

Supporting information for

Origin of the unusual UV absorption of Arsenicin A

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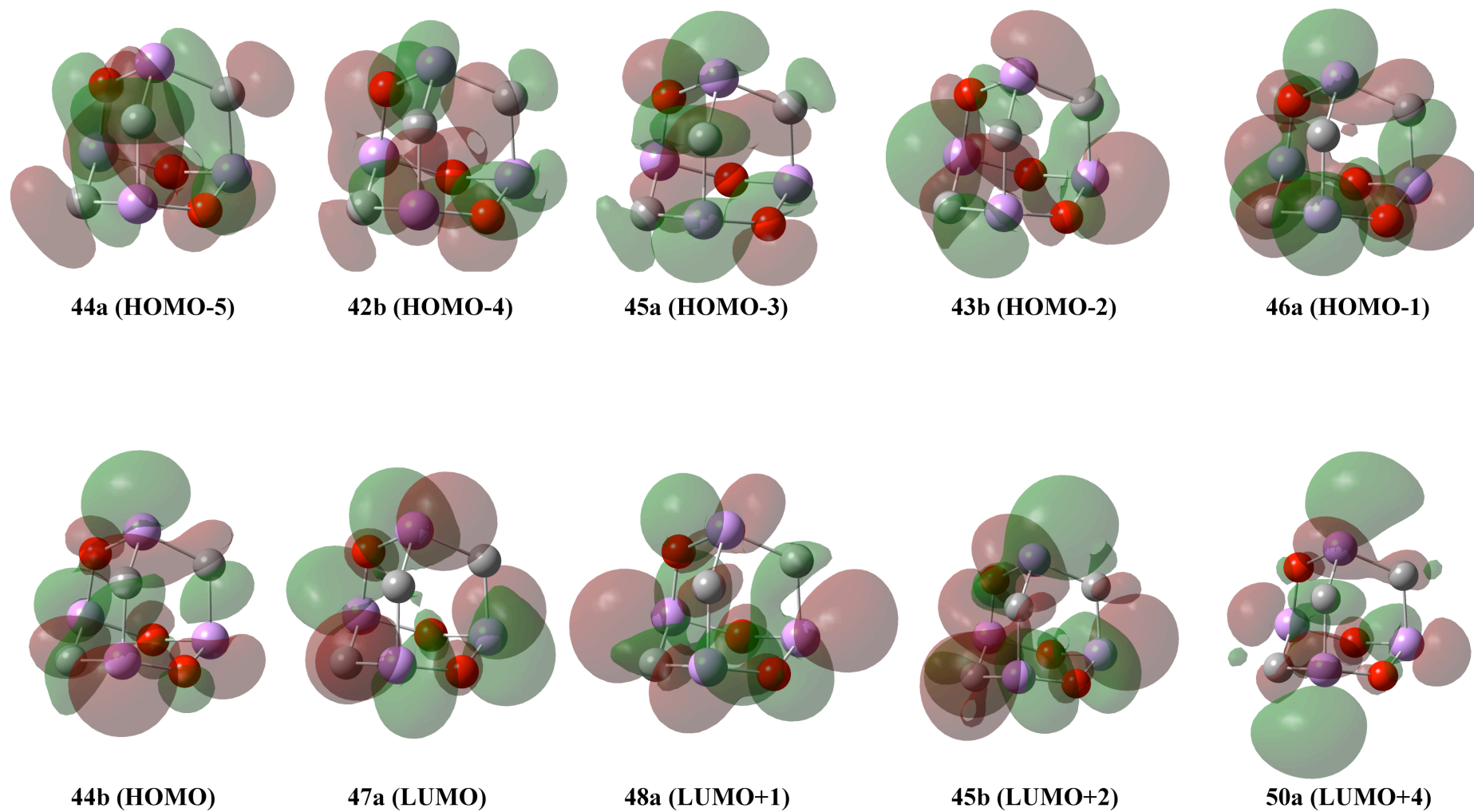


Figure S1. Some of the important molecular orbitals in Arsenicin A [Hydrogen atoms were removed for clarity]. Molecular orbitals are numbered according to their irreducible representations, a and b.

TABLE S1. Bond lengths (R) and vibrational modes (ν) obtained for various arsenic diatomic molecules using B3LYP functional with (A) 6-311+G(3*df*,2*pd*) and (B) Aug-cc-pVTZ basis sets along with the experimental values.

