

Supplementary Information

Table S1. Parameters for DMA.

Nonbonded Parameters			
	q	ϵ	σ
As	1.800	-0.785	2.25
O _{2A}	-0.875	-0.135	1.95
O _{SA}	-0.625	-0.195	2.05
Stretching Parameters			
	K_b (kcal/mole-Å ²)	b_0 (Å)	
O _{2A} -As	500	1.61	
O _{SA} -As	250	1.74	
O _{SA} -C _{T3}	330	1.40	
Bending Parameters			
	K_θ (kcal/mole-rad ²)	θ_0 (degree)	
O _{2A} -As-O _{2A}	70	126.5	
O _{SA} -As-O _{2A}	65	106.5	
O _{SA} -As-O _{SA}	55	98.0	
As-O _{SA} -C _{T3}	20	117.4	
O _{SA} -C _{T3} -H _A	60	109.5	
Torsion Parameters			
	K_ϕ (kcal/mol)	n	δ
O _{SA} -As-O _{SA} -C _{T3}	0.55	1	90
	0.85	2	0
	0.60	3	0
O _{2A} -As-O _{SA} -C _{T3}	0.10	3	0
X-C _{T3} -O _{SA} -X	-0.13	3	0

Table S2. Vibration frequencies and potential energy distributions from the empirical and scaled HF/6-31G* calculations for DMA ^a.

Scaled HF/6-31G *					Empirical				
Freq.	Assignment %				Freq.	Assignment %			
70	t(O-C)	91			74	t(O-C)	86	t(As-H)	15
76	t(O-C)	56	t(As-H)	42	88	t(O-C)	53	t(As-H)	43
98	t(As-H)	89			140	t(As-H)	75	t(O-C)	12
						β O-As-O	11		
132	t(As-H)	55	t(O-C)	41	189	t(As-H)	57	t(O-C)	43
186	twAs-O	48	β As-O-C	42	233	twAs-O	48	β As-O-C	29
						β O-As-O	15		
190	β As-O-C	57	rAs-O	41	235	rAs-O	51	β As-O-C	35
						wAs-O	13		
281	β O-As-O	45	β O=As=O	42	292	β O-As-O	73	twAs-O	24
310	twAs-O	43	β As-O-C	38	293	wAs-O	82		
339	wAs-O	82			358	β O=As=O	69	β As-O-C	23
370	β O=As=O	48	β O-As-O	34	384	β As-O-C	51	β O=As=O	28
	β As-O-C	12				twAs-O	20		

Table S2. Cont.

Scaled HF/6-31G *					Empirical				
Freq.	Assignment %				Freq.	Assignment %			
394	rAs–O	47	βAs–O–C	28	394	βAs–O–C	60	rAs–O	37
	wAs–O	15							
610	vO–As	87			617	vO–As	88		
622	vO–As	87			645	vO–As	88		
901	vO=As	99			903	vO=As	96		
985	vO=As	99			1003	vO=As	97		
1088	vC–O	96			1019	vC–O	81		
1098	vC–O	94			1017	vC–O	81		
1160	rCH ₃	95			1137	rCH ₃	75	δCH ₃	17
1162	rCH ₃	94			1137	rCH ₃	75	δCH ₃	17
1180	rCH ₃	90			1153	rCH ₃	71	δCH ₃	20
1180	rCH ₃	91			1156	rCH ₃	70	δCH ₃	21
1450	δCH ₃	96			1622	δCH ₃	90		
1451	δCH ₃	94			1623	δCH ₃	90		
1473	δCH ₃	92			1425	δCH ₃	78	rCH ₃	21
1474	δCH ₃	90			1426	δCH ₃	78	rCH ₃	21
1487	δCH ₃	91			1475	δCH ₃	76	rCH ₃	28
1489	δCH ₃	90			1476	δCH ₃	75	rCH ₃	28
2838	vCH ₃	93			2854	vCH ₃	100		
2840	vCH ₃	94			2854	vCH ₃	100		
2880	vCH ₃	100			2912	vCH ₃	100		
2880	vCH ₃	100			2912	vCH ₃	100		
2920	vCH ₃	93			2917	vCH ₃	100		
2921	vCH ₃	93			2917	vCH ₃	100		

^a Frequencies in cm⁻¹. Symbols represent; v, stretching; β, bending; w, out-of-plane deformations (wags); t, torsional deformations; r, rocking, δ, methyl group deformations, and tw twisting modes. The potential energy contribution is listed as a percentage in parentheses. Only internal coordinate contributing more than 10% to the potential energy distribution are reported.

Figure S1. Adiabatic torsional potential energy surface of DMA for the (a) O_{2A} -As- O_{SA} - C_{T3} , (b) O_{SA} -As- O_{SA} - C_{T3} and (c) As- O_{SA} - C_{T3} - H_A the black solid line was the HF/6-31G * results. The red dash line was the empirical results which fitted to the HF/6-31G * results.

