Electronic Supplementary Information

The Reactivity of Quaternary Ammonium- versus Potassium- Fluorides Supported on Metal Oxides: Paving the Way to an Instantaneous Detoxification of Chemical Warfare Agents

Yossi Zafrani, Lea Yehezkel, Michael Goldvaser, Daniele Marciano, Daniel Waysbort, Eytan Gershonov and Ishay Columbus

The Department of Organic Chemistry, Israel Institute for Biological Research, Ness-Ziona, 74100, Israel;
E-mail: yossiz@iibr.gov.il; ishayc@iibr.gov.il

Table of contents:

Fig. S2: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/Al$_2$O$_3$ (6, EtOH, 60), containing 1 mmol KF, and its degradation profile onto this sorbent.

Fig. S3: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TMAF/Al$_2$O$_3$ (16, EtOH, 60), containing 1 mmol TMAF, and its degradation profile onto this sorbent.

Fig. S4: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TMAF/Al$_2$O$_3$ (33, EtOH, 60), containing 2 mmol TMAF, and its degradation profile onto this sorbent.

Fig. S5: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TEAF/Al$_2$O$_3$ (18, EtOH, 60), containing 1 mmol TEAF, and its degradation profile onto this sorbent.

Fig. S6: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on DTMAF/Al$_2$O$_3$ (27, EtOH, 60), containing 1 mmol DTMAF, and its degradation profile onto this sorbent.

Fig. S7: $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on BTMAF/Al$_2$O$_3$ (20, EtOH, 60), containing 1 mmol TAAF, and its degradation profile onto this sorbent.

Fig. S8: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (5% wt) on TBAF/Al$_2$O$_3$ (20, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S9: $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/SiO$_2$ (12, EtOH, 60), containing 2 mmol KF, and its degradation profile onto this sorbent.

Fig. S10: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TEAF/SiO$_2$ (18, EtOH, 60), containing 1 mmol TEAF, and its degradation profile onto this sorbent.

Fig. S11: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TEAF/TiO$_2$ (18, EtOH, 60), containing 1 mmol TEAF, and its degradation profile onto this sorbent.

Fig. S12: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/TiO$_2$ (12, EtOH, 60), containing 2 mmol KF.

Fig. S13: Selected $^{31}$P MAS NMR spectra of adsorbed VX (1% wt) on KF/Al$_2$O$_3$ (25, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S14: Selected $^{31}$P MAS NMR spectra of adsorbed VX (1% wt) on TBAF/Al$_2$O$_3$ (20, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S15: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/Al$_2$O$_3$ (25, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S16: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (10% wt) on KF/Al$_2$O$_3$ (25, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S17: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (10% wt) on TBAF/KF/Al$_2$O$_3$ (20, 20, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S18: Selected $^{31}$P MAS NMR spectra of adsorbed VX (10% wt) on TBAF/KF/Al$_2$O$_3$ (20, 20, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S19: $^{31}$P MAS NMR spectra of adsorbed GB (10% wt) on TBAF/KF/Al$_2$O$_3$ (20, 20, EtOH, 60) and its degradation profile onto this sorbent.

Fig. S20: GC-MS chromatogram of the extraction mixture of HD* on KF/TiO$_2$ (12, EtOH, 60).
Fig. S2: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/Al$_2$O$_3$ (6, EtOH, 60), containing 1 mmol KF, and its degradation profile onto this sorbent.
Fig. S3: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TMAF/Al$_2$O$_3$ (16, EtOH, 60), containing 1 mmol TMAF, and its degradation profile onto this sorbent.
Fig. S4: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TMAF/Al$_2$O$_3$ (33, EtOH, 60), containing 2 mmol TMAF, and its degradation profile onto this sorbent.
Fig. S5: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TEAF/Al$_2$O$_3$ (18, EtOH, 60), containing 1 mmol TEAF, and its degradation profile onto this sorbent.
Fig. S6: Selected $^{13}$C MAS NMR spectra of adsorbed HD$^*$ (1% wt) on DTMAF/Al$_2$O$_3$ (27, EtOH, 60), containing 1 mmol DTMAF, and its degradation profile onto this sorbent.
**Fig. S7:** $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on BTMAF/Al$_2$O$_3$ (20, EtOH, 60), containing 1 mmol TAAF, and its degradation profile onto this sorbent.
**Fig. S8:** Selected $^{13}$C MAS NMR spectra of adsorbed HD* (5% wt) on TBAF/Al$_2$O$_3$ (20, EtOH, 60) and its degradation profile onto this sorbent.
**Fig. S9:** $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/SiO$_2$ (12, EtOH, 60), containing 2 mmol KF, and its degradation profile onto this sorbent.

$t_{1/2} = 546$ min

$R^2 = 0.973$
**Fig. S10:** Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TEAF/SiO$_2$ (18, EtOH, 60), containing 1 mmol TEAF, and its degradation profile onto this sorbent.
Fig. S11: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on TEAF/TiO$_2$ (18, EtOH, 60), containing 1 mmol TEAF, and its degradation profile onto this sorbent.
Fig. S12: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/TiO$_2$ (12, EtOH, 60), containing 2 mmol KF. One of the degradation products on this sorbent is (2-chloroethyl)(2-fluoroethyl) sulfide. The NMR chemical shifts of this product are overlapping with HD* and bis(2-fluoroethyl)sulfide.
Fig. S13: Selected $^{31}$P MAS NMR spectra of adsorbed VX (1% wt) on KF/Al$_2$O$_3$ (25, EtOH, 60) and its degradation profile onto this sorbent.
Fig. S14: Selected $^{31}$P MAS NMR spectra of adsorbed VX (1% wt) on TBAF/Al$_2$O$_3$ (20, EtOH, 60) and its degradation profile onto this sorbent.
**Fig S15:** Selected $^{13}$C MAS NMR spectra of adsorbed HD* (1% wt) on KF/Al$_2$O$_3$ (25, EtOH, 60) and its degradation profile onto this sorbent.
Fig. S16: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (10% wt) on KF/Al$_2$O$_3$ (25, EtOH, 60) and its degradation profile onto this sorbent.
Fig. S17: Selected $^{13}$C MAS NMR spectra of adsorbed HD* (10% wt) on TBAF/KF/Al$_2$O$_3$ (20, 20, EtOH, 60) and its degradation profile onto this sorbent.

$t_{1/2} (1) = 32$ min
$R^2 = 0.7822$
$t_{1/2} (2) = 620$ min
$R^2 = 0.94463$
Fig S18: Selected $^{31}$P MAS NMR spectra of adsorbed VX (10% wt) on TBAF/KF/Al$_2$O$_3$ (20, 20, EtOH, 60) and its degradation profile onto this sorbent.
**Fig S19:** $^{31}$P MAS NMR spectra of adsorbed GB (10% wt) on TBAF/KF/Al$_2$O$_3$ (20, 20, EtOH, 60) and its degradation profile onto this sorbent.
**Fig. S20:** The GC-MS-EI chromatogram and the EI and CI mass spectra of the degradation products from the extraction mixture of HD* on KF/TiO₂ (12, EtOH, 60).