System	R in Å			ν in cm ⁻¹		
	Theory		Expt.	Theory		Expt.
	A	B		A	B	
As ₂	2.1036	2.1051	2.1026	451.3	450.6	429.6
³ AsH	1.5340	1.5360	1.5231	2170.2	2157.6	2155.5
³ AsF	1.7629	1.7590	1.7360	664.9	672.2	685.9
AsN	1.6092	1.6116	1.618	1142.5	1140.0	1068.5
² AsO	1.6252	1.6265	1.6236	995.2	996.5	967.1
AsP	1.9986	2.0023	1.999	630.3	627.0	604.0
² AsS	2.0260	2.0300	2.0174	577.9	575.8	567.9

TABLE S2. IR and Raman vibrational modes (ν) of Arsenicin A calculated at the B3LYP/6-311+G(3df,2pd) level of theory. I refers intensity.

Mode	Calculated values			Experimental values ¹	
	ν cm ⁻¹	I (IR) Km mol ⁻¹	I (Raman) Å ⁴ amu ⁻¹	ν (IR) cm ⁻¹	ν (Raman) cm ⁻¹
A	3097.0	2.56	58.36	2953	2957
B	3096.9	1.64	67.71		2932
B	3091.6	2.59	57.21	2921	2899
A	3038.3	0.89	269.6		2887
B	3038.2	10.34	22.38	2851	
A	3036.8	4.45	56.75		
A	1412.3	4.82	3.53		
B	1402.8	12.15	0.87	1462	
A	1398.1	1.14	10.85		
B	1129.9	54.56	1.43	1105	
A	1115.7	19.58	1.51		
B	1095.4	5.56	0.13		
A	1055.1	4.97	3.58		
B	1026.4	2.78	0.19		
A	1014.2	1.49	1.92		
B	782.8	325.34	4.17	765	
B	726.7	3.06	0.39		
A	734.8	204.00	3.54	723	
A	690.8	5.01	0.27		
B	657.4	8.51	0.39		
B	668.3	108.05	4.96	674	
B	600.2	3.75	2.67		
A	600.0	4.00	3.84		
B	601.7	0.14	1.51		
A	571.3	0.60	47.93		579
B	509.0	7.09	3.59		

A	495.1	11.01	2.86	
A	464.4	20.12	1.20	
B	465.3	51.11	3.48	
A	462.6	1.38	0.56	
A	337.6	0.11	19.71	337
B	324.1	19.59	0.67	
A	287.7	4.12	1.54	
B	276.2	1.52	0.94	
B	216.7	1.92	3.57	215
A	211.1	2.98	3.43	
B	201.4	1.16	2.97	
A	182.7	0.15	3.58	
A	171.8	0.39	2.45	
B	159.8	1.59	0.23	
A	156.7	1.81	0.47	
B	148.5	0.46	0.13	

¹- Reference 3.

TABLE S3. Low-lying singlet excited states of Arsenicin A obtained using TD-DFT (B3LYP/ 6-311+G(3*df*,2*pd*) [excitation energies (*DE*) and oscillator strengths (*f*)] along with the experimental values and some important assignments]

State	Principle configuration	Nature	Theory		Expt.	
			ΔE (eV)	<i>f</i>	Wavelength (eV)	Abs.
1 ¹ <i>B</i>	(44b) → (47a)	As(<i>p</i>)+ $\sigma_{(As-C)}^*+O(p)$ → π^* -like [As(<i>p</i>)] TS due to the mixing of $\sigma_{(As-O)}^*$ and As(<i>p</i>)	3.789	0.0219	3.95	0.261
2 ¹ <i>A</i>	(46a) → (47a)		4.121	0.0041		
2 ¹ <i>B</i>	(44b) → (48a)		4.124	0.0039		
3 ¹ <i>A</i>	(46a) → (48a)	As(<i>p</i>)+ $\sigma_{(As-C)}^*+O(p) + \sigma_{(As-O)}^*$ forms a π -like bonding → π^* -like [As(<i>p</i>)] TS due to the mixing of $\sigma_{(As-O)}^*$ and As(<i>p</i>)	4.537	0.0206	4.31	0.174
4 ¹ <i>A</i>	(44b) → (45b)		4.613	0.0022		

