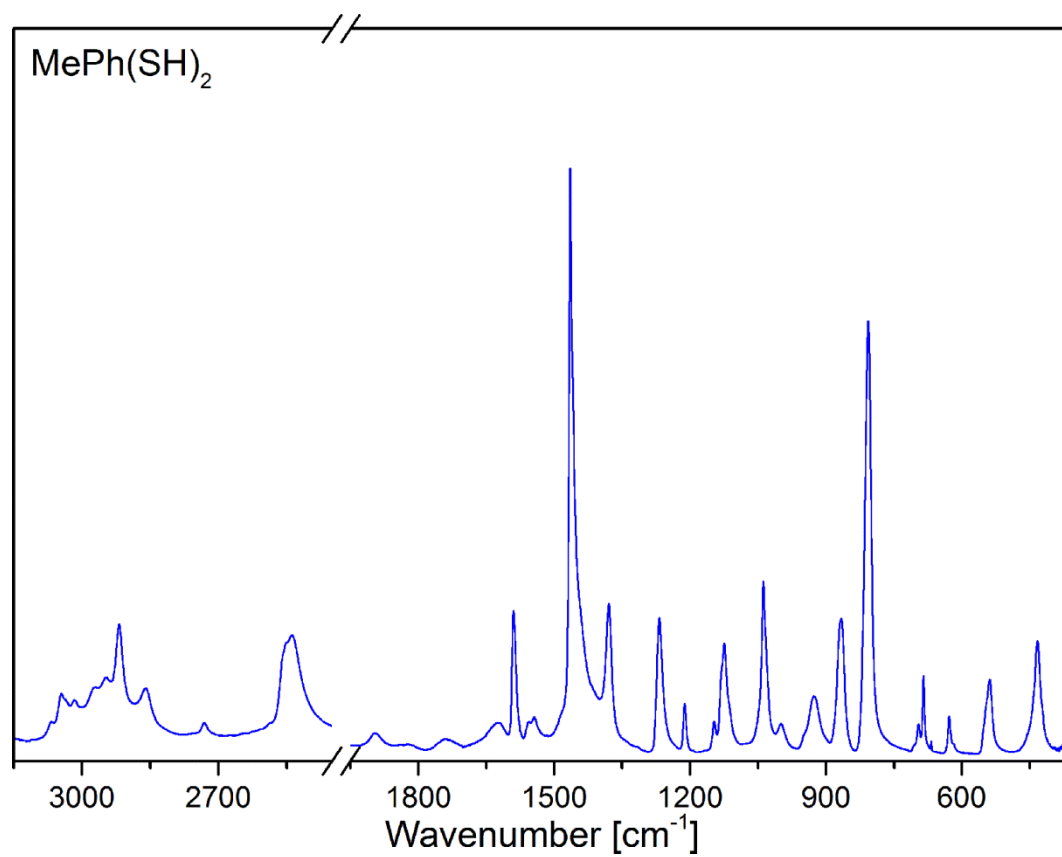


Figure S5.

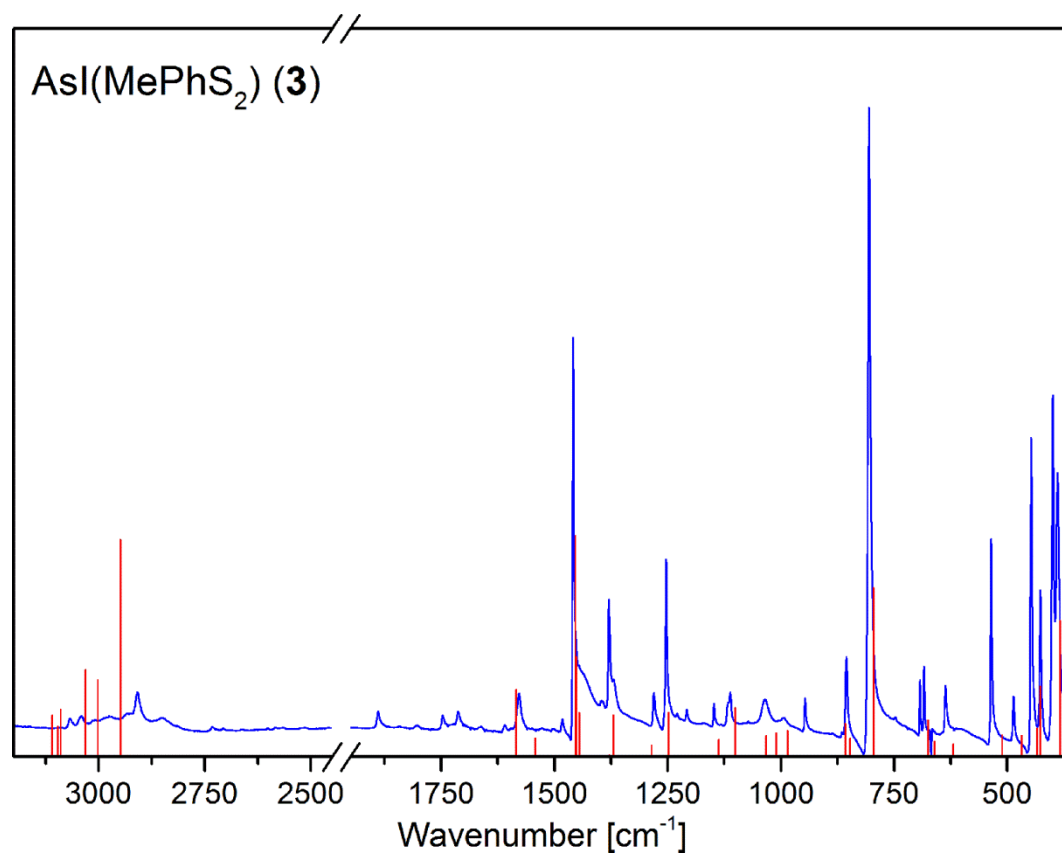


Figure S6.

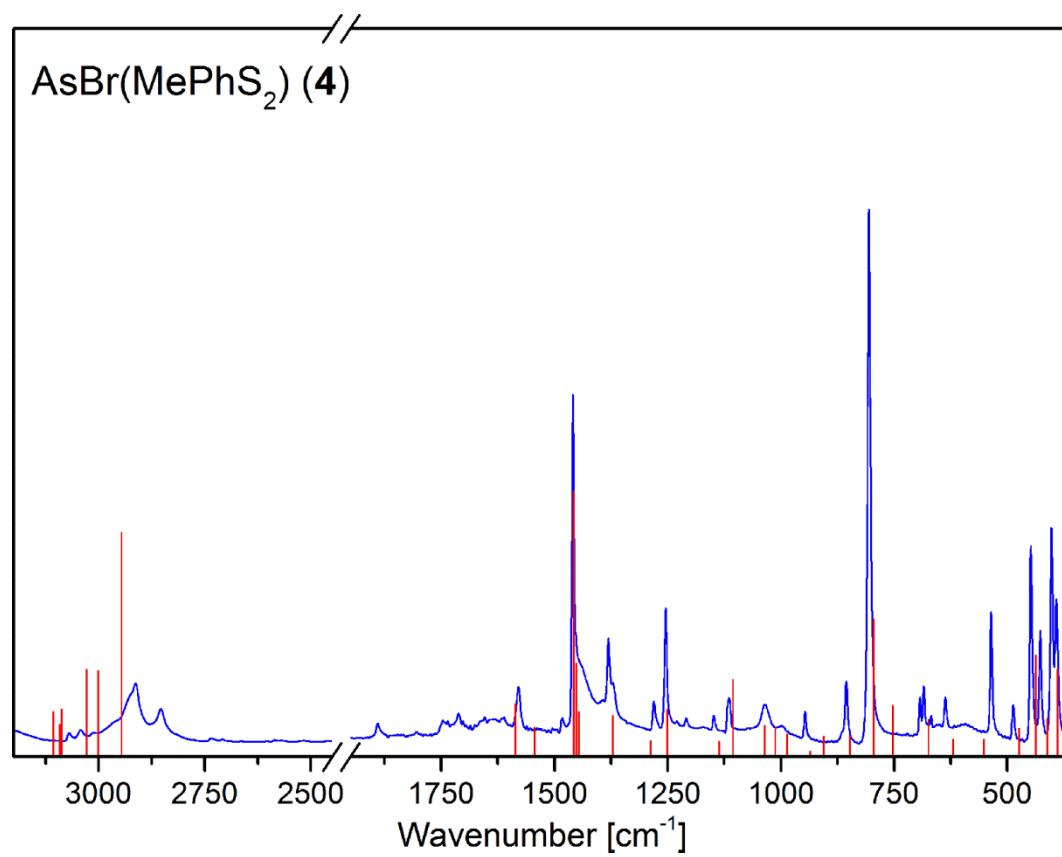


Figure S7.

