Supporting Information

The electrochemical reduction of perfluorooctanoic acid (PFOA): an experimental and theoretical approach

Jonathan J. Calvillo Solís,[†,‡] Christian Sandoval-Pauker,[†,‡] David Bai,[†,‡] Sheng Yin,[†,‡] Thomas P. Senftle,[§,‡] Dino Villagrán[†,‡]

†Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, TX 79968, USA
[§]Department of Chemical and Biomolecular Engineering, Rice University, 6100 Main Street, Houston, TX 770052, USA

‡Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment (NEWT), El Paso, Texas 79968, USA.

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Figure S1 Stability of the linear sweep voltammetry response for silver electrode

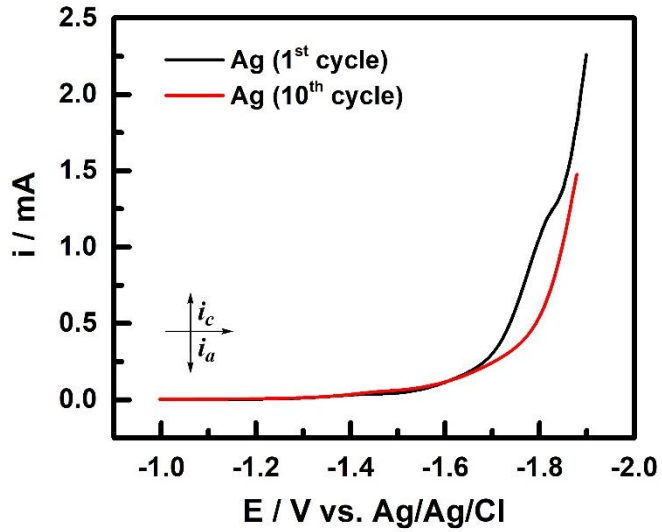

Figure S1. Linear sweep voltammetry of 1 mM PFOA in 0.5 M $KHCO_3$ (pH 9.5), electrochemical response of silver electrode before and after to 10 runs. v = 50 mV s^{-1}, φ = 3 mm.

Figure S2 Effect of the pH in the electrochemical reduction of PFOA on gold electrode

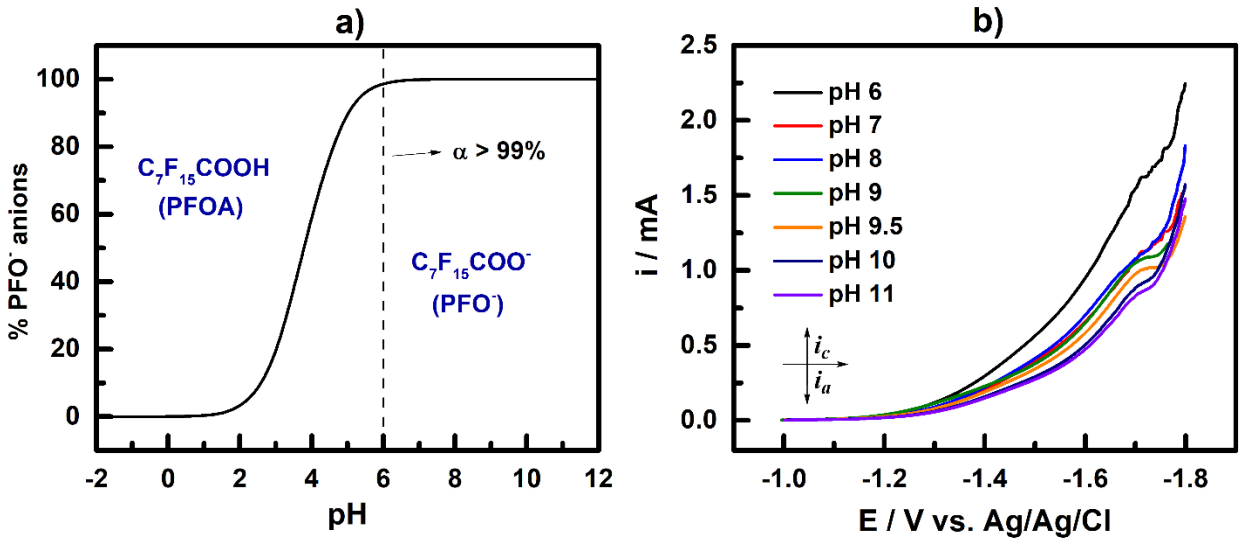

Figure S2. pH effect in the reduction of 1 mM PFOA + 0.5 M $KHCO_3$ for an Au electrode. (a) Fractional composition diagram for PFOA (pK_a = 3.8). (b) LSV response of the PFOA at different pH values. v = 50 mV s^{-1}, φ = 3 mm.

