

Supporting information

**Sterically Crowded Azulene-Based Dication Salts as Novel Guests; Synthesis  
and Complexation Studies with Crown Ethers and Calixarenes in Solution and  
in the Gas Phase**

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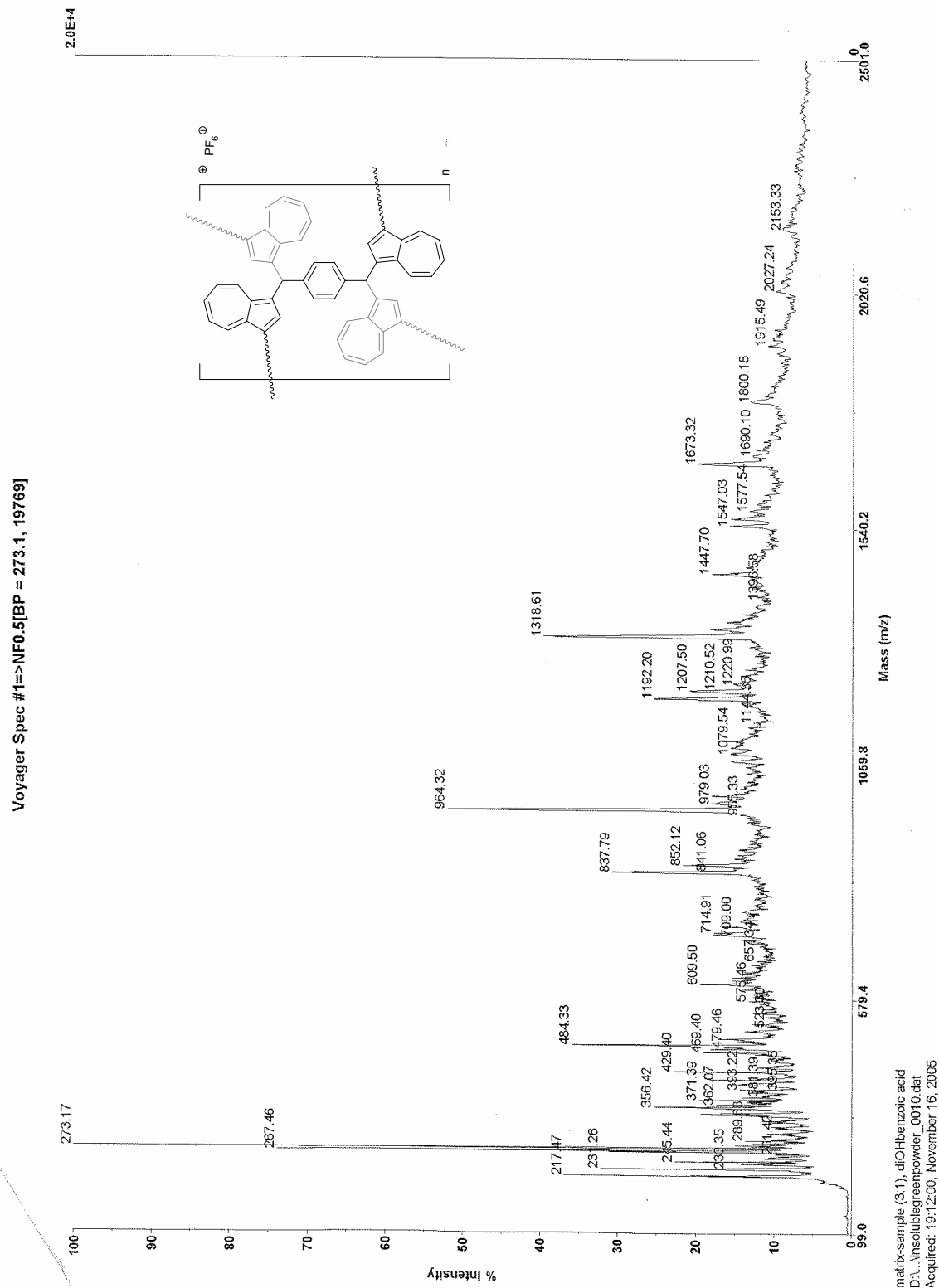
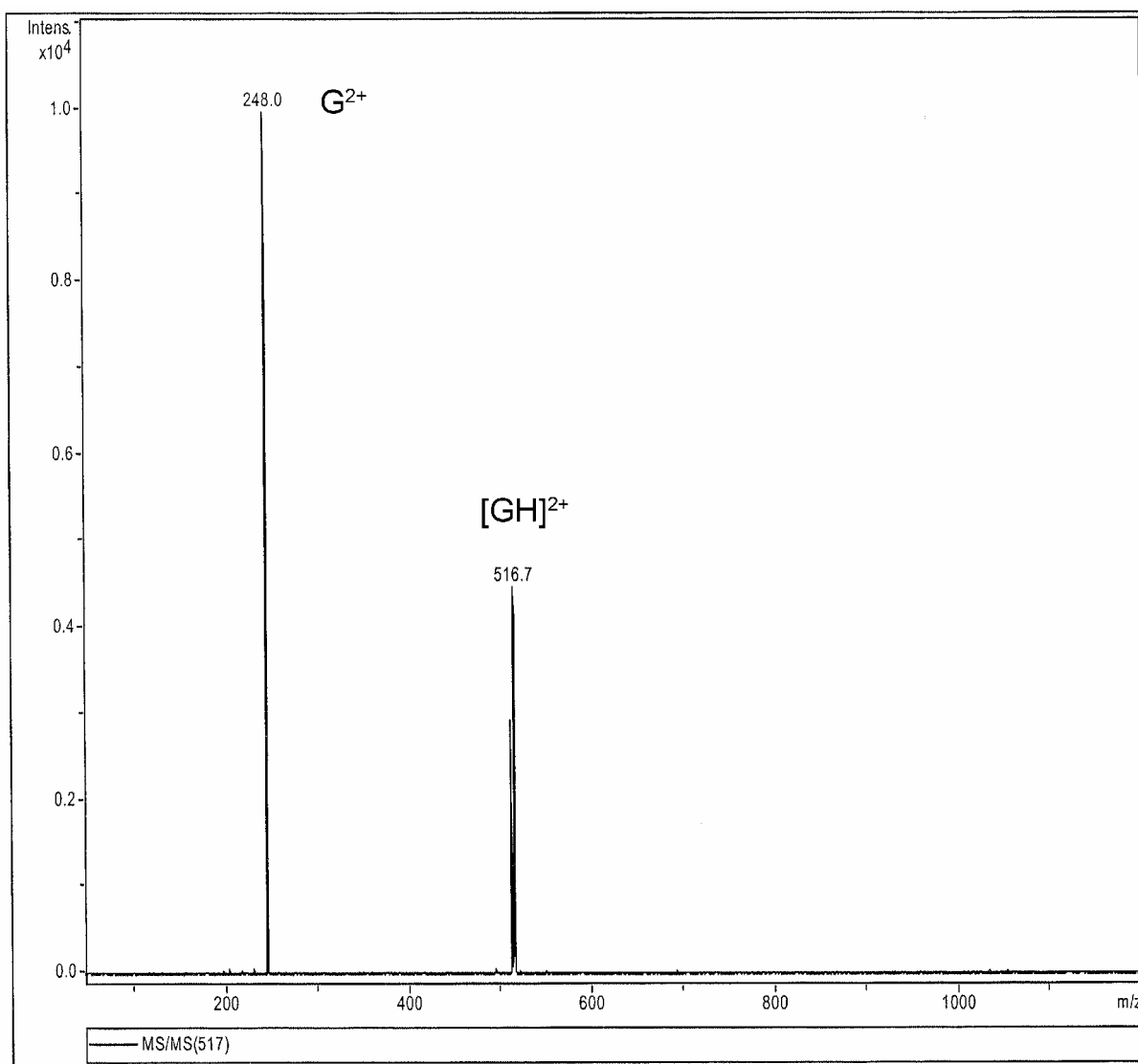
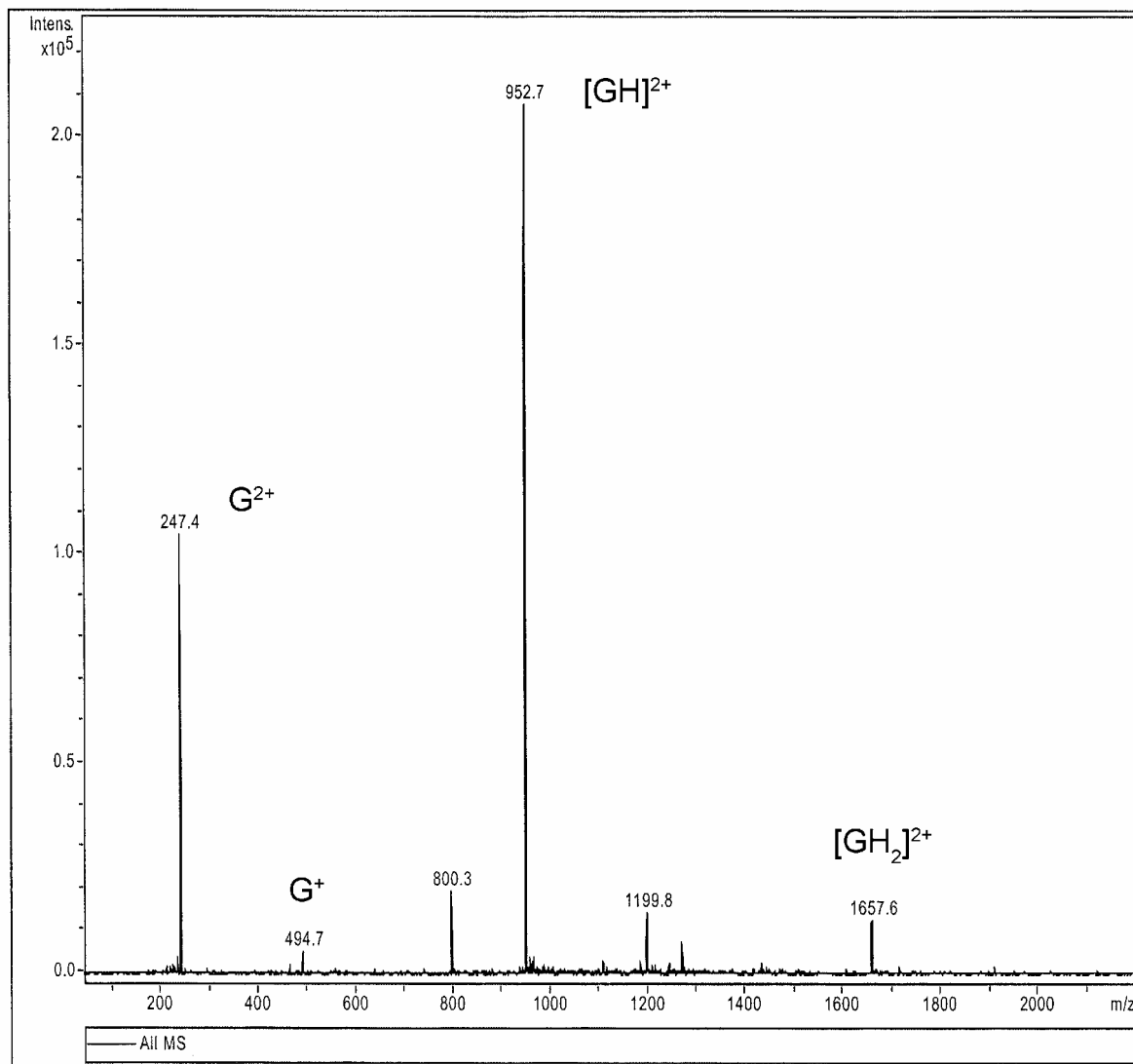