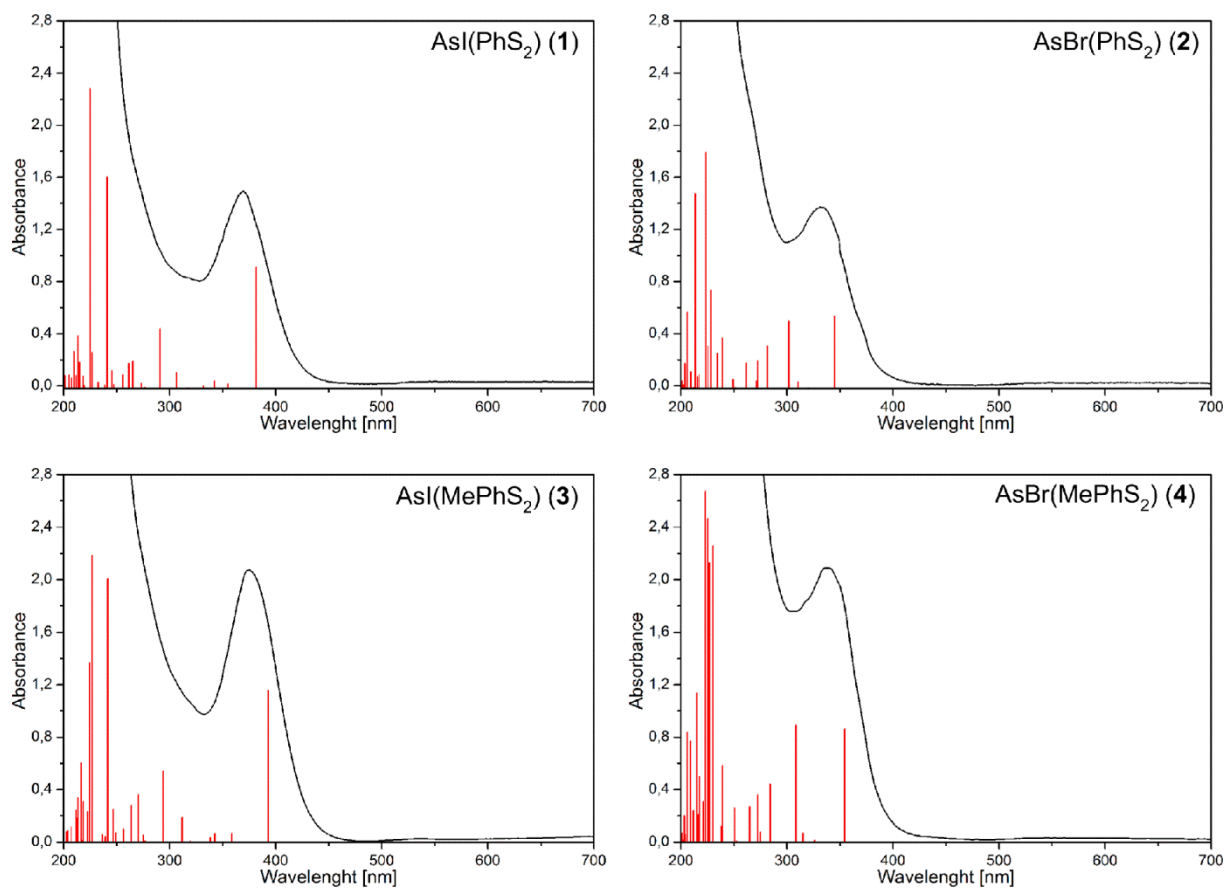
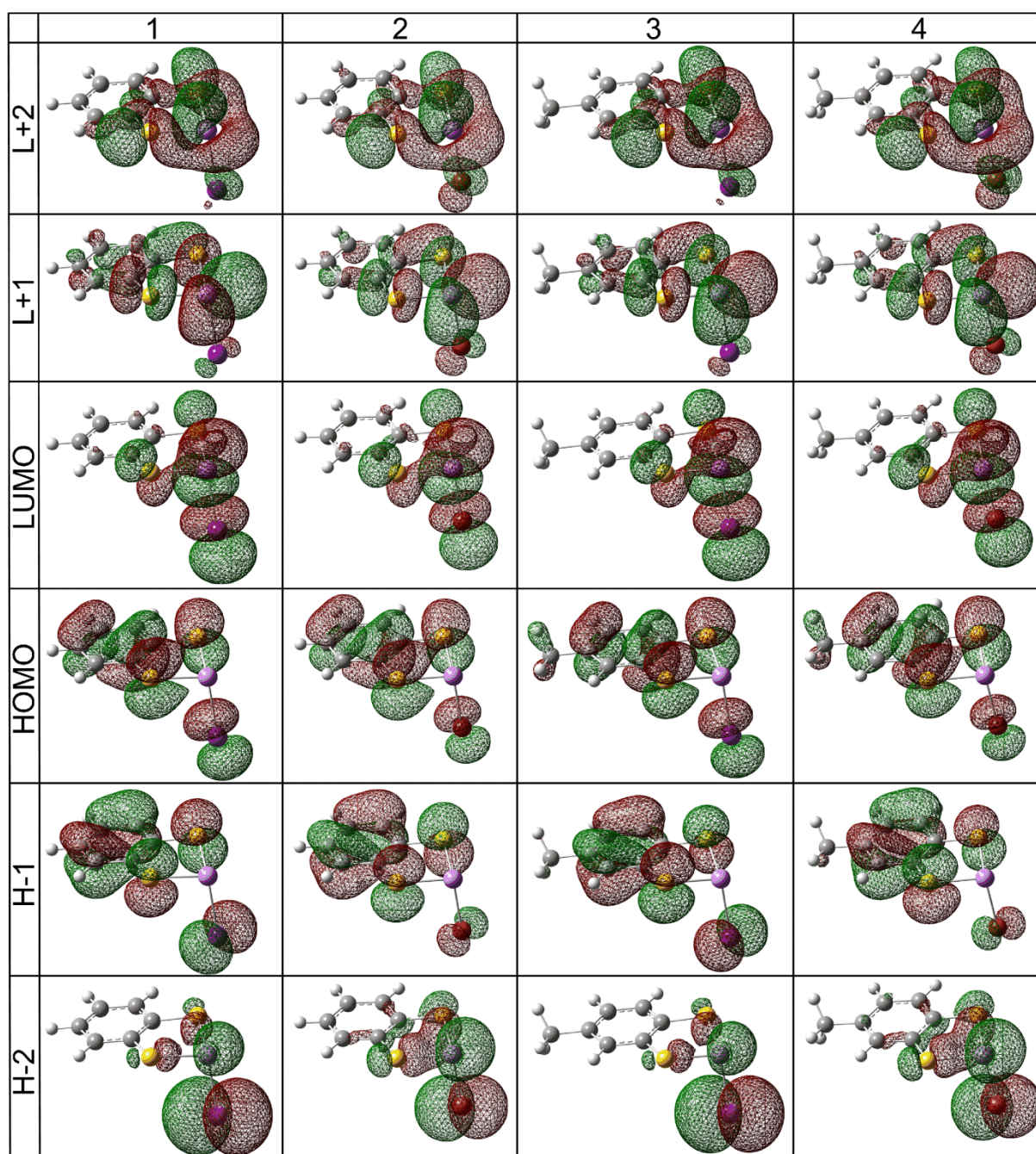


Figure S8.



