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Hydrogen bonding interactions between arsenious acid and dithiothreitol/dithioerythritol at different pH values: A computational study under explicit solvent model

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Supplementary material

Table S1 The forms of arsenious acid, DTT/DTE and solvent molecules at different pH values.

<table>
<tr><th>pH range</th><th>$H_{n+3}AsO_3^n$</th><th>DTT^m</th><th>DTE^m</th><th>$HEPES^k$</th></tr>
<tr><td>1.00</td><td rowspan="13">0</td><td rowspan="9">0</td><td rowspan="9">0</td><td rowspan="2">/</td></tr>
<tr><td>|</td></tr>
<tr><td>6.80</td><td rowspan="5">0</td></tr>
<tr><td>|</td></tr>
<tr><td>7.00</td></tr>
<tr><td>|</td></tr>
<tr><td>7.50</td></tr>
<tr><td>|</td><td rowspan="2">-1</td></tr>
<tr><td>8.30</td></tr>
<tr><td>|</td><td rowspan="4">-1</td><td rowspan="4">-1</td><td rowspan="8">/</td></tr>
<tr><td>9.23</td></tr>
<tr><td>|</td><td rowspan="4">-1</td></tr>
<tr><td>9.50</td></tr>
<tr><td>|</td><td rowspan="5">-2</td><td rowspan="5">-2</td></tr>
<tr><td>12.10</td></tr>
<tr><td>|</td></tr>
<tr><td>13.41</td></tr>
<tr><td>|</td><td rowspan="2">-3</td></tr>
<tr><td>14.00</td></tr>
</table>

Note: n, m and k in the table represent the valence states respectively

Table S2 The binding energy △E of the most stable optimized configurations in aqueous solution and HEPES buffer under DFT/B3LYP-D3 method.

Conformation	△E（kcal/mol)
H_3AsO_3-DTT-HEPES	-27.57
H_3AsO_3-DTE-HEPES	-32.47
H_3AsO_3-DTT-$HEPES^-$	-54.53
H_3AsO_3-DTE-$HEPES^-$	-61.51
H_3AsO_3-DTT-H_2O	-26.64
H_3AsO_3-DTE-H_2O	-25.14
H_3AsO_3-DTT^--H_2O	-44.97
H_3AsO_3-DTE^--H_2O	-48.83
$H_2AsO_3^-$-DTT^--H_2O	4.58
$H_2AsO_3^-$-DTE^--H_2O	-8.49

Table S3 QTAIM topology analysis parameters of the most stable configurations under explicit solvent model calculated by DFT/B3LYP method. (The unit is a.u.)