3 ¹ B	(43b) → (47a)		4.862	0.0056		
4 ¹ B	(46a) → (45b)		5.023	0.0101		
5 ¹ B	(44b) → (49a)		5.152	0.0160		
6 ¹ B	(44b) → (50a)	As(<i>p</i>)+σ _(As-C) +O(<i>p</i>) → σ* _(As-C) +σ* _(As-O)	5.197	0.0332	4.83	0.432
5 ¹ A	(44b) → (46b)		5.329	0.0114		
7 ¹ B	(43b) → (48a)	As(<i>p</i>)+σ _(As-C) +O(<i>p</i>)+σ _(As-O) forms a σ-like bonding → π*-like [As(<i>p</i>)] TS due to the mixing of σ* _(As-O) and As(<i>p</i>)	5.333	0.1060	5.39	1.287
6 ¹ A	(46a) → (49a)*		5.544	0.0173		
7 ¹ A	(46a) → (50a)*		5.573	0.0154		
8 ¹ B	(46a) → (46b)		5.755	0.0318		
8 ¹ A	(43b) → (45b)*		5.798	0.0683		
9 ¹ A	(44b) → (47b)*		5.837	0.0019		
9 ¹ B	(44b) → (51a)		5.864	0.0164		
10 ¹ A	(45a) → (47a)*		5.885	0.0167		
11 ¹ A	(44b) → (48b)		5.968	0.0431		
10 ¹ B	(42b) → (47a)		5.996	0.0003		

12 ¹ A	(44a) → (47a)	6.179	0.0029
13 ¹ A	(46a) → (51a)*	6.226	0.0120
11 ¹ B	(46a) → (47b)	6.234	0.0396
14 ¹ A	(44b) → (49b)*	6.255	0.0000
12 ¹ B	(46a) → (48b)*	6.263	0.0301
13 ¹ B	(41b) → (47a)*	6.294	0.0205
15 ¹ A	(45a) → (48a)	6.325	0.0190
14 ¹ B	(43b) → (49a) *	6.337	0.0041
15 ¹ B	(44b) → (52a)	6.368	0.0468
16 ¹ A	(44b) → (50b)	6.410	0.0000
16 ¹ B	(43b) → (50a)*	6.411	0.1061
17 ¹ A	(43b) → (46b)	6.423	0.0069
17 ¹ B	(42b) → (48a)*	6.429	0.1115
18 ¹ B	(44b) → (53a)*	6.448	0.0128
18 ¹ A	(43a) → (47a)	6.559	0.0017

*-Refers significant contribution of additional excitations(s), TS-through space.

TABLE S4. Low-lying singlet excited states of Arsenicin A obtained using TD-DFT (M06-L / 6-311+G(3*df*,2*pd*) [excitation energies (*DE*) and oscillator strengths (*f*)] along with the experimental values and some important assignments.

State	Principle configuration	Nature	Theory		Expt.	
			ΔE (eV)	<i>f</i>	Wavelength (eV)	Abs.
1 ¹ <i>B</i>	(44b) → (47a)	As(<i>p</i>)+ $\sigma_{(As-C)}+O(p)$ → π^* -like [As(<i>p</i>)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(<i>p</i>)	3.742	0.0209	3.95	0.261
2 ¹ <i>A</i>	(46a) → (47a)		4.037	0.0038		
2 ¹ <i>B</i>	(44b) → (48a)		4.055	0.0041		
3 ¹ <i>A</i>	(46a) → (48a)	As(<i>p</i>)+ $\sigma_{(As-C)}+O(p) + \sigma_{(As-O)}$ forms a π -like bonding → π^* -like [As(<i>p</i>)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(<i>p</i>)	4.465	0.0196	4.31	0.174
4 ¹ <i>A</i>	(44b) → (45b)		4.632	0.0008		