Figure S3 Adsorption study of PFOA into glassy carbon, boron-doped diamond, silver, and gold electrodes.

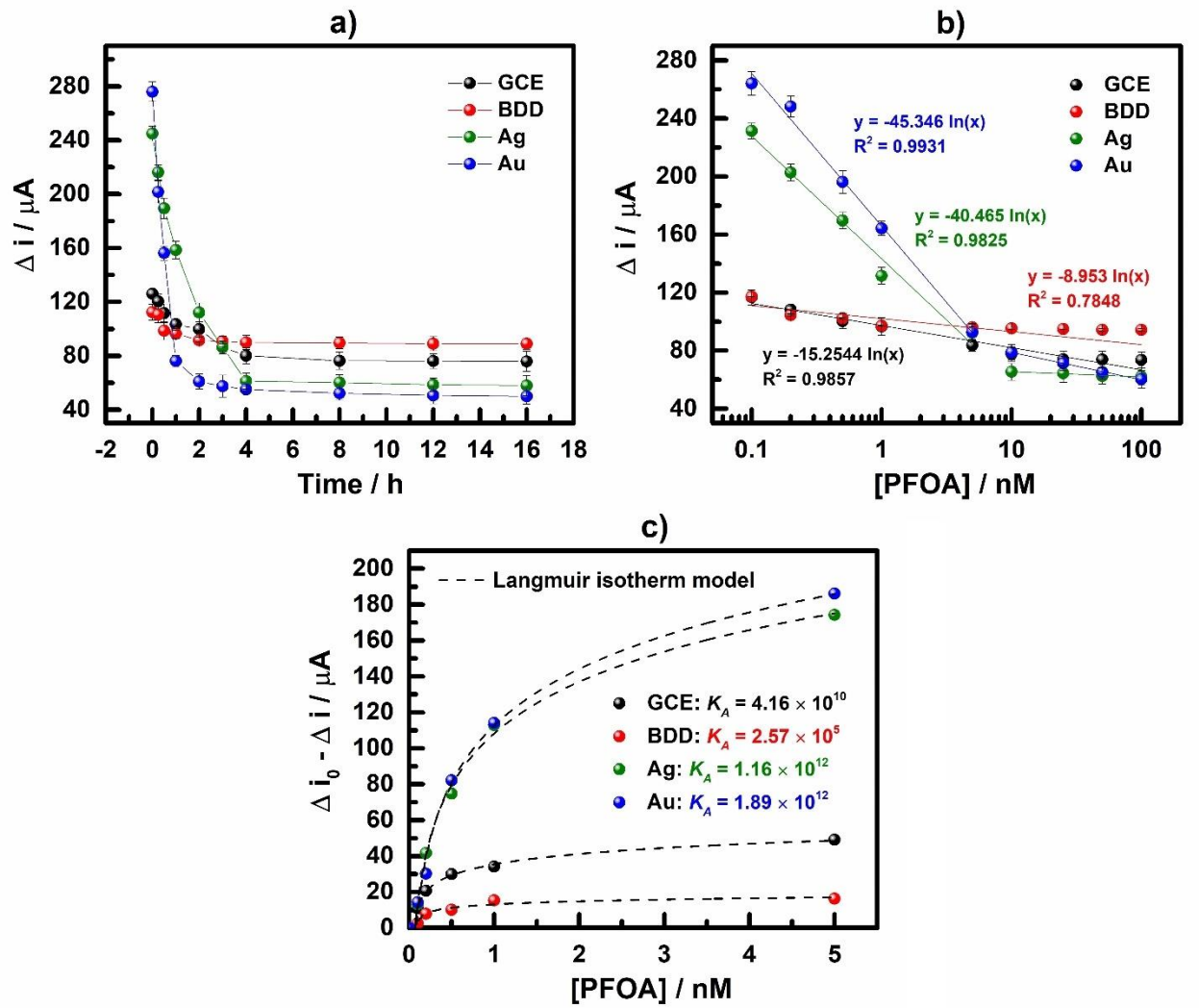

Figure S3. Adsorption equilibrium of PFOA into the different electrode materials (glassy carbon, BDD, silver and gold electrodes. (a) Adsorption kinetics in a 100 nM PFOA + 0.5 M $KHCO_3$ along 16 hours. (b) Square wave voltammetry response (Δi) vs ln [PFOA] plot. (c) Experimental data to the Langmuir isotherm model, calculation of the adsorption constants (K_A) for each electrode.

Figure S4 Adsorption study of PFOA into gold electrode in the absence and presence of a negative potential.