Configurations	Hydrogen bonds	ρ（r）	$\nabla^2\rho$（r）	$H_{BCP}/10^{-4}$	$LBO/10^{-4}$
H_3AsO_3-DTT^--H_2O	O25···H7-O6	0.0498	0.1387	-18.30	3.36
H_3AsO_3-DTT^--H_2O	S18···H27-O25	0.0414	0.0469	-68.40	5.47
H_3AsO_3-DTT^--H_2O	O6···H24-O23	0.0307	0.0904	-5.76	0.75
H_3AsO_3-DTT^--H_2O	O21···H3-O2	0.0397	0.1185	1.99	1.79
H_3AsO_3-DTT^--H_2O	O23···H5-O4	0.0302	0.0909	-0.61	0.97
H_3AsO_3-DTT^--H_2O	O2···H29-O28	0.0153	0.0449	-1.44	0.34
H_3AsO_3-DTT^--H_2O	O4···H30-O28	0.0237	0.0661	-8.75	1.13
H_3AsO_3-DTT^--H_2O	O28···H20-S19	0.0160	0.0387	-5.21	0.61
H_3AsO_3-DTE^--H_2O	O25···H22-O21	0.0405	0.1112	-8.90	1.95
H_3AsO_3-DTE^--H_2O	S13···H26-O25	0.0300	0.0483	-30.50	1.82
H_3AsO_3-DTE^--H_2O	S13···H20-O19	0.0330	0.0442	-39.90	1.53
H_3AsO_3-DTE^--H_2O	O23···H15-O24	0.0270	0.0753	-8.40	0.58
H_3AsO_3-DTE^--H_2O	O28···H24-O23	0.0258	0.0707	-7.79	0.49
H_3AsO_3-DTE^--H_2O	S11···H30-O28	0.0082	0.0267	13.20	0.05
H_3AsO_3-DTE^--H_2O	O14···H29-O28	0.0326	0.0938	-5.69	0.21
H_3AsO_3-DTT-$HEPES^-$	S20···H57-O56	0.0138	0.0338	5.22	0.24
H_3AsO_3-DTT-$HEPES^-$	O54···H19-S18	0.0098	0.0266	2.64	0.09
H_3AsO_3-DTT-$HEPES^-$	S18···H7-O6	0.0277	0.0782	-8.01	0.08
H_3AsO_3-DTT-$HEPES^-$	O22···H3-O2	0.0413	0.1230	-4.60	2.01
H_3AsO_3-DTT-$HEPES^-$	O53···H23-O22	0.0607	0.1623	-59.40	8.19
H_3AsO_3-DTE-$HEPES^-$	O20···H12-S11	0.0146	0.0410	0.75	0.51
H_3AsO_3-DTE-$HEPES^-$	O54···H21-O20	0.0304	0.0916	-1.20	0.95
H_3AsO_3-DTE-$HEPES^-$	O53···H23-O22	0.0540	0.1574	-27.00	4.89
H_3AsO_3-DTE-$HEPES^-$	O22···H16-O15	0.0387	0.1155	-1.86	2.07
H_3AsO_3-DTE-$HEPES^-$	O56···H14-S13	0.0076	0.0248	7.95	0.06
H_3AsO_3-DTE-$HEPES^-$	O15···H57-O56	0.0273	0.0762	-5.30	0.73

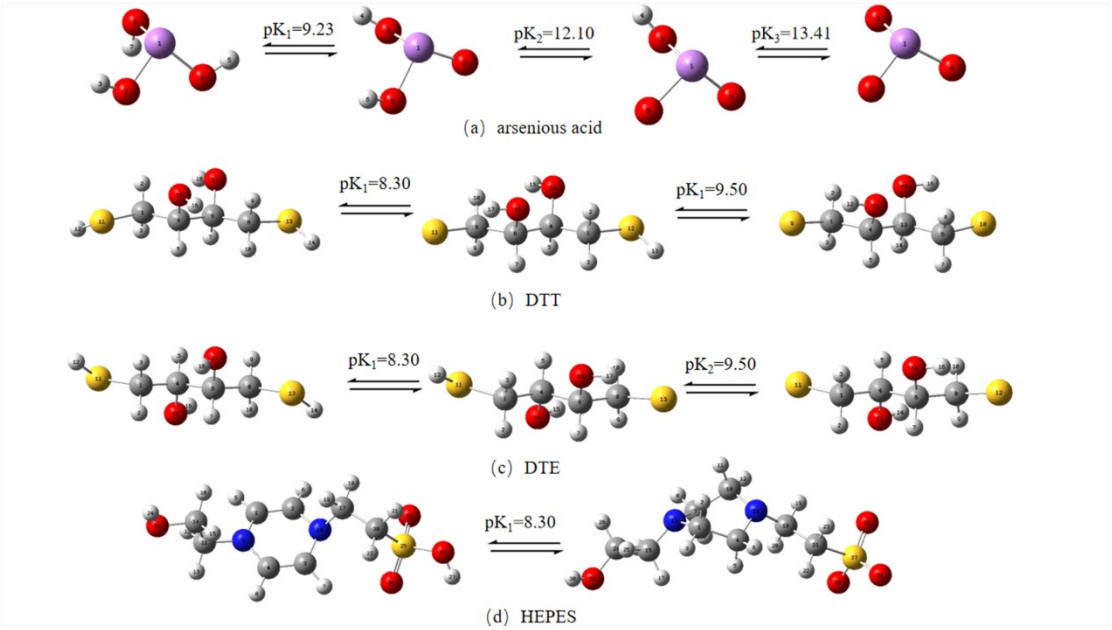

Fig. S1 Dissociated structures of arsenious acid, DTT/DTE and HEPES.