3 ¹ B	(43b) → (47a)		4.735	0.0058		
4 ¹ B	(46a) → (45b)		5.014	0.0121		
5 ¹ B	(44b) → (49a)		5.109	0.0051		
6 ¹ B	(44b) → (50a)*	As(p)+σ _(As-C) +O(p) → σ* _(As-C) +σ* _(As-O)	5.131	0.0156	4.83	0.432
5 ¹ A	(44b) → (46b)		5.274	0.0112		
7 ¹ B	(43b) → (48a)*	As(p)+σ _(As-C) +O(p)+σ _(As-O) forms a σ-like bonding → π*-like [As(p)] TS due to the mixing of σ* _(As-O) and As(p)	5.313	0.1279	5.39	1.287
6 ¹ A	(46a) → (49a)		5.465	0.0093		
7 ¹ A	(46a) → (50a)		5.521	0.0000		
8 ¹ B	(46a) → (46b)		5.647	0.0168		
8 ¹ A	(43b) → (45b)*		5.689	0.0040		
9 ¹ B	(44b) → (51a)		5.705	0.0199		
9 ¹ A	(44b) → (47b)		5.719	0.0173		
10 ¹ A	(45a) → (47a)*		5.747	0.0000		
10 ¹ B	(42b) → (47a)		5.790	0.0028		
11 ¹ A	(43b) → (45b)*		5.804	0.1222		

12 ¹ A	(44a) → (47a)	6.048	0.0016
11 ¹ B	(46a) → (48b)*	6.068	0.0187
12 ¹ B	(46a) → (47b)	6.076	0.0021
13 ¹ A	(46a) → (51a)	6.077	0.0077
14 ¹ A	(44b) → (49b)	6.108	0.0000
13 ¹ B	(41b) → (47a)*	6.109	0.0264
15 ¹ A	(45a) → (48a)	6.146	0.0363
14 ¹ B	(43b) → (49a)	6.146	0.0160
15 ¹ B	(44b) → (52a)	6.185	0.0471
16 ¹ B	(42b) → (48a)	6.201	0.0272
16 ¹ A	(44b) → (50b)	6.249	0.0000
17 ¹ B	(44b) → (53a)	6.289	0.0220
17 ¹ A	(43b) → (46b)	6.297	0.0001
18 ¹ B	(43b) → (53a)*	6.325	0.1663
18 ¹ A	(43a) → (47a)	6.326	0.0095

*-Refers significant contribution of additional excitations(s), TS-through space.

TABLE S5. Low-lying singlet excited states of Arsenicin A obtained using TD-DFT (M06-2X / 6-311+G(3df,2pd))
[excitation energies (ΔE) and oscillator strengths (f)] along with the experimental values and some important assignments.

State	Principle configuration	Nature	Theory		Expt.	
			ΔE (eV)	f	Wavelength (eV)	Abs.
1 1B	(44b) \rightarrow (47a)	As(p)+ $\sigma_{(As-C)}+O(p)$ $\rightarrow \pi^*$ -like [As(p)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(p)	4.286	0.0454	3.95	0.261
2 1B	(44b) \rightarrow (48a)		4.615	0.0049		
2 1A	(46a) \rightarrow (47a)		4.664	0.0032		
3 1A	(46a) \rightarrow (48a)	As(p)+ $\sigma_{(As-C)}+O(p)$ + $\sigma_{(As-O)}$ forms a π -like bonding $\rightarrow \pi^*$ -like [As(p)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(p)	5.086	0.0548	4.31	0.174
4 1A	(44b) \rightarrow (46b)*	As(p)+ $\sigma_{(As-C)}+O(p)$	5.172	0.0161	4.83	0.432

		$\rightarrow \sigma^*_{(\text{As-C})} + \sigma^*_{(\text{As-O})}$				
3 1B	(44b) \rightarrow (49a)*		5.284	0.0101		
4 1B	(44b) \rightarrow (49a)		5.365	0.0131		
5 1A	(44b) \rightarrow (45b)*		5.609	0.0005		
5 1B	(44b) \rightarrow (50a)*	As(<i>p</i>)+ $\sigma_{(\text{As-C})}$ +O(<i>p</i>)+ $\sigma_{(\text{As-O})}$ forms a σ -like bonding $\rightarrow \pi^*$ -like [As(<i>p</i>)] TS due to the mixing of $\sigma^*_{(\text{As-O})}$ and As(<i>p</i>)	5.679	0.1406	5.39	1.287
6 1B	(46a) \rightarrow (46b)*		5.789	0.0258		
6 1A	(46a) \rightarrow (48a)		5.899	0.0575		
7 1B	(43b) \rightarrow (48a)		5.944	0.0755		
7 1A	(46a) \rightarrow (50a)*		5.988	0.0018		
8 1B	(44b) \rightarrow (51a)*		6.125	0.0226		
8 1A	(44b) \rightarrow (47b)*		6.199	0.0025		
9 1B	(46a) \rightarrow (45b)*		6.249	0.0344		
9 1A	(44b) \rightarrow (48b)		6.293	0.0400		
10 1A	(43b) \rightarrow (46b)		6.448	0.1004		
11 1A	(44b) \rightarrow (49b)*		6.481	0.0075		

