

Table 1: Charge distributions of MG molecule in two different environments**Partial charges of MG in different environments**

	Atom Index	Atom Type	MG-Alone	MG-RNA Field
Ring A	7	C	-0.279	-0.504
	8	C	0.326	0.573
	9	C	-0.269	-0.419
	10	C	0.009	0.054
	11	C	0.036	-0.146
	12	C	0.017	0.152
	25	H	0.157	0.208
	26	H	0.157	0.219
	27	H	0.050	0.128
	28	H	0.052	0.035
	39	N	-0.176	-0.326
	40	C	-0.026	0.096
	41	H	0.090	-0.048
	42	H	0.050	0.074
	43	H	0.050	0.052
	44	C	-0.039	-0.138
	45	H	0.095	0.168
	46	H	0.052	0.273
	47	H	0.055	-0.074
Ring B	13	C	-0.278	-0.501
	14	C	0.017	0.115
	15	C	0.037	-0.120
	16	C	0.008	0.108
	17	C	-0.268	-0.467
	18	C	0.326	0.564
	29	H	0.157	0.197
	30	H	0.052	0.060
	31	H	0.051	0.027
	32	H	0.157	0.199
	33	N	-0.176	-0.434
	34	C	-0.024	0.061
	35	H	0.089	-0.049
	36	H	0.050	0.104
	37	H	0.050	0.074
	38	C	-0.039	0.071
	48	H	0.095	0.069
	49	H	0.052	0.151
	50	H	0.055	-0.073
Ring C	1	C	0.129	0.065
	2	C	-0.052	-0.052
	3	C	-0.110	-0.162
	4	C	-0.042	0.052

	5	C	-0.111	-0.164
	6	C	-0.051	-0.076
	20	H	0.054	0.107
	21	H	0.123	0.155
	22	H	0.106	0.149
	23	H	0.123	0.153
	24	H	0.053	0.108
Center				
C+	19	C	-0.036	0.133

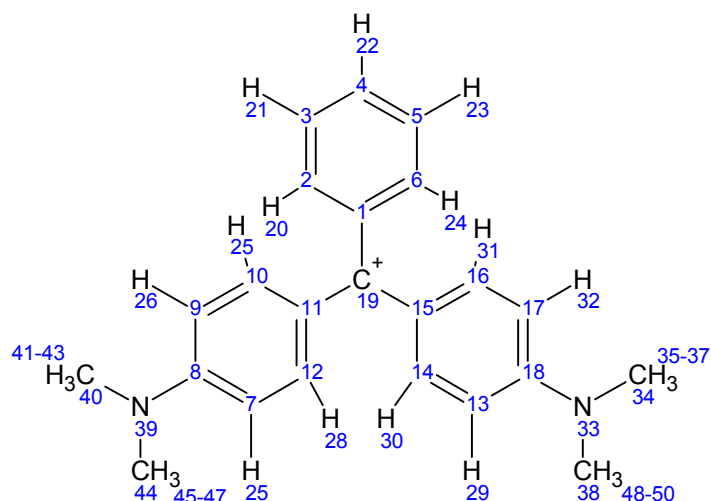


Table 2: Calculated and experimental absorption wavelengths for MG

	Absorption Wavelength (nm)	
	Computed	Experiment
MG (free)	376	616
MG in RNA	379	630
Difference	3	14

Figure SF1. Optimized Valence Angles and Bond Distances for MG in Vacuum.

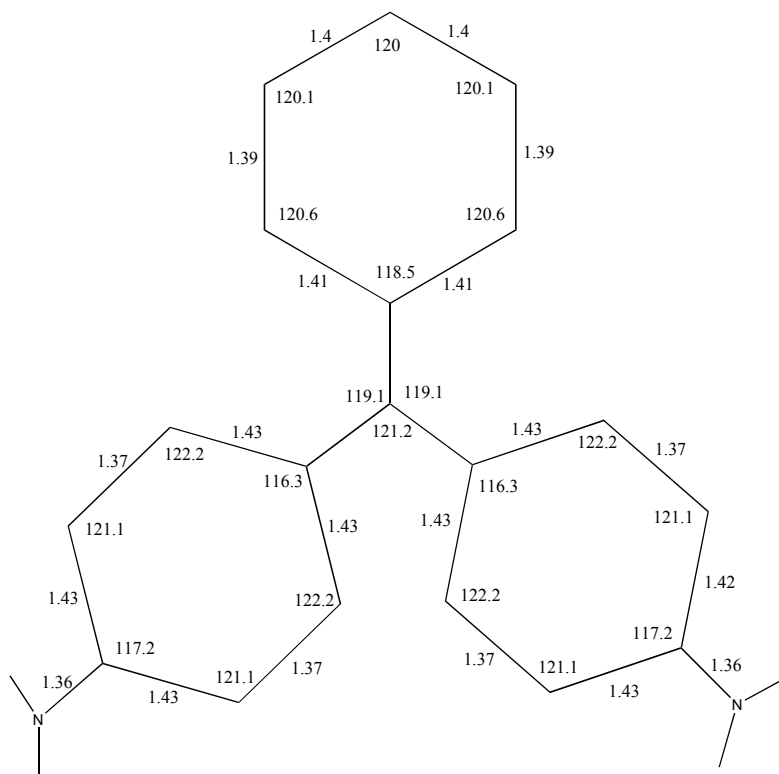


Figure SF2. Optimized Valence Angles and Bond Distances for MG in RNA Charge Field.