Tables S5. Calculated transitions for AsI(PhS₂) (1).

Wavelength [nm]	Oscillator strength	Main components	%
381.49	0.1485	HOMO → LUMO	94.17
		HOMO → LUMO+2	2.63
355.05	0.0055	HOMO-1 → LUMO	94.17
		HOMO-3 → LUMO	3.29
342.02	0.0086	HOMO-2 → LUMO	98.70
332.22	0.0031	HOMO → LUMO+1	95.58
316.86	0.0009	HOMO-3 → LUMO	93.73
		HOMO-1 → LUMO	3.37
306.61	0.0194	HOMO → LUMO+2	86.24
		HOMO-1 → LUMO+1	10.81
291.00	0.0729	HOMO-1 → LUMO+1	84.80%
		HOMO → LUMO+2	9.28%
		HOMO → LUMO+3	2.36%
276.42	0.0012	HOMO-2 → LUMO+1	90.80%
		HOMO-1 → LUMO+2	7.36%
273.45	0.0066	HOMO-1 → LUMO+2	88.07%
		HOMO-2 → LUMO+1	6.94%
265.42	0.0335	HOMO-4 → LUMO	51.41%
		HOMO-3 → LUMO+1	27.52%
		HOMO → LUMO+3	10.94%
		HOMO-2 → LUMO+2	4.71%
		HOMO-1 → LUMO+4	3.46%
261.42	0.0305	HOMO → LUMO+3	58.10%
		HOMO-4 → LUMO	18.07%

255.86	0.0169	HOMO-1 →	9.36%
		LUMO+4	
		HOMO-2 →	8.62%
		LUMO+2	
		HOMO-3 →	46.52%
		LUMO+1	
		HOMO-2 →	37.29%
		LUMO+2	
		HOMO →	9.87%
		LUMO+3	
247.28	0.0049	HOMO-1 →	2.58%
		LUMO+4	
		HOMO-5 →	67.00%
		LUMO	
		HOMO →	23.69%
		LUMO+4	
		HOMO-1 →	4.25%
		LUMO+3	
		HOMO-3 →	2.31%
		LUMO+2	
245.36	0.0218	HOMO-5 →	67.00%
		LUMO	
		HOMO →	50.69%
		LUMO+4	
		HOMO-3 →	10.36%
		LUMO+2	
		HOMO-1 →	3.16%
		LUMO+3	
		HOMO-2 →	43.86%
		LUMO+2	
240.87	0.2587	HOMO-4 →	19.85%
		LUMO	
		HOMO-3 →	19.57%
		LUMO+1	
		HOMO-1 →	4.82%
		LUMO+4	
		HOMO-8 →	3.85%
		LUMO	
		HOMO-10 →	2.44%
		LUMO	
238.46	0.0042	HOMO-3 →	84.18%
		LUMO+2	
		HOMO →	7.46%
		LUMO+4	
232.53	0.0076	HOMO-1 →	3.65%
		LUMO+3	
		HOMO-4 →	96.12%
		LUMO+1	
226.59	0.0442	HOMO-1 →	83.09%
		LUMO+3	
		HOMO →	7.02%

		LUMO+4	
		HOMO-5 →	2.22%
		LUMO+3	
224.78	0.3672	HOMO-1 →	61.36%
		LUMO+4	
		HOMO →	11.92%
		LUMO+3	
		HOMO-4 →	10.96%
		LUMO+2	
		HOMO-6 →	3.73%
		LUMO	
		HOMO-4 →	3.39%
		LUMO+3	
219.55	0.0038	HOMO-2 →	98.58%
		LUMO+3	
218.21	0.0151	HOMO-4 →	59.14%
		LUMO+2	
		HOMO-6 →	20.85%
		LUMO	
		HOMO-5 →	6.01%
		LUMO+1	
		HOMO →	3.52%
		LUMO+5	
		HOMO →	3.34%
		LUMO+6	
		HOMO-1 →	3.00%
		LUMO+4	
215.00	0.0011	HOMO-2 →	97.11%
		LUMO+4	
214.82	0.0316	HOMO →	87.84%
		LUMO+5	
		HOMO-5 →	5.74%
		LUMO+1	
		HOMO-4 →	2.50%
		LUMO+2	
213.31	0.0644	HOMO-5 →	64.25%
		LUMO+1	
		HOMO-4 →	14.49%
		LUMO+2	
		HOMO-6 →	5.54%
		LUMO	
		HOMO →	3.53%
		LUMO+5	
		HOMO-1 →	3.18%
		LUMO+4	
		HOMO-4 →	2.51%
		LUMO+3	
211.69	0.0160	HOMO-7 →	75.11%
		LUMO	
		HOMO-5 →	18.97%
		LUMO+2	

209.96	0.0448	HOMO-6 →	55.51%
		LUMO	
		HOMO-5 →	17.60%
		LUMO+1	
		HOMO-4 →	7.69%
		LUMO+2	
		HOMO →	5.28%
		LUMO+6	
		HOMO-3 →	3.55%
209.55	0.0221	LUMO+4	
		HOMO-1 →	3.27%
		LUMO+4	
		HOMO →	82.25%
		LUMO+6	
		HOMO-6 →	6.24%
		LUMO	
		HOMO →	2.86%
		LUMO+8	
207.46	0.0132	HOMO-3 →	2.14%
		LUMO+4	
205.05	0.0167	HOMO-3 →	94.26%
		LUMO+3	
		HOMO-3 →	82.74%
		LUMO+4	
		HOMO-4 →	8.17%
		LUMO+3	
201.14	0.0156	HOMO-6 →	3.15%
		LUMO	
		HOMO-1 →	42.77%
		LUMO+5	
		HOMO-5 →	30.69%
		LUMO+2	
		HOMO-7 →	9.76%
		LUMO	
		HOMO →	3.58%
		LUMO+8	
		HOMO →	2.91%
		LUMO+7	
		HOMO-6 →	2.12%
		LUMO+1	

Tables S6. Calculated transitions for AsBr(PhS₂) (**2**).

Wavelength [nm]	Oscillator strength	Main components	%
345.16	0.0686	HOMO → LUMO	88.42
		HOMO →	
		LUMO+2	9.63
320.20	0.0006	HOMO → LUMO+1	89.84
		HOMO-1 → LUMO	8.54
310.46	0.0060	HOMO-1 → LUMO	85.77
		HOMO →	8.67

		LUMO+1	
		HOMO-1 →	2.88
		LUMO+2	
301.80	0.0640	HOMO →	84.65
		LUMO+2	
		HOMO → LUMO	8.29
		HOMO-1 →	4.40
		LUMO+1	
281.26	0.0407	HOMO-1 →	90.74
		LUMO+1	
		HOMO →	3.57
		LUMO+2	
		HOMO →	3.23
		LUMO+3	
272.15	0.0262	HOMO-2 → LUMO	88.80
		HOMO-1 →	7.69
		LUMO+2	
271.59	0.0070	HOMO-1 →	84.02
		LUMO+2	
		HOMO-2 →	8.01
		LUMO+	
		HOMO-1 → LUMO	2.48
		HOMO →	2.19
		LUMO+4	
261.55	0.0238	HOMO →	74.28
		LUMO+3	
		HOMO-1 →	19.62
		LUMO+4	
		HOMO-1 →	2.49
		LUMO+1	
251.53	0.0008	HOMO-3 → LUMO	90.62
		HOMO-2 →	5.45
		LUMO+1	
248.97	0.0085	HOMO →	56.12
		LUMO+4	
		HOMO-2 →	33.13
		LUMO+1	
		HOMO-1 →	4.53
		LUMO+3	
		HOMO-3 → LUMO	3.08
239.03	0.0482	HOMO-2 →	57.58
		LUMO+1	
		HOMO →	24.42
		LUMO+4	
		HOMO-1 →	7.53
		LUMO+3	
		HOMO-3 → LUMO	2.10
234.48	0.0334	HOMO-2 →	66.20
		LUMO+2	
		HOMO-4 → LUMO	29.74