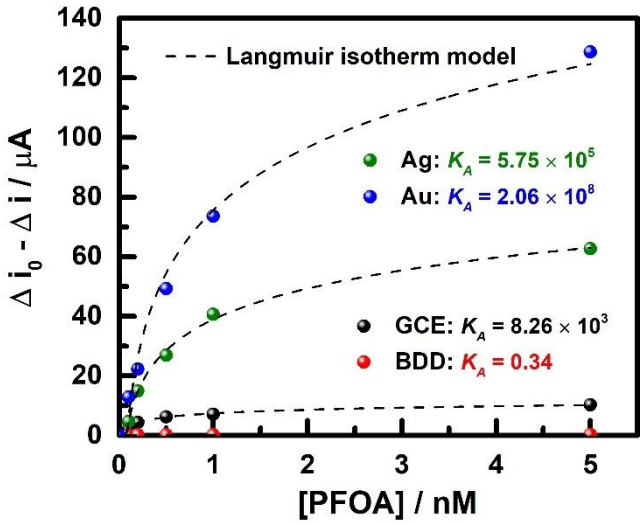

Figure S4. Experimental data to the Langmuir isotherm model, for the PFOA adsorption under a potential of –1.0 V vs Ag/AgCl. Calculation of the adsorption constants (K_A) for each electrode.

Figure S5 Adsorption kinetics of PFOA into gold electrode at E = –1.0 V

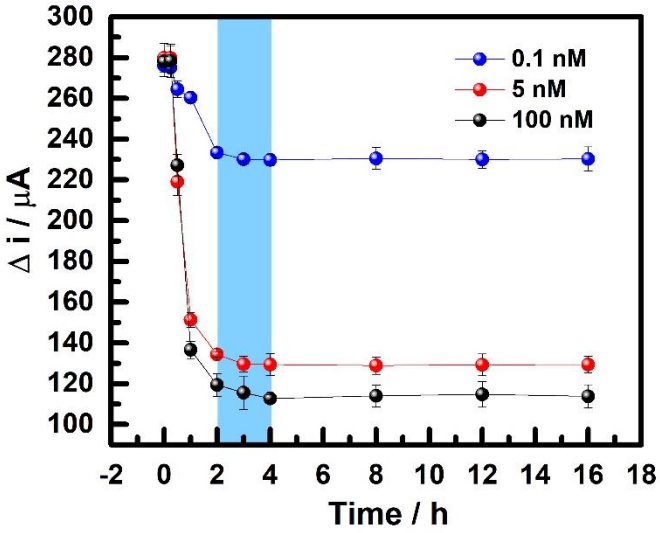

Figure S5. Adsorption kinetics of PFOA into Au electrode immersed in a 0.1 nM, 5 nM, and 100 nM PFOA solution, applying a potential of –1.0 V vs Ag/AgCl.

Figure S6 Calculation of the electrochemical active surface-area (ECSA) for gold electrode in the absence and presence of negative potential.