10 ¹ B	(46a) → (47b)	6.543	0.0163
11 ¹ B	(46a) → (48b)*	6.648	0.1852
12 ¹ B	(44b) → (52a)	6.715	0.0088
12 ¹ A	(46a) → (51a)*	6.751	0.0011
13 ¹ A	(44b) → (49b)*	6.804	0.0009
13 ¹ B	(44b) → (54a)*	6.824	0.0009
14 ¹ B	(43b) → (49a)	6.867	0.0055
14 ¹ A	(43b) → (45b)	6.874	0.0462
15 ¹ B	(44b) → (53a)*	6.889	0.0723
16 ¹ B	(44b) → (55a)	6.973	0.0091
15 ¹ A	(45a) → (47a)*	6.990	0.0053
17 ¹ B	(44b) → (55a)*	7.018	0.0843
18 ¹ B	(42b) → (47a)*	7.045	0.0115
16 ¹ A	(44b) → (50b)*	7.065	0.0065
17 ¹ A	(44b) → (51b)*	7.092	0.0180
19 ¹ B	(46a) → (49b)	7.143	0.0052

*-Refers significant contribution of additional excitations(s), TS-through space.

TABLE S6. Low-lying singlet excited states of Arsenicin A obtained using SAC-CI (LevelTwo) / 6-311+G(*d,p*) [excitation energies (*DE*) and oscillator strengths (*f*)] along with the experimental values and some important assignments.

State	Nature	Theory		Expt.	
		ΔE (eV)	<i>f</i>	Wavelength (eV)	Abs.
1 ¹ <i>B</i>	As(<i>p</i>)+ $\sigma_{(As-C)}+O(p)$ → π^* -like [As(<i>p</i>)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(<i>p</i>)	3.619	0.0526	3.95	0.261
2 ¹ <i>B</i>		4.014	0.0039		
2 ¹ <i>A</i>		4.063	0.0050		
3 ¹ <i>A</i>	As(<i>p</i>)+ $\sigma_{(As-C)}+O(p)$ + $\sigma_{(As-O)}$ forms a π -like bonding → π^* -like [As(<i>p</i>)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(<i>p</i>)	4.565	0.0781	4.31	0.174
4 ¹ <i>A</i>		4.710	0.0112		
3 ¹ <i>B</i>		4.761	0.0149		

4 ¹ B		4.900	0.0057		
5 ¹ A		5.204	0.0160		
5 ¹ B	As(p)+ $\sigma_{(As-C)}+O(p)$ $\rightarrow \sigma^*_{(As-C)}+\sigma^*_{(As-O)}$	5.393	0.0419	4.83	0.432
6 ¹ A		5.461	0.0513		
6 ¹ B	As(p)+ $\sigma_{(As-C)}+O(p)+\sigma_{(As-O)}$ forms a σ -like bonding $\rightarrow \pi^*$ -like [As(p)] TS due to the mixing of $\sigma^*_{(As-O)}$ and As(p)	5.497	0.1569	5.39	1.287
7 ¹ A		5.608	0.0000		
7 ¹ B		5.709	0.0153		
8 ¹ A		5.837	0.0002		
8 ¹ B		5.875	0.0033		
9 ¹ A		6.041	0.1114		
9 ¹ B		6.153	0.0153		
10 ¹ A		6.201	0.0436		
10 ¹ B		6.273	0.1232		
11 ¹ A		6.303	0.0256		
11 ¹ B		6.417	0.0118		

12 ¹ <i>A</i>	6.533	0.0015
12 ¹ <i>B</i>	6.538	0.0090
13 ¹ <i>A</i>	6.561	0.0243
13 ¹ <i>B</i>	6.599	0.0686
14 ¹ <i>A</i>	6.683	0.0063
14 ¹ <i>B</i>	6.742	0.0205
15 ¹ <i>B</i>	6.781	0.0889
15 ¹ <i>A</i>	6.858	0.0079
16 ¹ <i>A</i>	6.989	0.0065

TABLE S7. Comparison between the excitation energies of Arsenicin A calculated using various levels of theory [excitation energies (ΔE) and oscillator strengths (f)] along with the observed experimental peaks.