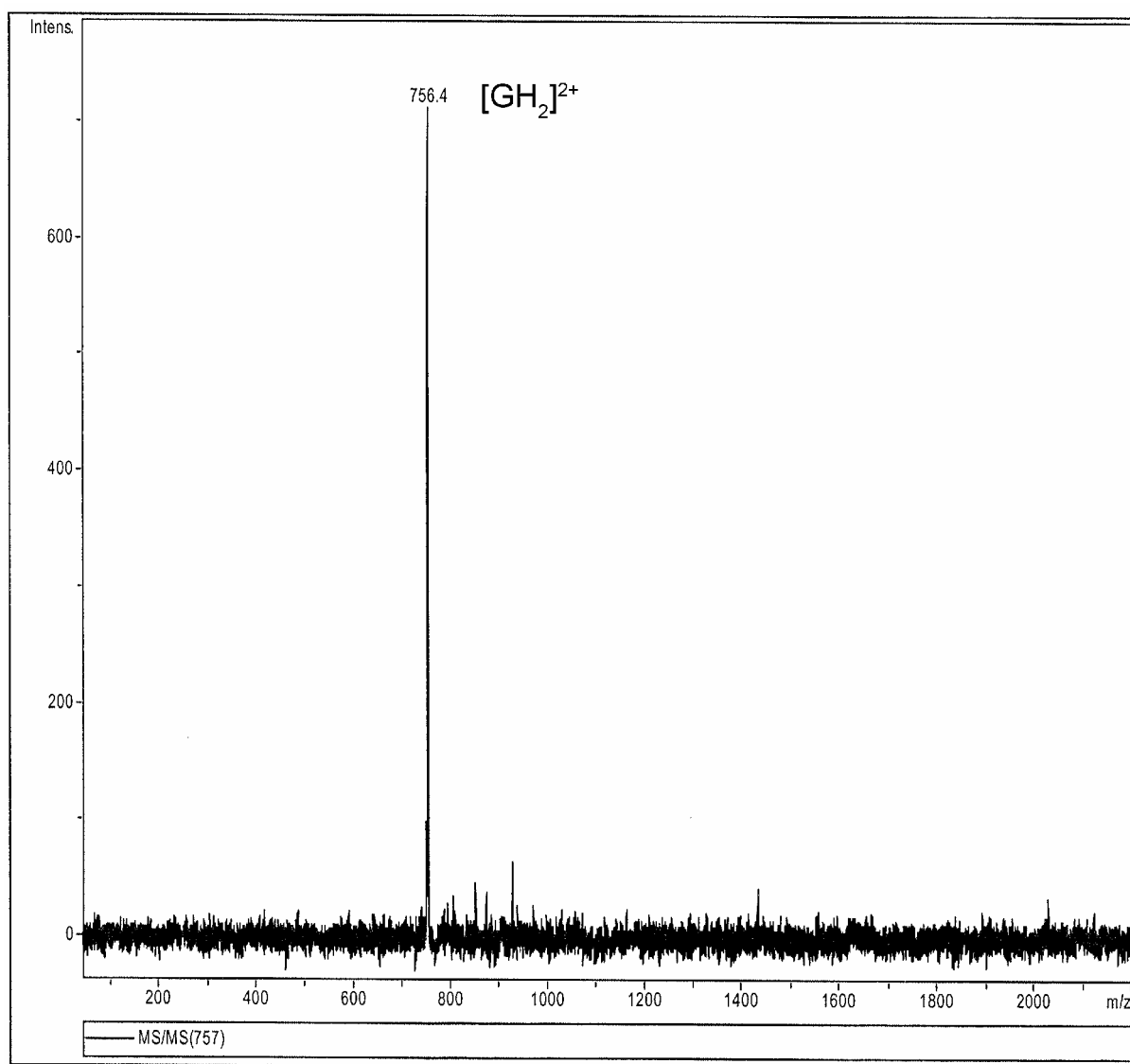
Fig. S1. MALDI-TOF-MS of oligomeric green powder via attempted dication salt synthesis with parent azulene