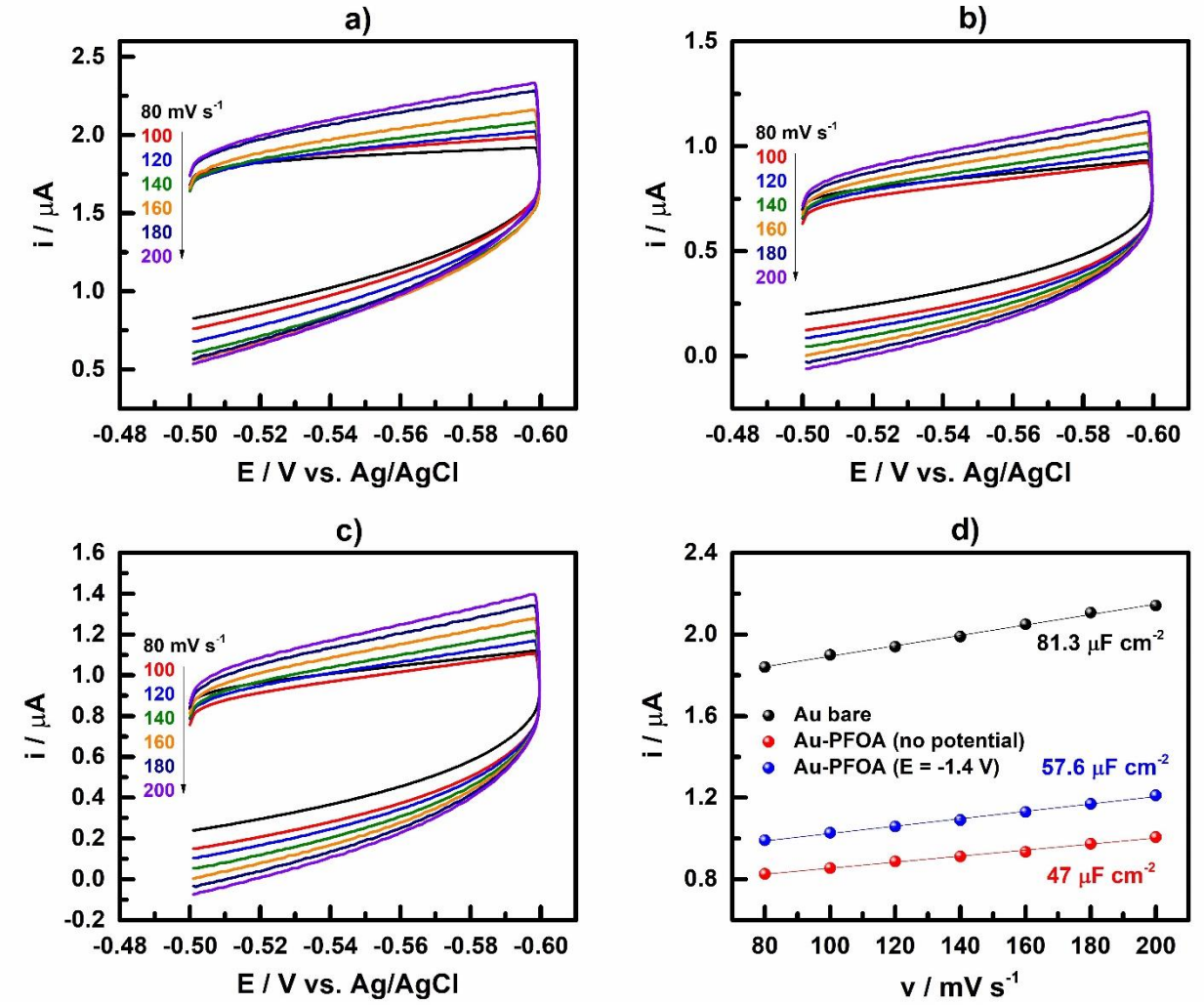

Figure S6. Calculation of the double-layer capacitance (C_{dl}) of gold electrode at different conditions in 0.5 $KHCO_3$ (pH 9.5). (a) Gold electrode in the absence of potential and without PFOA previously preconcentrated. (b) Gold electrode with PFOA adsorbed in the absence of potential. (d) Gold electrode with PFOA adsorbed at –1.4 V vs Ag/AgCl. (d) i_{dl} vs v plot. φ = 3 mm.

Table S1. Calculation of electrochemical active surface-area (ECSA) for gold electrode under different conditions. The specific capacitance (C_s) for gold electrode is 15.28 µF cm^{-2}.