B3LYP/ 6-311+G(3df,2pd)		M06-L/ 6-311+G(3df,2pd)		M06-2X/ 6-311+G(3df,2pd)		SAC-CI/ 6-311+G(d,p)		Expt.	
ΔE (eV)	f	ΔE (eV)	f	ΔE (eV)	f	ΔE (eV)	f	Wavelength (eV)	Abs.
3.789	0.0219	3.742	0.0209	4.286	0.0454	3.619	0.0526	3.95	0.261
4.537	0.0206	4.465	0.0196	5.086	0.0548	4.565	0.0781	4.31	0.174
5.197	0.0332	5.131	0.0156	5.172	0.0161	5.393	0.0419	4.83	0.432
5.333	0.1060	5.313	0.1279	5.679	0.1406	5.497	0.1569	5.39	1.287

TABLE S8. B3LYP/6-31G(*d*) overlap integrals calculated between lone As lone pairs, As(*p*), and various As-C and As-O sigma bonds. All the values are in a.u. Atom numberings are as shown in the figure below.

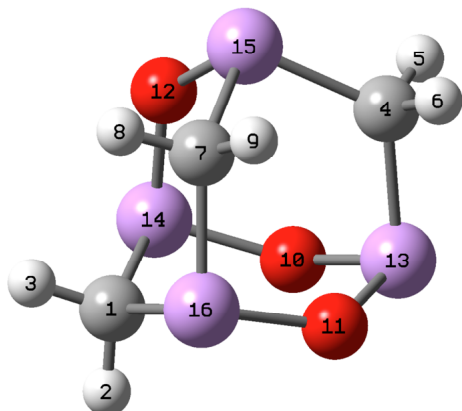


TABLE S9. Most important $n \rightarrow \sigma^*$ interactions calculated at B3LYP/6-311+G(3*df*,2*pd*) level of theory.

$n \rightarrow \sigma^*$	in eV
$n_{\text{O}} \rightarrow \sigma^*_{\text{As-C}}$	0.15
$n_{\text{O}} \rightarrow \sigma^*_{\text{As-O}}$	0.24
$n_{\text{As}} \rightarrow \sigma^*_{\text{As-C}}$	0.16
$n_{\text{As}} \rightarrow \sigma^*_{\text{As-O}}$	0.23

TABLE S10. B3LYP/6-311+G(3df,2pd) optimized coordinates of Arsenicin A and Adamantane

Optimized structures (Arsenicin A as well as Adamantane) do not possess any imaginary frequency. For Arsenicin A, calculations were done on both enantiomers and, as expectedly same results, within ± 0.1 kJ/mol difference, were obtained.

Arsenicin A

C	-1.569008	1.417262	0.007283
H	-1.680597	2.301657	0.635752
H	-2.450804	1.357290	-0.634460
C	1.569008	-1.417262	0.007283
H	1.680597	-2.301657	0.635752
H	2.450804	-1.357290	-0.634460
C	0.000000	0.000000	-2.141599
H	-0.877361	-0.004001	-2.790896
H	0.877361	0.004001	-2.790896
O	0.000000	0.000000	1.973296
O	1.361545	1.463664	-0.000415
O	-1.361545	-1.463664	-0.000415
As	1.628000	0.165582	1.211482
As	-1.628000	-0.165582	1.211482
As	0.000000	-1.735229	-1.172669
As	0.000000	1.735229	-1.172669

Adamantane

H	1.520751	-1.520751	1.520751
C	0.889743	-0.889743	0.889743
C	-0.889743	0.889743	0.889743
C	0.889743	0.889743	-0.889743
C	0.000000	1.775580	0.000000
C	1.775580	0.000000	0.000000
C	0.000000	0.000000	1.775580
H	0.621163	2.427089	0.621163
H	2.427089	0.621163	0.621163
H	0.621163	0.621163	2.427089
H	-1.520751	1.520751	1.520751
H	1.520751	1.520751	-1.520751
H	-0.621163	2.427089	-0.621163
H	2.427089	-0.621163	-0.621163
H	-0.621163	-0.621163	2.427089
C	0.000000	0.000000	-1.775580
H	0.621163	-0.621163	-2.427089
H	-0.621163	0.621163	-2.427089
C	0.000000	-1.775580	0.000000
H	-0.621163	-2.427089	0.621163

