Supporting Information for

Dipolar Molecules inside C_{70}; Electric Field-Driven Room-Temperature Single-Molecule Switch

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Table S1. Encapsulation energies for conformers **a** and **b** shown in Figure 3 in the absence of an external electric field in kcal/mol.

MX	LiF	LiCl	NaF	NaCl
Conformer (a)	-33.6	-38.6	-35.9	-29.3
Conformer (b)	-33.8	-39.0	-36.4	-29.4

Table S2

Table S1. Relative energies of the low-energy minima **c**, **d** and corresponding transition states for turning the MX@C_{70}, with respect to the high-energy minima **a** and **b** in kcal/mol. The differences ΔE_{ac} and ΔE_{bd} are defined as $E_a - E_c$ and $E_b - E_d$. Field strength is presented in au and energies in kcal/mol.

LiCl@C_{70}				
EF	ΔE_{ac}	TS_{ac}	ΔE_{bd}	TS_{bd}
0.000	0.4	10.4	-0.4	10.0
0.002	-1.3	9.2	-2.1	9.5
0.004	-3.0	8.2	-3.8	8.9
0.006	-4.7	7.1	-5.4	8.5
0.008	-6.4	6.1	-7.0	8.1
0.010	-8.1	5.1	-8.5	7.7
0.012	-9.8	4.1	-9.9	7.3
0.014	-11.3	3.2	-11.2	7.0

NaF@C_{70}				
EF	ΔE_{ac}	ΔE_{ac}	ΔE_{ac}	ΔE_{ac}
0.000	-0.5	12.5	0.5	13.0
0.002	-2.4	11.3	-1.4	12.4
0.004	-4.3	10.1	-3.2	11.8
0.006	-6.2	9.0	-5.0	11.2
0.008	-8.0	8.0	-6.7	10.7
0.010	-9.9	7.0	-8.3	10.2
0.012	-11.7	6.1	-9.9	9.8
0.014	-13.4	5.3	-11.3	9.5

NaCl@C_{70}				
EF	ΔE_{ac}	ΔE_{ac}	ΔE_{ac}	ΔE_{ac}
0.000	0.1	28.7	-0.1	28.6
0.002	-2.0	28.0	-2.1	27.3
0.004	-4.1	27.5	-4.1	26.0
0.006	-6.2	27.0	-6.1	24.7
0.008	-8.2	26.5	-8.0	23.6
0.010	-10.3	26.0	-9.9	22.5
0.012	-12.3	25.6	-11.6	21.5
0.014	-14.2	25.1	-13.2	20.7

Table S3. Dipole moments, μ, for conformers a and b, presented in Figure 3 of the manuscript.

MX	LiF	LiCl	NaF	NaCl
Conformer (a)	6.18	6.57	6.63	6.87
Conformer (b)	3.49	3.50	3.19	3.23