Electrode	C_{dl} (µF cm^{-2})	ECSA (cm^2)
Au bare (no potential)	81.3	5.31
Au-PFOA (no potential)	47.0	3.07
Au-PFOA (E = –1.4 V)	57.6	3.77

Figure S7 Voltammetry study of the reduction of PFOA in gold electrode

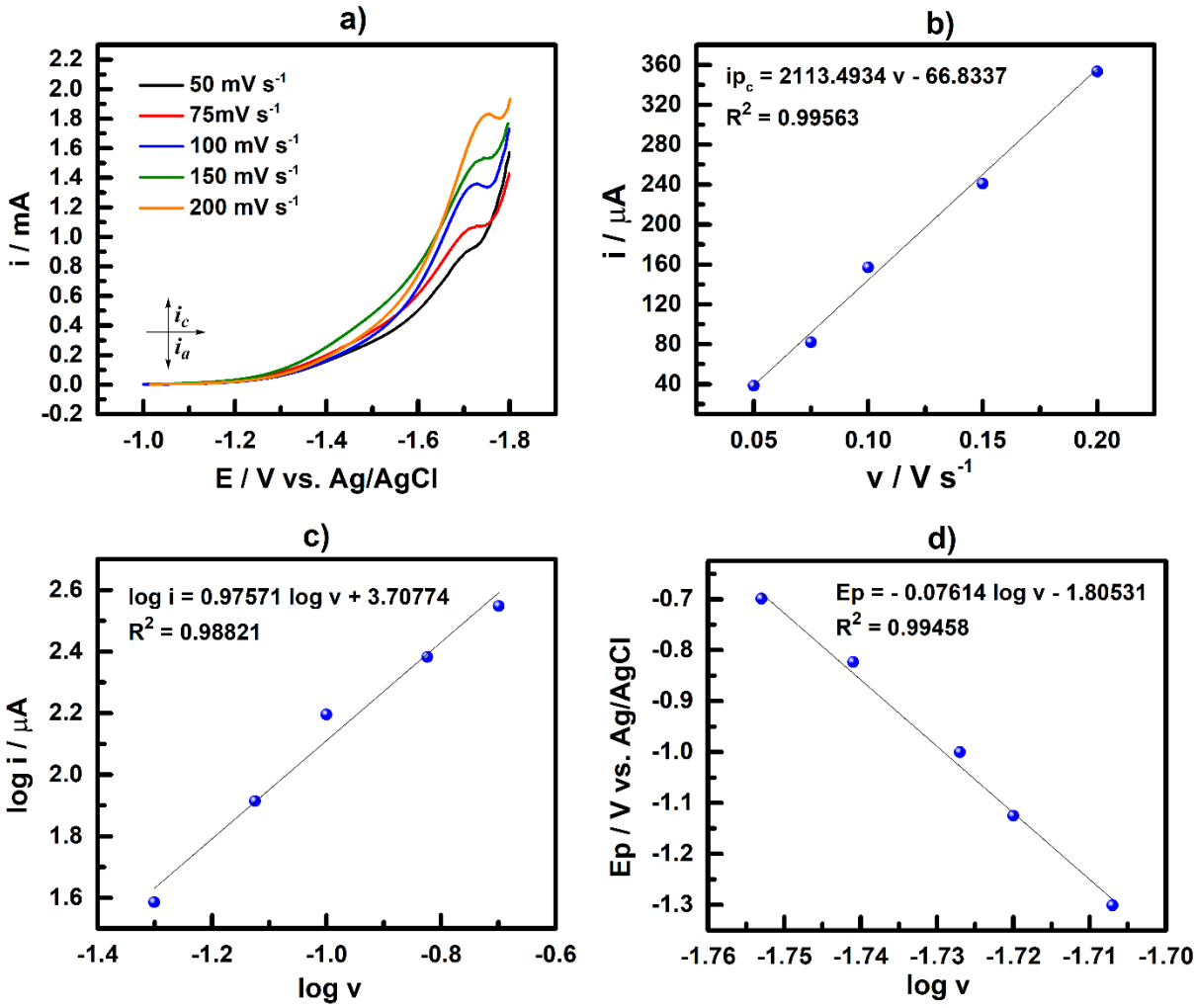

Figure S7. Electrochemical characterization of 1 mM PFOA + 0.5 M $KHCO_3$ (pH 9.5) for an Au electrode. (a) Linear sweep voltammograms from 25 mV s^{-1} to 200 mV s^{-1}. (b) ip_c vs. v plot. (c) log v vs log ip_c plot. (d) Ep_c vs. log v plot. φ = 3 mm.