H	0.621163	-2.427089	-0.621163
C	-1.775580	0.000000	0.000000
H	-2.427089	-0.621163	0.621163
H	-2.427089	0.621163	-0.621163
C	-0.889743	-0.889743	-0.889743
H	-1.520751	-1.520751	-1.520751

TABLE S11. B3LYP/6-311+G(*d,p*) optimized coordinates for the model systems AsH₃, AsH₂OH, As(CH₃)₂H, AsH₂OAsH₂, and AsH₂CH₂AsH₂

In all cases, optimized structures do not possess any imaginary frequency.

AsH₃

As	0.000264	-0.000070	-0.070541
H	-0.583990	1.128015	0.773267
H	1.264745	-0.060081	0.779875
H	-0.689480	-1.065639	0.774711

AsH₂OH

As	-0.374282	-0.062173	-0.000011
H	-0.574955	0.998683	-1.093372
H	-0.574973	0.998311	1.093693
O	1.458033	-0.092279	-0.000006
H	1.836974	0.792960	0.000075

As(CH₃)₂H

C	1.501387	0.834412	0.016926
H	2.431540	0.298277	0.211666
H	1.581712	1.323423	-0.955493
C	-1.501432	0.834379	0.016856
H	-1.582631	1.322824	-0.955754
H	-2.431344	0.298248	0.212773
As	0.000023	-0.474835	-0.052882
H	-0.000265	-0.761550	1.449487
H	-1.346405	1.587988	0.789588
H	1.346891	1.587588	0.790164

AsH₂OAsH₂

O	0.000147	-0.776998	-0.000028
As	1.636865	0.029055	-0.000045
As	-1.636893	0.029038	-0.000052
H	1.350553	1.073935	1.091914

H	-1.350740	1.073777	1.092041
H	-1.349852	1.075556	-1.090231
H	1.349783	1.075618	-1.090280

AsH₂CH₂AsH₂

C	0.000011	0.900378	-0.000190
H	0.000187	1.555812	-0.874389
H	-0.000126	1.553992	0.875460
As	1.749495	-0.064834	-0.000034
As	-1.749496	-0.064829	-0.000018
H	1.380048	-1.057590	1.098795
H	1.380227	-1.058989	-1.097688
H	-1.379830	-1.057753	1.098573
H	-1.380543	-1.058850	-1.097885

TABLE S12. B3LYP/6-31G(d) optimized coordinates for the Model A and Model B

Model A

C	0.000000	2.158212	0.000000
H	0.617467	2.819475	0.617467
H	-0.617467	2.819475	-0.617467
C	0.000000	-2.158212	0.000000
H	-0.617467	-2.819475	0.617467
H	0.617467	-2.819475	-0.617467
C	0.000000	0.000000	-2.158212
H	-0.617467	0.617467	-2.819475
H	0.617467	-0.617467	-2.819475
As	1.233517	-1.233517	1.233517
As	-1.233517	1.233517	1.233517
As	-1.233517	-1.233517	-1.233517
As	1.233517	1.233517	-1.233517
C	-2.158212	0.000000	0.000000
H	-2.819475	0.617467	-0.617467
H	-2.819475	-0.617467	0.617467
C	0.000000	0.000000	2.158212
H	0.617467	0.617467	2.819475
H	-0.617467	-0.617467	2.819475
C	2.158212	0.000000	0.000000
H	2.819475	-0.617467	-0.617467
H	2.819475	0.617467	0.617467

Model B

As	-1.848791	1.848791	1.848791
As	1.848791	-1.848791	1.848791
As	1.848791	1.848791	-1.848791
As	-1.848791	-1.848791	-1.848791
H	-0.826687	2.380692	0.826687
H	0.826687	2.380692	-0.826687
H	2.380692	0.826687	-0.826687
H	2.380692	-0.826687	0.826687
H	0.826687	0.826687	-2.380692
H	-0.826687	-0.826687	-2.380692
H	0.826687	-2.380692	0.826687
H	-0.826687	-2.380692	-0.826687
H	-2.380692	0.826687	0.826687
H	-2.380692	-0.826687	-0.826687
H	0.826687	-0.826687	2.380692
H	-0.826687	0.826687	2.380692