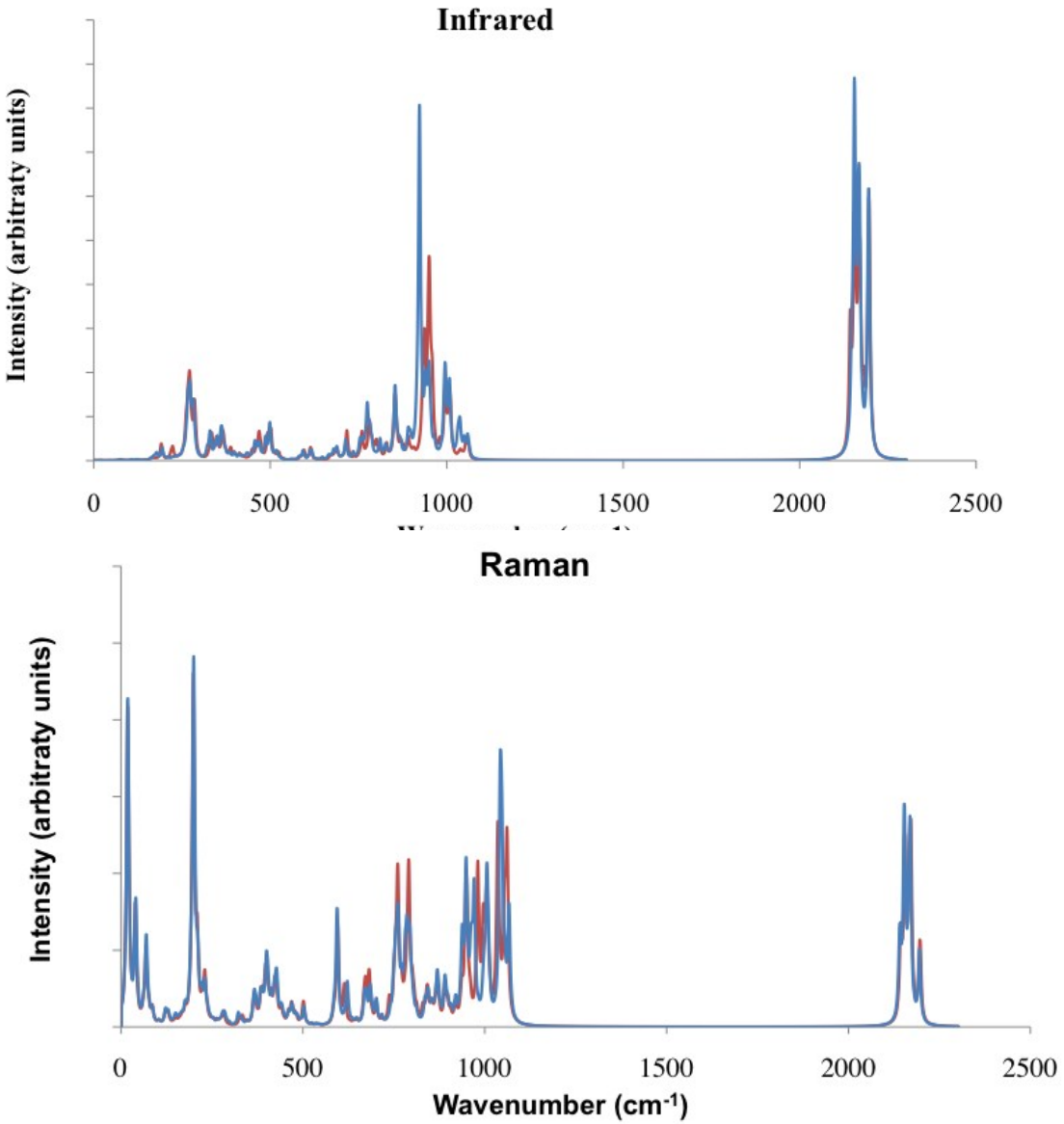

Figure S4. Comparison of calculated infrared (top) and Raman (bottom) spectra of conformers **a(d)** and **b(c)** of NaF@**1** (Figure 3) with the EEF set to zero.

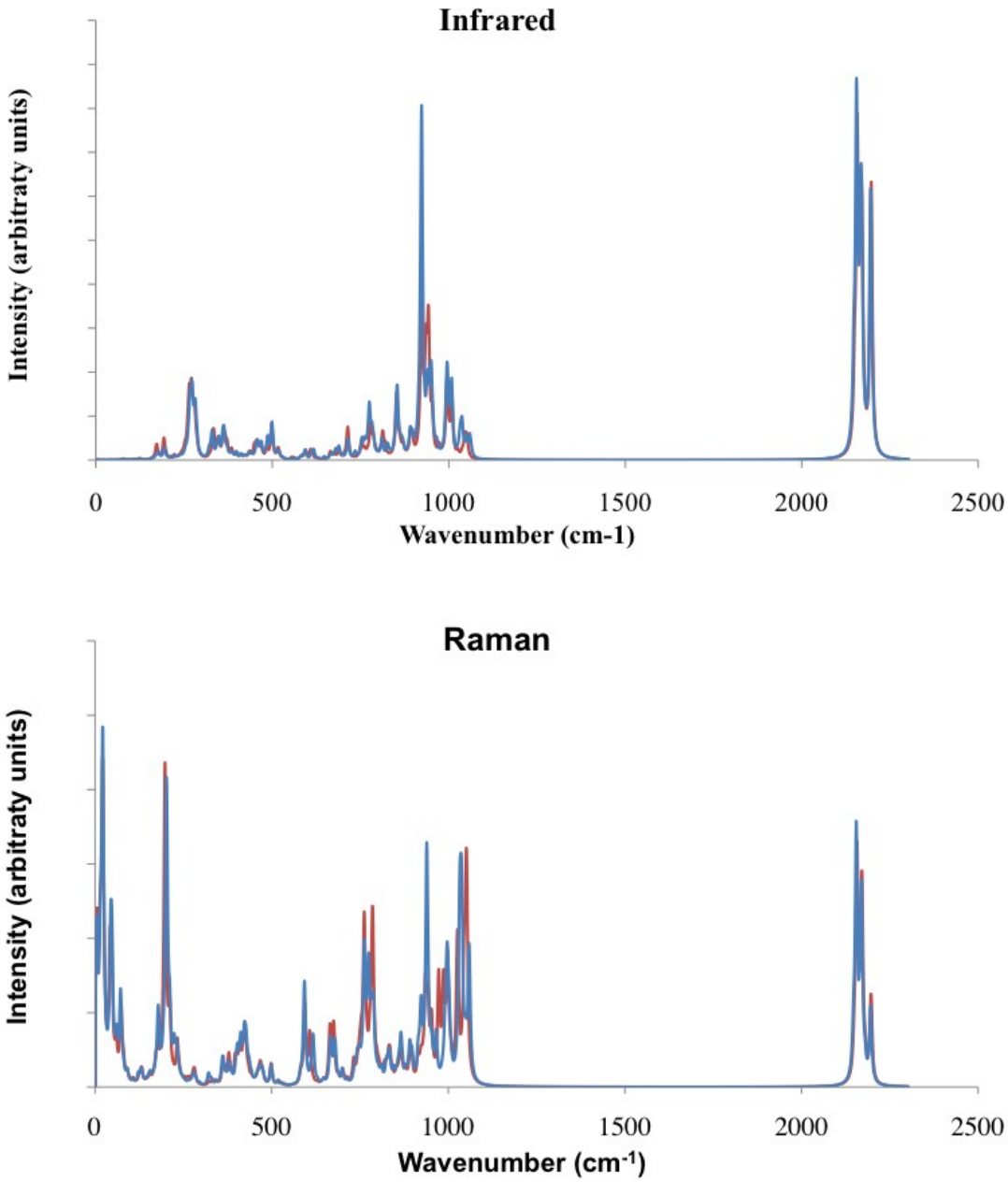

Figure S5. Comparison of calculated infrared (top) and Raman (bottom) spectra of conformers **a(d)** and **b(c)** of NaCl@**1** (Figure 3) with the EEF set to zero.