Figure S8 UV-Vis characterization of the bulk-electrolysis products

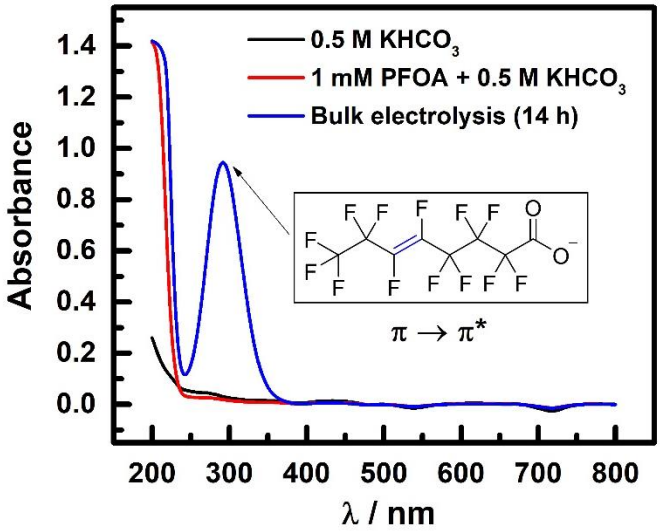

Figure S8. Comparison of UV-Vis spectra of 1 mM PFOA + 0.5 M $KHCO_3$ and the working solution after 14 h of bulk electrolysis on a gold electrode. T = 20°C, E_{app} = –1.80 V vs Ag/AgCl.

Figure S9 Mass spectrometry characterization of the PFOA and bulk-electrolysis products.

