

Supplementary Materials:

Modeling of Carbonyl/Ammonium Sulfate Aqueous Brown Carbon Chemistry via UV/Vis Spectral Decomposition

Mengjie Fan ^{1,2}, Shiqing Ma ¹, Nahin Ferdousi ¹, Ziwei Dai ^{1,3}, and Joseph L. Woo ^{1,*}

¹ Department of Chemical and Biomolecular Engineering, Lafayette College, Easton, PA 18042, USA; fanmj@seas.upenn.edu (M.F.); mas@lafayette.edu (S.M.); ferdousn19@gmail.com (N.F.); zdai2@nd.edu (Z.D.)

² Now Located: Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA.

³ Now Located: Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556, USA.

* Correspondence: wooj@lafayette.edu; Tel.: +1-610-330-3291

Table S1. Normalized Root Mean Square Deviation (NRMSD) values for simulations performed at varying times, numbers of Gaussian lineshapes, and CVOC/AS reaction systems.

Time (hrs)	G			GA			MG		
	Double	Triple	Quad	Double	Triple	Quad	Double	Triple	Quad
0	0.0189	0.0100	0.0091	0.0436	0.0125	0.0124	0.0267	0.0146	0.0146
1	0.0206	0.0119	0.0108	0.0427	0.0117	0.0118	0.0152	0.0110	0.0121
2	0.0211	0.0117	0.0103	0.0405	0.0122	0.0124	0.0122	0.0104	0.0109
3	0.0219	0.0123	0.0109	0.0432	0.0131	0.0133	0.0121	0.0100	0.0102
4	0.0229	0.0129	0.0113	0.0436	0.0130	0.0131	0.0126	0.0099	0.0100
5	0.0238	0.0135	0.0119	0.0430	0.0125	0.0126	0.0130	0.0097	0.0094
6	0.0237	0.0135	0.0119	0.0406	0.0121	0.0121	0.0139	0.0102	0.0092

Table S2. Maximum percentage error in the 205-300nm region for simulations performed at varying times, numbers of Gaussian lineshapes, and CVOC/AS reaction systems.

Time (hrs)	G			GA			MG		
	Double	Triple	Quad	Double	Triple	Quad	Double	Triple	Quad
0	60.0%	55.9%	56.4%	30.0%	27.8%	27.9%	41.8%	43.8%	55.1%
1	59.6%	72.6%	74.7%	41.9%	22.8%	22.9%	28.0%	30.0%	43.9%
2	27.8%	39.9%	41.6%	32.6%	30.5%	30.6%	19.8%	21.6%	36.7%
3	37.4%	35.8%	37.7%	41.1%	27.8%	27.8%	15.3%	17.1%	32.4%
4	27.2%	35.7%	37.2%	50.7%	30.3%	30.3%	11.2%	12.3%	27.6%
5	49.8%	59.9%	61.7%	45.6%	30.5%	30.6%	11.9%	12.0%	25.6%
6	33.1%	42.6%	44.1%	88.8%	65.5%	65.6%	14.9%	11.7%	24.0%

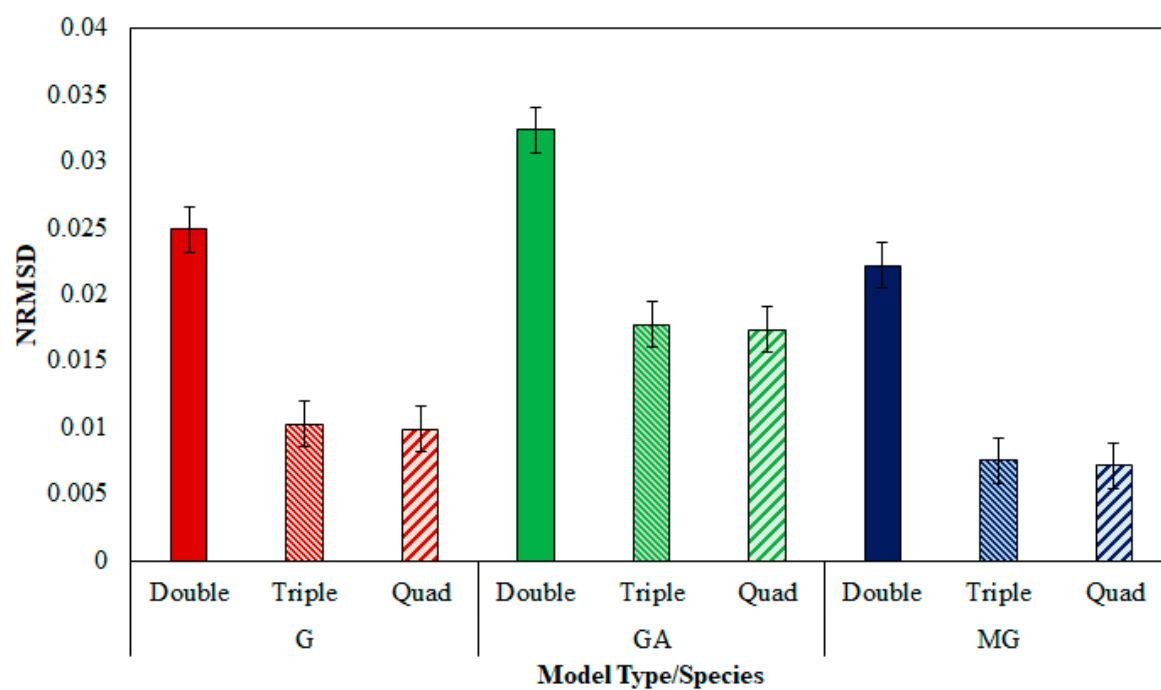


Figure S1. Multiple comparison test of population marginal means for the NRMSD of different CVOC/AS reaction systems and number of Gaussian curves used in model regression, across all times (0-6 hours).