228.15	0.0938	HOMO-4 → LUMO	38.16
		HOMO-3 →	31.43
		LUMO+1	
		HOMO-2 →	12.42
		LUMO+2	
		HOMO-1 →	9.42
		LUMO+4	
		HOMO →	3.44
225.64	0.0404	LUMO+3	
		HOMO-5 → LUMO	46.48
		HOMO-1 →	39.39
		LUMO+3	
		HOMO →	4.83
		LUMO+4	
223.84	0.2711	HOMO-3 →	2.03
		LUMO+1	
		HOMO-5 → LUMO	29.41
		HOMO-1 →	23.19
		LUMO+4	
		HOMO-1 →	18.51
		LUMO+3	
		HOMO-3 →	11.81
		LUMO+1	
		HOMO →	5.40
223.44	0.2250	LUMO+3	
		HOMO →	2.07
		LUMO+4	
		HOMO-1 →	32.27
		LUMO+4	
		HOMO-1 →	21.81
		LUMO+3	
		HOMO-5 → LUMO	16.06
		HOMO-3 →	12.92
		LUMO+1	
		HOMO →	5.31
		LUMO+3	
216.99	0.0129	HOMO-3 →	2.24
		LUMO+2	
		HOMO →	87.11
		LUMO+5	
215.37	0.0110	HOMO-3 →	3.80
		LUMO+1	
		HOMO-3 →	89.09
213.58	0.1855	LUMO+2	
		HOMO-3 →	31.25
		LUMO+1	
		HOMO-4 → LUMO	21.61
		HOMO-2 →	13.35
		LUMO+2	
		HOMO →	7.52
		LUMO+5	

		HOMO-1 →	5.37
		LUMO+4	
		HOMO-4 →	5.77
		LUMO+2	
		HOMO →	2.79
		LUMO+3	
		HOMO-10 →	2.52
		LUMO	
		HOMO-5 →	2.01
		LUMO+1	
211.94	0.0012	HOMO-4 →	96.71
		LUMO+1	
209.41	0.0157	HOMO →	82.82
		LUMO+6	
		HOMO-4 →	4.28
		LUMO+2	
		HOMO →	3.99
		LUMO+8	
205.97	0.0727	HOMO-5 →	80.73
		LUMO+1	
		HOMO-4 →	3.46
		LUMO+2	
		HOMO-6 → LUMO	2.39
		HOMO →	2.30
		LUMO+6	
204.15	0.0233	HOMO-4 →	77.97
		LUMO+2	
		HOMO-5 →	7.95
		LUMO+1	
		HOMO →	4.38
		LUMO+6	
203.54	0.0240	HOMO-2 →	93.99
		LUMO+3	
		HOMO-5 →	2.13
		LUMO+1	
202.34	0.0034	HOMO-1 →	47.90
		LUMO+5	
		HOMO-5 →	27.17
		LUMO+2	
		HOMO-6 → LUMO	9.28
		HOMO-7 → LUMO	4.49
		HOMO →	2.41
		LUMO+7	
		HOMO-1 →	2.21
		LUMO+6	
201.19	0.0028	HOMO-5 →	35.11
		LUMO+2	
		HOMO-1 →	33.30
		LUMO+5	
		HOMO-2 →	13.62
		LUMO+4	

		HOMO-6 → LUMO	6.34
		HOMO-7 → LUMO	3.92
		HOMO →	2.27
		LUMO+7	
200.82	0.0070	HOMO-2 →	81.82
		LUMO+4	
		HOMO-1 →	7.59
		LUMO+5	
		HOMO-5 →	2.71
		LUMO+2	
		HOMO-7 → LUMO	2.07

Tables S7. Calculated transitions for AsI(MePhS₂) (**3**).

Wavelength [nm]	Oscillator strength	Main components	%
392.75	0.1447	HOMO → LUMO	94.89
		HOMO →	
		LUMO+2	2.36
		HOMO-1 →	
358.86	0.0082	LUMO	93.18
		HOMO-3 →	
		LUMO	2.73
		HOMO →	
		LUMO+1	2.07
		HOMO-2 →	
342.56	0.0079	LUMO	98.65
		HOMO →	
338.15	0.0041	LUMO+1	95.63
		HOMO-3 →	
319.14	0.0009	LUMO	94.97
		HOMO-1 →	
		LUMO	2.76
		HOMO →	
311.86	0.0236	LUMO+2	89.82
		HOMO-1 →	
		LUMO+1	6.83
		HOMO-1 →	
293.73	0.0674	LUMO+1	88.63
		HOMO →	
		LUMO+2	5.81
		HOMO →	
		LUMO+3	2.25
		HOMO-1 →	
276.55	0.0012	LUMO+2	62.67
		HOMO-2 →	
		LUMO+1	34.66
		HOMO-2 →	
274.97	0.0065	LUMO+1	62.64
		HOMO-1 →	
		LUMO+2	32.63
		HOMO-4 →	
270.23	0.0454	LUMO	71.14
		HOMO-3 →	
		LUMO+1	16.82
		HOMO-2 →	
		LUMO+2	6.88
		HOMO →	
263.63	0.0349	LUMO+3	68.21
		HOMO-1 →	
		LUMO+4	12.08
		HOMO-3 →	
		LUMO+1	4.36

		HOMO-4 →	
		LUMO	3.94
		HOMO-2 →	
		LUMO+2	2.71
		HOMO →	
		LUMO+4	2.50
		HOMO-3 →	
256.17	0.0122	LUMO+1	53.29
		HOMO-2 →	
		LUMO+2	35.34
		HOMO →	
		LUMO+3	6.26
		HOMO-5 →	
249.24	0.0090	LUMO	68.30
		HOMO →	
		LUMO+4	21.28
		HOMO-1 →	
		LUMO+3	3.70
		HOMO →	
246.83	0.0312	LUMO+4	51.25
		HOMO-5 →	
		LUMO	26.58
		HOMO-3 →	
		LUMO+2	7.07
		HOMO-1 →	
		LUMO+3	4.79
		HOMO →	
		LUMO+3	2.21
		HOMO-2 →	
241.77	0.2510	LUMO+2	48.25
		HOMO-3 →	
		LUMO+1	20.30
		HOMO-4 →	
		LUMO	14.40
		HOMO-1 →	
		LUMO+4	3.32
		HOMO-8 →	
		LUMO	2.74
		HOMO-3 →	
239.18	0.0053	LUMO+2	88.98
		HOMO →	
		LUMO+4	4.68
		HOMO-1 →	
		LUMO+3	2.07
		HOMO-4 →	
236.45	0.0072	LUMO+1	95.76
		HOMO-1 →	
227.03	0.2733	LUMO+3	58.86
		HOMO-4 →	
		LUMO+2	9.48
		HOMO →	8.33

		LUMO+4	
		HOMO-1 →	
		LUMO+4	6.88
		HOMO-6 →	
		LUMO	3.15
		HOMO →	
		LUMO+3	2.70
224.66	0.1706	HOMO-1 →	
		LUMO+4	47.39
		HOMO-1 →	
		LUMO+3	20.77
		HOMO-4 →	
		LUMO+2	14.74
		HOMO →	
		LUMO+3	6.47
		HOMO-4 →	
		LUMO+3	2.06
222.35	0.0292	HOMO-4 →	
		LUMO+2	42.21
		HOMO-6 →	
		LUMO	40.59
		HOMO-1 →	
		LUMO+4	5.80
		HOMO-5 →	
		LUMO+1	4.20
		HOMO →	
218.50	0.0389	LUMO+5	95.61
		HOMO-2 →	
217.82	0.0018	LUMO+3	97.00
		HOMO-6 →	
216.58	0.0751	LUMO	36.37
		HOMO-4 →	
		LUMO+2	26.68
		HOMO-1 →	
		LUMO+4	11.88
		HOMO-5 →	
		LUMO+1	8.34
		HOMO-4 →	
		LUMO+3	2.71
		HOMO →	
		LUMO+3	2.62
		HOMO-4 →	
		LUMO	2.05
		HOMO-5 →	
213.38	0.0422	LUMO+1	72.45
		HOMO-6 →	
		LUMO	12.11
		HOMO-7 →	
		LUMO	5.34
		HOMO-2 →	
		LUMO+4	3.59