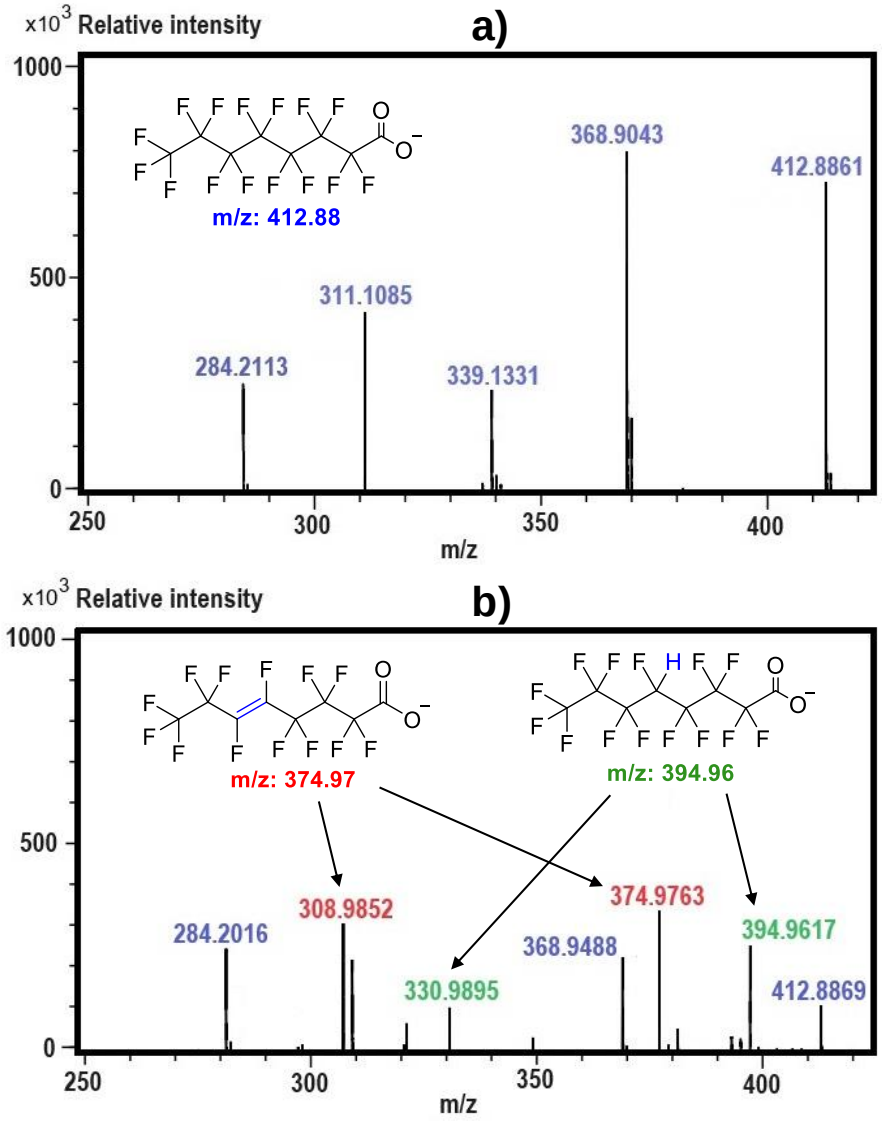

Figure S9. The mass/charge spectra for a) PFOA and b) for the solution after 14 h of bulk electrolysis on a gold electrode.

Computational details

Geometry optimizations and vibrational frequencies

Geometry optimizations were performed using DFT as implemented in the Orca software v.5.0.3[1]. As an illustration, the following input file was used for PFOA anion $[C_7F_{15}COO]^-$ (The lines for controlling the RAM allocation (%maxcore) and processors (%pal) are omitted for simplicity).

```
!TPSSh def2-TZVP opt d3 TightSCF SlowConv defgrid2

!CPCM
%cpcm smd true
SMDsolvent "WATER"
surfacetype gepol_ses
rsolv 1.40
radius[1] 1.250
radius[6] 2.000
radius[8] 1.600
radius[9] 1.682
end

* xyz 0 1
C       4.787576000     0.096990000    -0.374068000
O       5.440841000    -0.596843000    -1.091587000
O       5.034249000     1.373726000    -0.064926000
H       5.837623000     1.644568000    -0.535720000
.
.
.
F      -5.360953000     0.534038000     0.257000000
F      -4.437068000    -0.229003000    -1.546255000
*
```

The structures were optimized in the solvent phase using the meta GGA hybrid TPSSh functional and the def2-TZVP basis set[2–4]. The D3 keyword activates Grimme's D3 dispersion correction and the Becke-Johnson (D3BJ) damping scheme. The resolution of the identity approximation for Coulomb and chain of spheres approximation for exchange interactions (RIJCOSX)[5] is activated by default. The TightSCF command requests a tight convergence of the wavefunction, SlowConv selects the convergence strategy, and defgrid2 sets the numerical integration grid quality. The universal solvation model based on solute electron density (SMD)[6] accounted for the solvent effects (!CPCM section of the input). The atomic radii of the default method were adjusted to H (1.250 Å), C (2.000 Å), O (1.600 Å), and F (1.682). The radius of water was set at 1.40 Å. The gepol algorithm[7–9] generated the solvent cavity as a solvent-excluded surface.

The following input was employed to compute numerical vibrational frequencies in water at the same level of theory as optimizations to evaluate that the optimized equilibrium structures correspond to the minima of the potential energy surface and to obtain the thermodynamic corrections needed for compute the $G^{0,sol}$ value of each species.

```
!TPSSh def2-TZVP numfreq d3 TightSCF SlowConv defgrid2

!CPCM
%cpcm smd true
SMDsolvent "WATER"
surfacetype gepol_ses
```

```
rsolv 1.40
radius[1] 1.250
radius[6] 2.000
radius[8] 1.600
radius[9] 1.682
end

* xyz 0 1
C       4.777610000     0.108323000    -0.376967000
O       5.400666000    -0.594882000    -1.127140000
O       5.036365000     1.362972000    -0.040002000
H       5.837814000     1.667757000    -0.506041000
.
.
.
F      -5.353990000     0.536580000     0.254444000
F      -4.415371000    -0.191858000    -1.558422000
*
```

$E^{0,sol}$ and $G^{0,sol}$ values in E_h were extracted from the .out files of the previous calculations located in the sections as follows:

```
-------------------------   --------------------
FINAL SINGLE POINT ENERGY     -1954.334154121396
-------------------------   --------------------
```

For optimization calculations and

```
------------------
GIBBS FREE ENERGY
------------------

The Gibbs free energy is G = H - T*S

Total enthalpy                  ...  -1954.20053988 Eh
Total entropy correction        ...     -0.07500502 Eh    -47.07 kcal/mol
-----------------------------------------------------------------------------
Final Gibbs free energy         ...  -1954.27554490 Eh
```

For numerical frequency calculations.

