

**Trapped-molecule charge-transfer complexes with huge dipoles:
M-C₂F₆-X (M = Na to Cs, X = Cl to I)**

Fedor Y. Naumkin

Supplement

Table 4 (full) Vibrational frequencies and IR intensities (in cm⁻¹ and D²/Å²) of M-C₂F₆-X

System	ν	I
C ₂ F ₆	73.839	0.000
	212.751	0.059
	212.751	0.059
	348.029	0.000
	371.680	0.000
	371.680	0.000
	503.886	0.095
	503.886	0.095
	606.198	0.000
	606.198	0.000
	692.925	0.791
	789.143	0.000
	1101.694	6.403
	1212.148	0.000
	1212.148	0.000
	1236.800	12.764
1236.800	12.764	
1457.071	0.000	
Na-C ₂ F ₆ -Cl	29.094	0.069
	29.094	0.069
	72.321	0.000
	79.899	0.175
	79.899	0.175
	120.487	1.488
	199.982	0.699
	228.618	0.052
	228.618	0.052
	355.719	0.233
	372.546	0.027
	372.546	0.027
	499.770	0.096
	499.770	0.096
	599.079	0.025
	599.079	0.025
	685.070	1.821
	777.138	0.484
1072.194	8.774	
1135.199	4.614	
1135.199	4.614	
1282.038	6.164	
1282.038	6.164	
1416.920	0.000	
K-C ₂ F ₆ -Cl	24.192	0.005
	26.199	0.003
	74.978	0.133
	75.729	0.135
	76.052	0.002
	101.492	1.621
139.122	0.000	

	229.073 0.049
	229.637 0.050
	353.823 0.125
	373.123 0.022
	373.263 0.022
	498.764 0.080
	498.781 0.080
	600.908 0.025
	600.977 0.025
	681.696 1.629
	777.367 0.410
	1076.449 8.763
	1148.915 4.552
	1150.599 4.533
	1276.276 6.351
	1276.406 6.356
	1423.455 0.001
Rb-C ₂ F ₆ -Cl	22.008 0.028
	22.008 0.028
	74.216 0.102
	74.216 0.102
	77.233 0.006
	77.785 0.932
	126.003 0.248
	229.451 0.047
	229.451 0.047
	353.584 0.108
	373.191 0.020
	373.191 0.020
	498.321 0.076
	498.321 0.076
	601.237 0.023
	601.237 0.023
	681.112 1.636
	777.817 0.380
	1076.639 8.862
	1153.589 4.426
	1153.589 4.426
	1274.551 6.412
	1274.551 6.412
	1424.373 0.000
Cs-C ₂ F ₆ -Cl	19.790 0.065
	19.790 0.065
	65.188 0.679
	72.381 0.095
	72.381 0.095
	77.600 0.000
	123.534 0.379
	230.440 0.050
	230.440 0.050
	353.479 0.111
	373.642 0.018
	373.642 0.018
	498.126 0.072
	498.126 0.072
	601.682 0.022
	601.682 0.022
	680.696 1.660
	778.373 0.351
	1077.936 9.032
	1157.156 4.295
	1157.156 4.295

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
 This journal is © The Owner Societies 2008

	1273.416 6.457
	1273.416 6.457
	1425.963 0.000
Cs-C ₂ F ₆ -Br	15.802 0.005
	15.802 0.005
	52.851 0.582
	62.439 0.017
	62.439 0.017
	78.971 0.000
	94.958 0.025
	228.502 0.060
	228.502 0.060
	353.876 0.064
	373.350 0.021
	373.350 0.021
	498.325 0.072
	498.325 0.072
	601.903 0.021
	601.903 0.021
	680.613 1.832
	779.020 0.360
	1079.187 9.430
	1159.452 4.264
	1159.452 4.264
	1272.880 6.378
	1272.880 6.378
	1429.240 0.001
Cs-C ₂ F ₆ -I	14.524 0.000
	14.524 0.000
	47.906 0.461
	56.263 0.005
	56.263 0.005
	76.428 0.000
	88.402 0.006
	226.177 0.062
	226.177 0.062
	352.365 0.045
	372.999 0.020
	372.999 0.020
	499.026 0.068
	499.026 0.068
	602.642 0.018
	602.642 0.018
	682.014 1.910
	780.290 0.360
	1081.603 9.940
	1162.645 4.232
	1162.645 4.232
	1270.066 5.953
	1270.066 5.953
	1433.884 0.003