213.12	0.0018	HOMO-2 →	
		LUMO+4	76.67
		HOMO-7 →	
		LUMO	16.97
		HOMO-5 →	
212.23	0.0227	LUMO+2	3.17
		HOMO-7 →	
		LUMO	53.78
		HOMO-2 →	
		LUMO+4	17.04
211.76	0.0306	HOMO-5 →	
		LUMO+2	15.68
		HOMO-5 →	
		LUMO+1	8.32
		HOMO →	
207.13	0.0145	LUMO+6	82.57
		HOMO →	
		LUMO+8	5.01
		HOMO →	
		LUMO+7	4.12
203.54	0.0107	HOMO-3 →	
		LUMO+3	85.79
		HOMO-3 →	
202.66	0.0101	LUMO+4	5.95
		HOMO-3 →	
		LUMO+4	78.46
		HOMO-4 →	
		LUMO+3	7.07
		HOMO-3 →	
		LUMO+3	6.53
		HOMO-1 →	
		LUMO+5	65.40
		HOMO-5 →	
		LUMO+2	9.36
		HOMO →	
		LUMO+7	4.99
		HOMO →	
		LUMO+8	4.40
		HOMO-7 →	
		LUMO	3.81
		HOMO →	
		LUMO+9	3.10
		HOMO-3 →	
		LUMO+4	2.09

Tables S8. Calculated transitions for AsBr(MePhS₂) (**4**).

Wavelength [nm]	Oscillator strength	Main components	%
354.59	0.0676	HOMO → LUMO	89.21
		HOMO →	
		LUMO+2	8.97
		HOMO-1 →	
326.12	0.0009	LUMO	93.11
		HOMO →	
		LUMO+1	5.16
		HOMO-1 →	
314.95	0.0052	LUMO	87.02
		HOMO-1 →	
		LUMO+2	5.15
		HOMO →	
		LUMO+1	3.06
		HOMO →	
		LUMO+2	2.13
		HOMO-1 →	
308.52	0.0700	LUMO	84.73
		HOMO-1 →	
		LUMO+1	7.80
		HOMO → LUMO	2.62
		HOMO →	
		LUMO+2	2.36
		HOMO-1 →	
283.96	0.0346	LUMO+1	91.15
		HOMO →	
		LUMO+2	3.00
		HOMO →	
		LUMO+3	2.20
		HOMO-1 →	
274.81	0.0061	LUMO	89.98
		HOMO-1 →	
		LUMO+2	2.60
		HOMO →	
		LUMO+3	2.11
		HOMO-2 →	
272.50	0.0284	LUMO	96.25
		HOMO-1 →	
264.68	0.0213	LUMO+3	69.03
		HOMO →	
		LUMO+4	15.25
		HOMO-1 →	
		LUMO+1	5.99
		HOMO-1 →	
		LUMO+4	3.20
		HOMO →	
		LUMO+3	2.32
252.30	0.0009	HOMO-2 →	90.76

		LUMO+1	
		HOMO-4 →	
		LUMO	2.83
		HOMO-3 →	
		LUMO	2.52
		HOMO →	
250.39	0.0205	LUMO+3	57.49
		HOMO →	
		LUMO+4	23.91
		HOMO-2 →	
		LUMO+1	8.22
		HOMO-1 →	
		LUMO+3	6.72
		HOMO →	
239.29	0.0458	LUMO+4	68.61
		HOMO-3 →	
		LUMO	12.71
		HOMO-1 →	
		LUMO+3	6.02
		HOMO →	
		LUMO+3	2.95
		HOMO-2 →	
		LUMO+1	2.27
		HOMO-4 →	
237.95	0.0094	LUMO	57.52
		HOMO-2 →	
		LUMO+2	36.55
		HOMO-4 →	
230.28	0.1775	LUMO	40.71
		HOMO-3 →	
		LUMO+1	22.28
		HOMO-2 →	
		LUMO+2	16.83
		HOMO-1 →	
		LUMO+3	5.75
		HOMO-1 →	
		LUMO+4	4.62
		HOMO →	
		LUMO+4	2.27
		HOMO-5 →	
226.79	0.1671	LUMO	42.29
		HOMO →	
		LUMO+4	36.7
		HOMO-3 →	
		LUMO+1	8.06
		HOMO-1 →	
		LUMO+3	3.9
		HOMO-5 →	
225.26	0.1936	LUMO	45.54
		HOMO-3 →	
		LUMO+1	20.91

		HOMO-1 →	
		LUMO+3	17.26
		HOMO-1 →	
		LUMO+4	3.74
		HOMO →	
		LUMO+4	2.83
		HOMO-3 →	
223.04	0.2100	LUMO+2	61.5
		HOMO-3 →	
		LUMO+1	9.42
		HOMO-5 →	
		LUMO	6.66
		HOMO-1 →	
		LUMO+3	6.37
		HOMO →	
		LUMO+3	4.01
		HOMO-1 →	
		LUMO+4	2.26
		HOMO →	
221.11	0.0245	LUMO+5	92.16
		HOMO-3 →	
217.21	0.0392	LUMO+1	57.15
		HOMO-4 →	
		LUMO	19.34
		HOMO-4 →	
		LUMO+2	3.93
		HOMO-4 →	
		LUMO+1	3.77
		HOMO-2 →	
		LUMO+2	3.54
		HOMO-1 →	
		LUMO+3	2.20
		HOMO-5 →	
216.42	0.0165	LUMO	82.39
		HOMO-4 →	
		LUMO+1	6.98
		HOMO-3 →	
		LUMO+2	2.18
		HOMO-3 →	
214.89	0.0892	LUMO+1	30.46
		HOMO-2 →	
		LUMO+2	18.55
		HOMO-4 →	
		LUMO+2	14.20
		HOMO-3 →	
		LUMO+2	8.83
		HOMO-4 →	
		LUMO+1	8.30
		HOMO-4 →	
		LUMO	4.60
		HOMO-1 →	2.58

		LUMO+4	
		HOMO →	
211.67	0.0189	LUMO+7	60.82
		HOMO →	
		LUMO+6	8.49
		HOMO →	
		LUMO+8	8.48
		HOMO-1 →	
		LUMO+4	6.59
		HOMO-4 →	
		LUMO+2	2.81
		HOMO-6 →	
208.92	0.0605	LUMO	64.21
		HOMO-2 →	
		LUMO+2	12.59
		HOMO-4 →	
		LUMO+2	3.48
		HOMO-3 →	
		LUMO+1	3.26
		HOMO-4 →	
		LUMO	2.57
		HOMO →	
		LUMO+7	2.52
		HOMO →	
		LUMO+6	2.34
		HOMO-6 →	
206.16	0.0660	LUMO	89.20
		HOMO-5 →	
		LUMO+1	3.56
		HOMO-2 →	
204.06	0.0046	LUMO+3	75.69
		HOMO →	
		LUMO+7	5.70
		HOMO →	
		LUMO+8	4.95
		HOMO-1 →	
		LUMO+5	3.21
		HOMO-5 →	
		LUMO+2	2.91
		HOMO-1 →	
203.29	0.0158	LUMO+5	89.38
		HOMO-5 →	
		LUMO+2	3.23
		HOMO-2 →	
		LUMO+3	2.25
		HOMO-1 →	
202.30	0.0012	LUMO+5	57.53
		HOMO-5 →	
		LUMO+2	19.25
		HOMO →	
		LUMO+8	5.29

		HOMO →	
		LUMO+10	3.02
		HOMO-6 →	
		LUMO	2.82
		HOMO-7 →	
		LUMO	2.52
200.95	0.0053	HOMO →	
		LUMO+6	75.02
		HOMO →	
		LUMO+7	16.03
		HOMO →	
		LUMO+8	2.31

Figure S9 a).