**Fig. S2.** Electrospray MS/MS spectrum of 1/DB30C10. 1:1 complex .



**Fig. S3.** ES-MS spectrum of 1/*p*-*t*Bu-methoxycalix[8]arene showing [GH]<sup>2+</sup> and [GH<sub>2</sub>]<sup>2+</sup> cation/molecule clusters



**Fig. S4.** ES-MS detection of the 1:2 complex between **2** and DB30C10

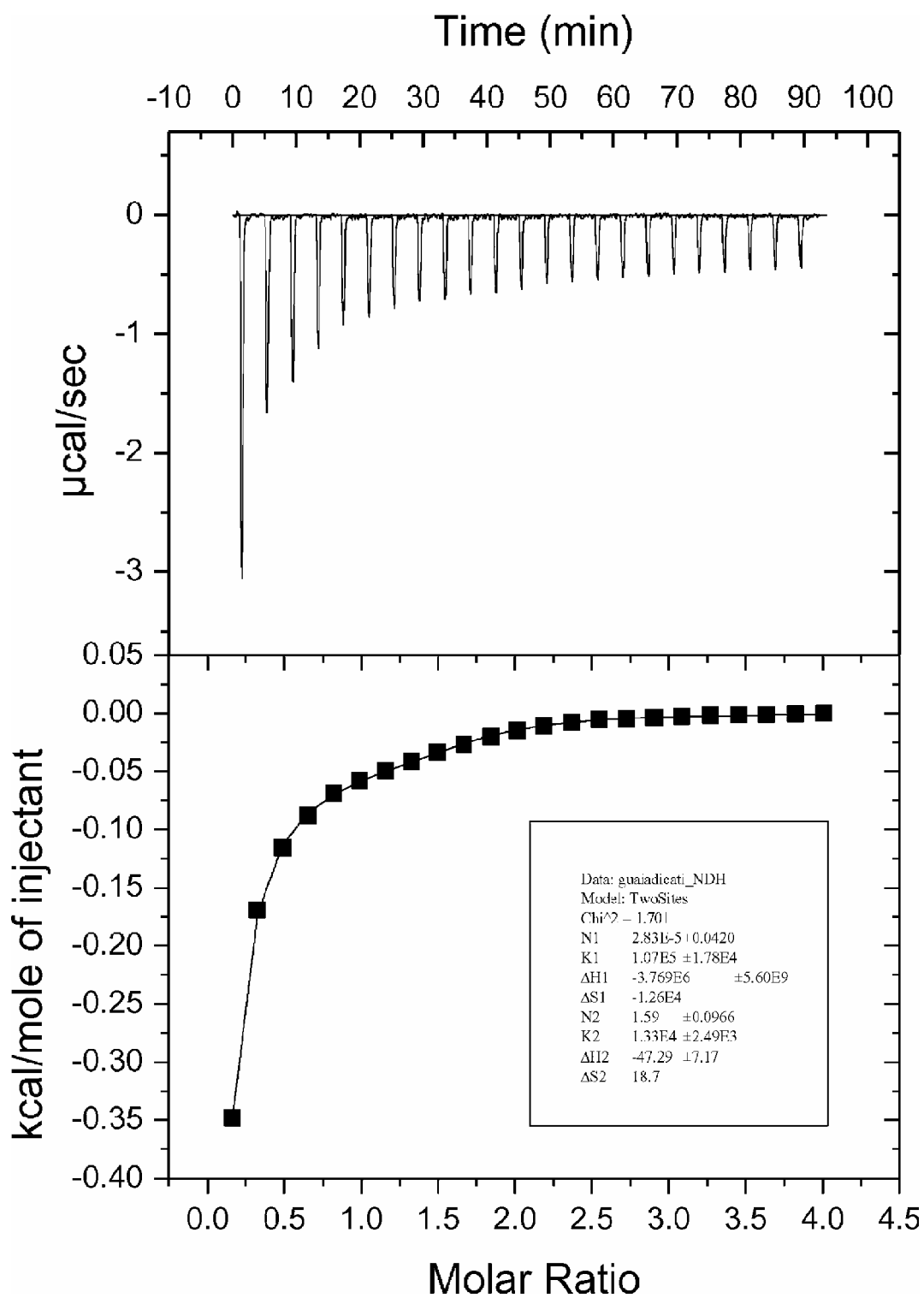


Fig. S5: Enlarged version of Fig. 7

**Table S1:** Binding constant and thermodynamic parameters

Number of complexation sites (n)	$\log K$	$\Delta H$ (kJ.mol <sup>-1</sup> )	$T\Delta S$ (kJ.mol <sup>-1</sup> )	$\Delta G$ (kJ.mol <sup>-1</sup> )
$n_1 = 0.00 \pm 0.04$	$5.0 \pm 0.4$	nt	nt.	nt
$n_2 = 1.6 \pm 0.1$	$4.1 \pm 0.3$	$-0.20 \pm 0.03$	23.29	-23.49

nt: not reported due to uncertainty in accuracy