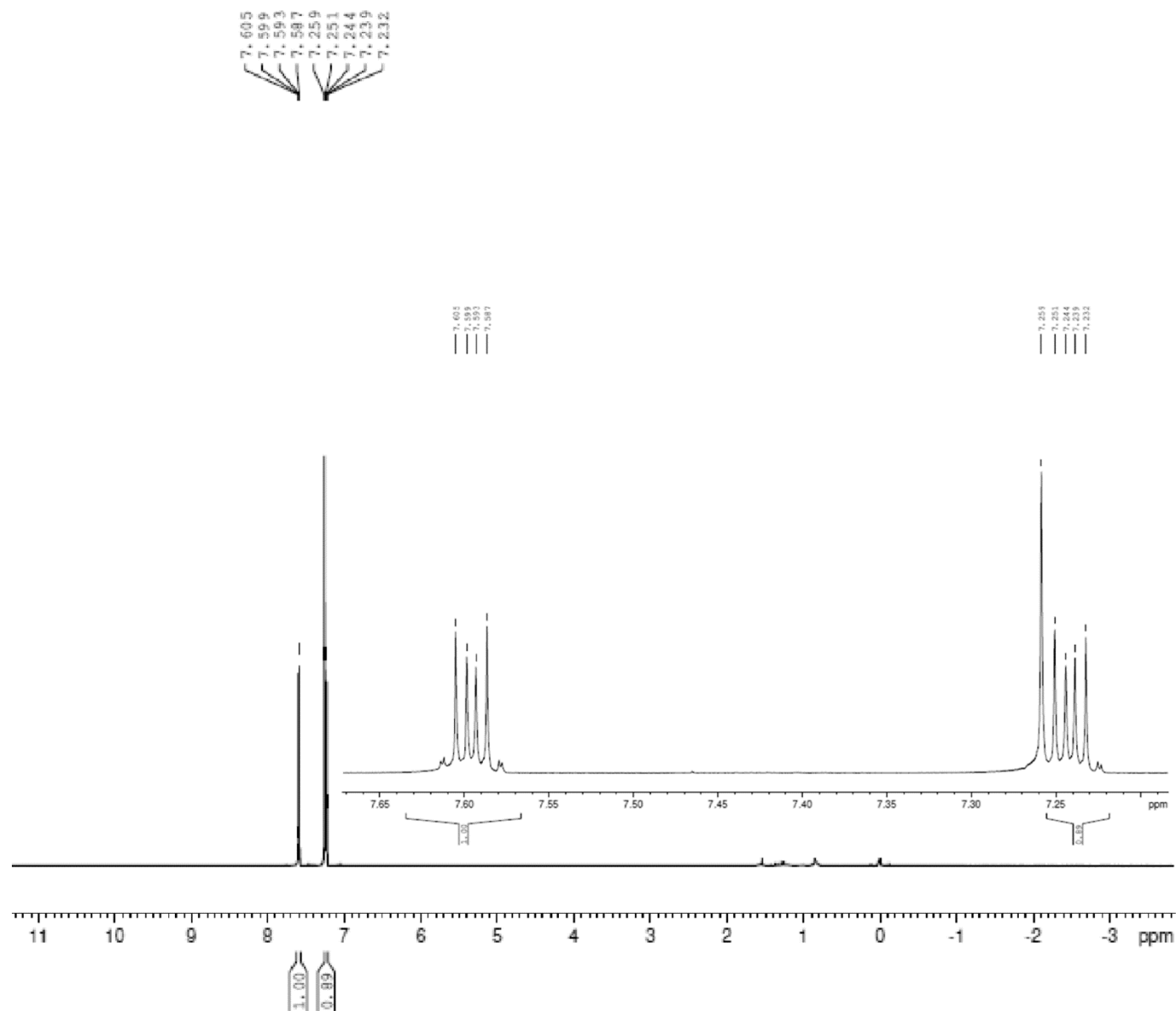
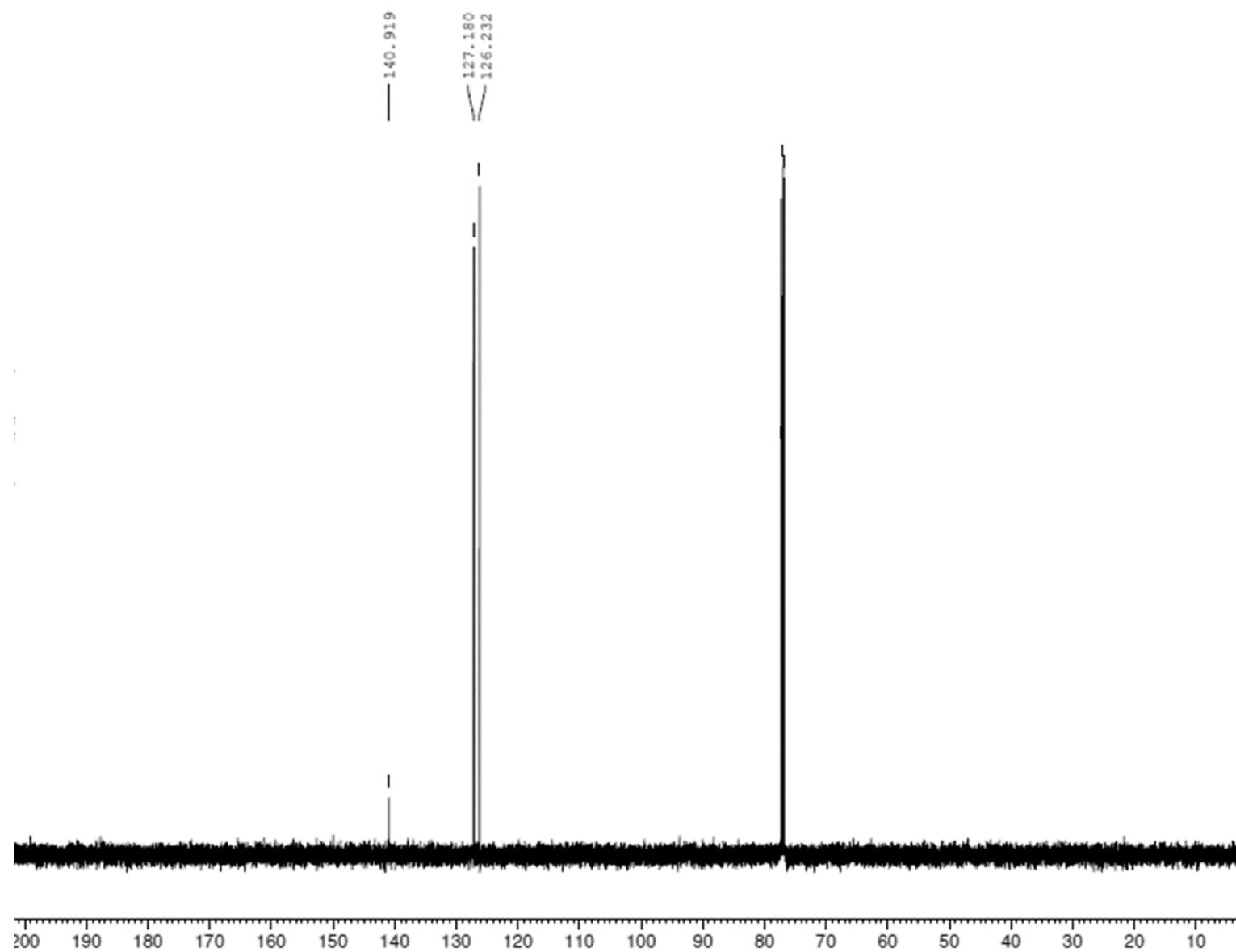


Figure S9 b).



1.00 1.20

Figure S10 b).

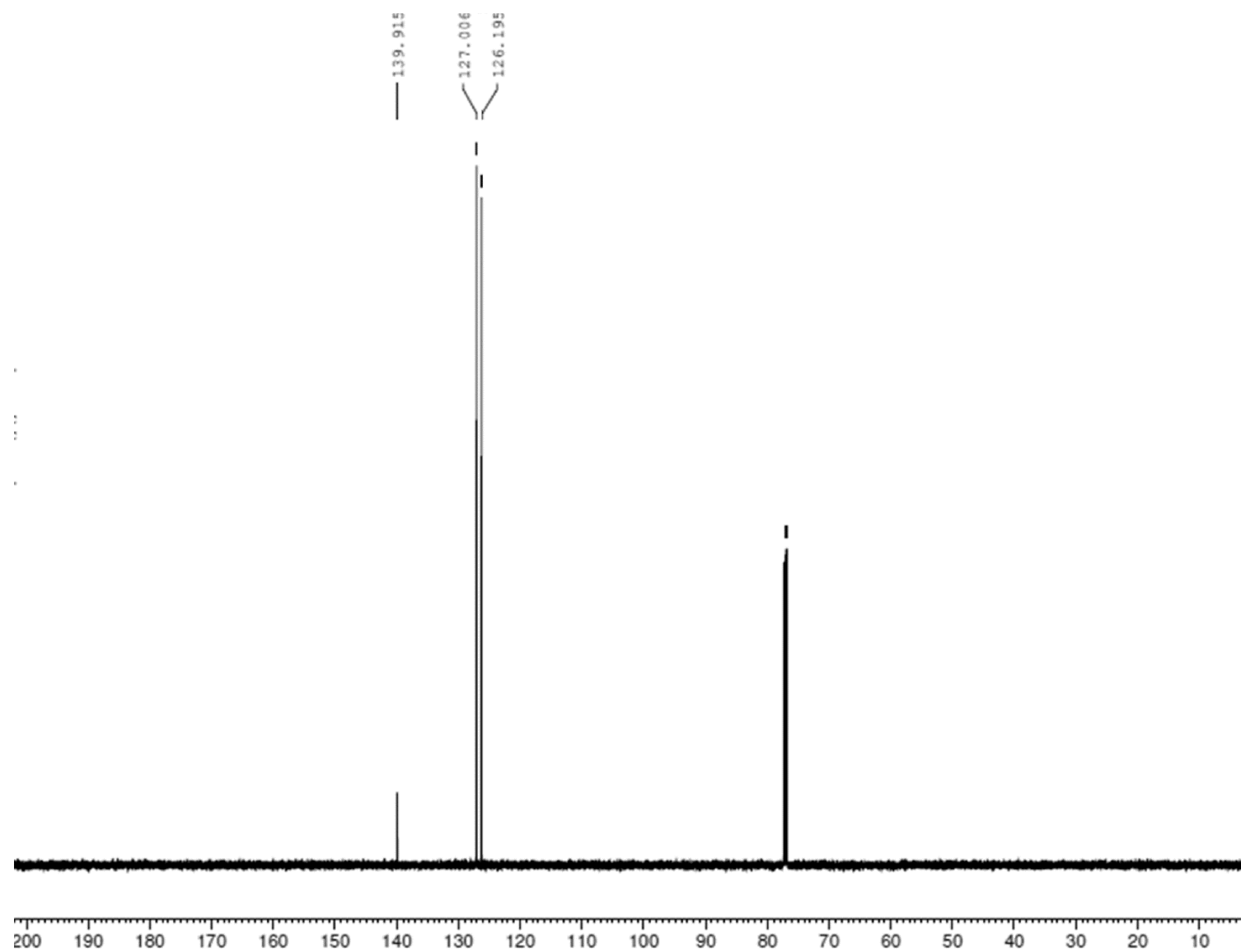


Figure S11 a).

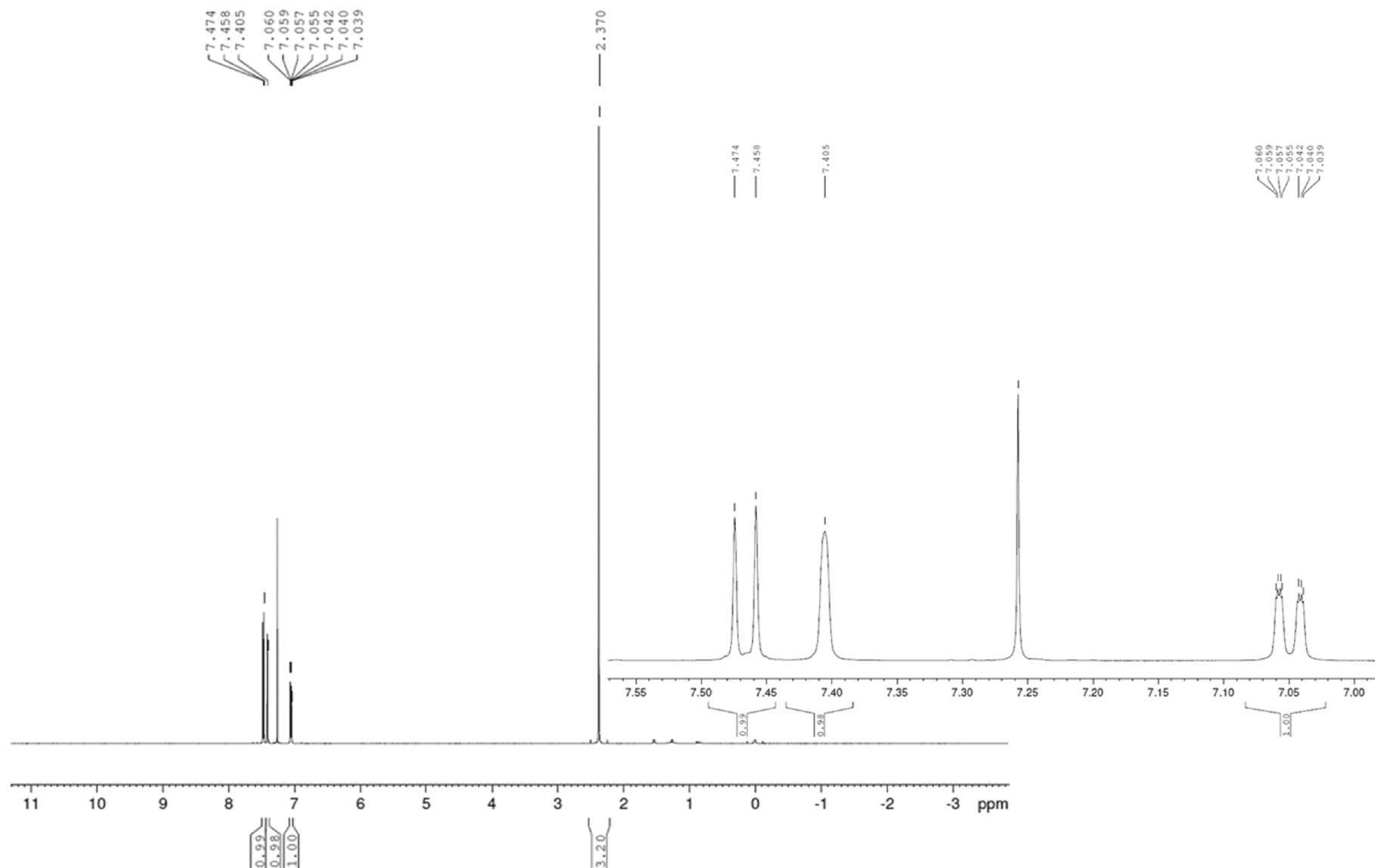


Figure S11 b).

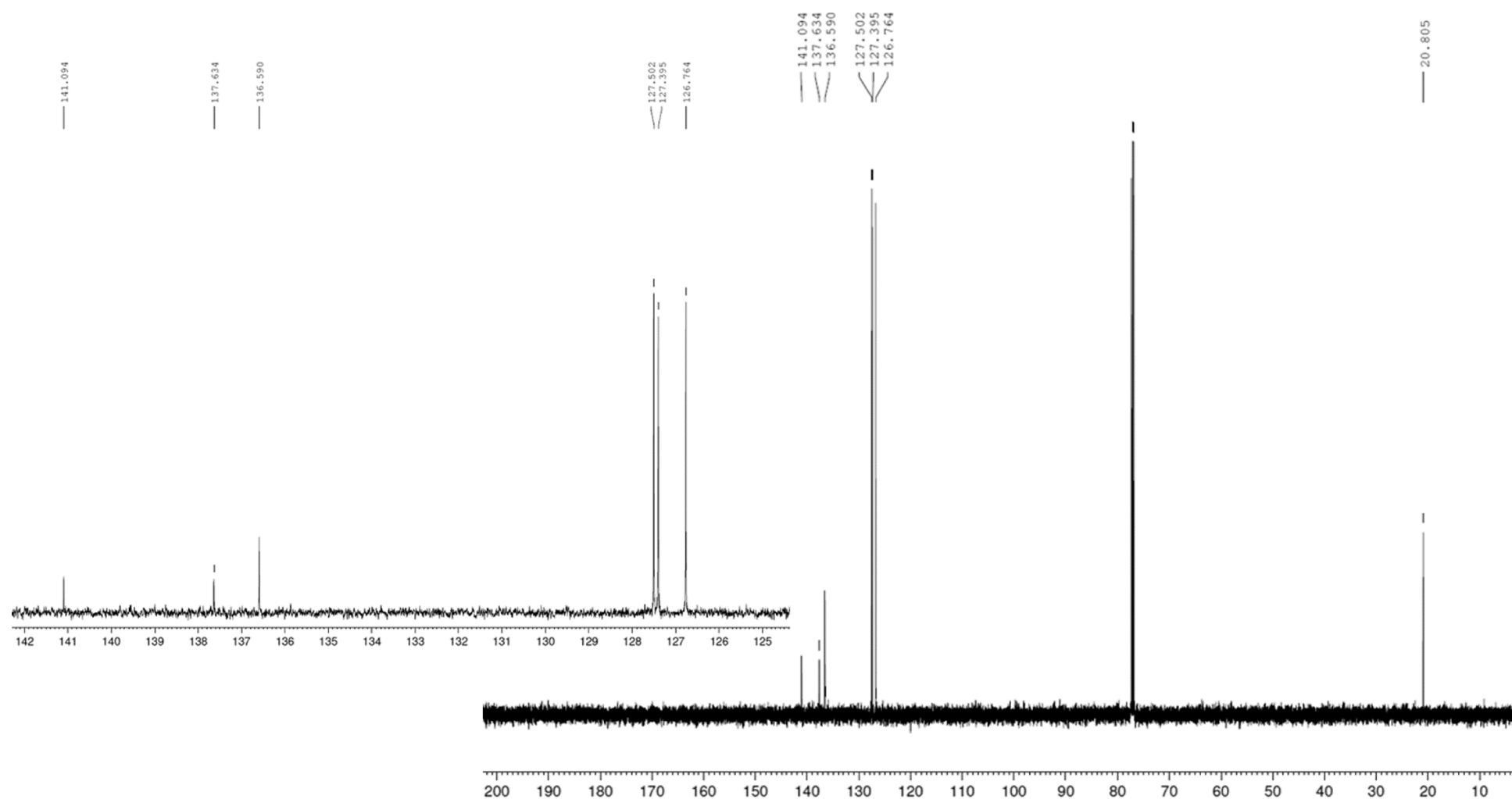


Figure S12 a).

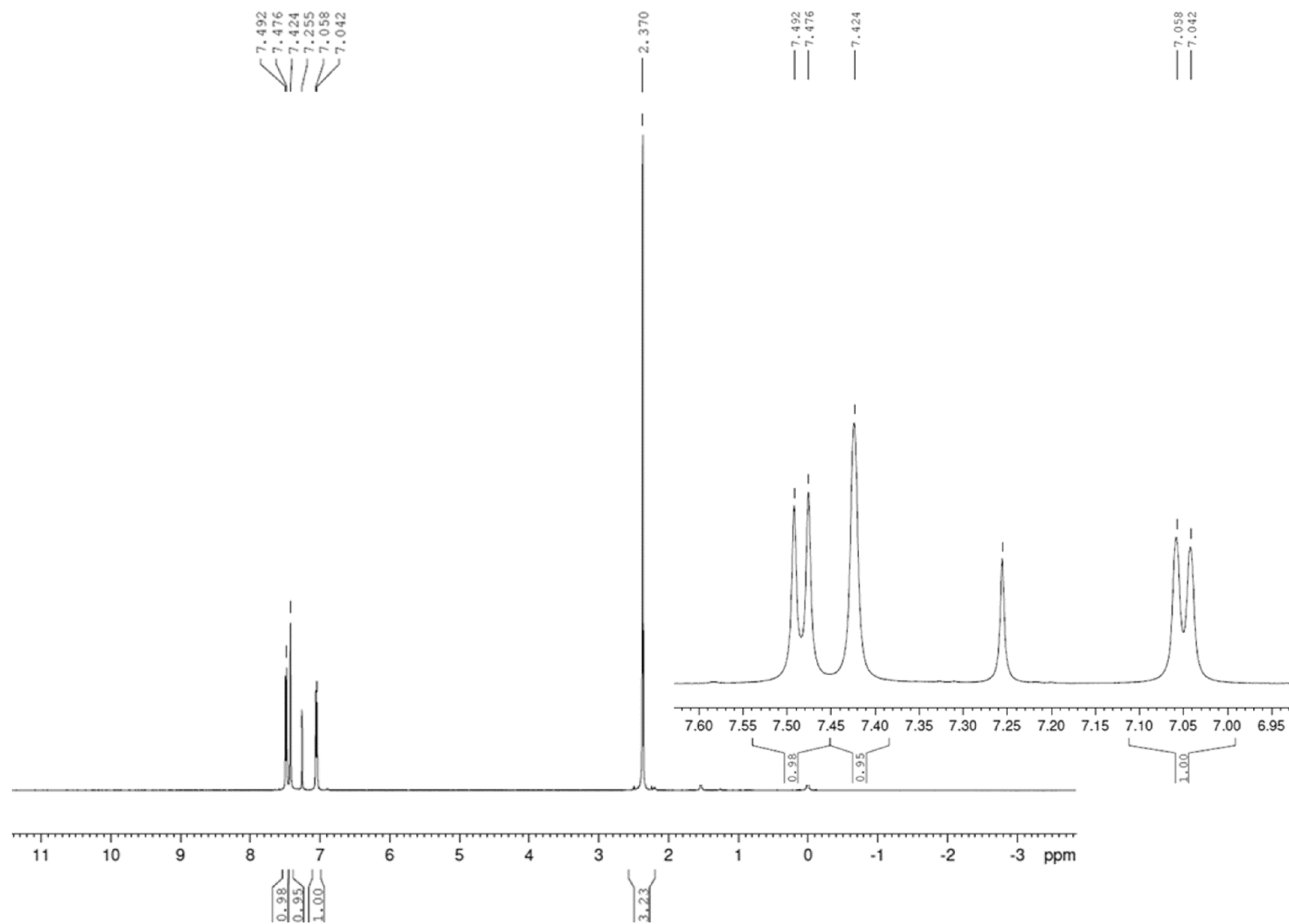


Figure S12 b).