Table S2. Summary of energies calculated at the TPSSh-D3/def2-TZVP level in water for the PFOA anion electroreduction mechanism. C_n (n= 1, 2, 3, …, 8) represents the carbon site where the C–F dissociation occurs.

Species	$E^{0,sol}$ (kcal mol^{-1})	$G^{0,sol}$ (kcal mol^{-1})
$[C_7F_{15}COO]^-$	−1226084.69	−1226055.64
$[C_7F_{15}COO]^{\bullet 2-}$	−1226115.52	−1226092.58
F−	–	−62767.80
H_2O	−47984.03	−47981.96
OH^-	−47665.02	−47669.86
TS (C_2)	−1226110.29	−1226087.00
TS (C_3)	−1226111.62	−1226089.53
TS (C_4)	−1226113.159	−1226090.74
TS (C_5)	−1226114.03	−1226091.52
TS (C_6)	−1226114.08	−1226091.45
TS (C_7)	−1226113.17	−1226090.81
TS (C_8)	−1226112.69	−1226089.55
$[C_7F_{14}COO]^{\bullet -}$ (C_2)	−1163373.43	−1163347.15
$[C_7F_{14}COO]^{\bullet -}$ (C_3)	−1163372.29	−1163346.19
$[C_7F_{14}COO]^{\bullet -}$ (C_4)	−1163373.07	−1163347.64
$[C_7F_{14}COO]^{\bullet -}$ (C_5)	−1163373.05	−1163347.49
$[C_7F_{14}COO]^{\bullet -}$ (C_6)	−1163373.18	−1163347.77
$[C_7F_{14}COO]^{\bullet -}$ (C_7)	−1163370.86	−1163344.81
$[C_7F_{14}COO]^{\bullet -}$ (C_8)	−1163362.63	−1163336.49
$[C_7F_{14}COO]^{2-}$ (C_2)	−1163457.39	−1163431.19
$[C_7F_{14}COO]^{2-}$ (C_3)	−1163463.26	−1163438.05
$[C_7F_{14}COO]^{2-}$ (C_4)	−1163467.91	−1163441.27
$[C_7F_{14}COO]^{2-}$ (C_5)	−1163471.64	−1163446.61
$[C_7F_{14}COO]^{2-}$ (C_6)	−1163473.63	−1163448.65
$[C_7F_{14}COO]^{2-}$ (C_7)	−1163472.39	−1163446.94
$[C_7F_{14}COO]^{2-}$ (C_8)	−1163454.10	−1163428.90
$[C_7HF_{14}COO]^-$ (C_2)	−1163787.56	−1163752.54
$[C_7HF_{14}COO]^-$ (C_3)	−1163789.98	−1163755.10
$[C_7HF_{14}COO]^-$ (C_4)	−1163791.29	−1163756.45
$[C_7HF_{14}COO]^-$ (C_5)	−1163791.44	−1163756.95
$[C_7HF_{14}COO]^-$ (C_6)	−1163791.76	−1163757.30
$[C_7HF_{14}COO]^-$ (C_7)	−1163791.88	−1163757.07
$[C_7HF_{14}COO]^-$ (C_8)	−1163783.86	−1163748.99

Calculation of standard reduction potentials

We computed the reduction potentials for the redox steps of the concerted mechanisms according to Eq. 1 and Eq. 2.

$$[C_7F_{15}COO]^- + e^- \rightarrow [C_7F_{14}COO]^{\bullet -} + F^- \quad (1)$$

$$[C_7F_{14}COO]^{\bullet -} + e^- \rightarrow [C_7F_{14}COO]^{2-} \quad (2)$$

We also calculated the reduction potential of the first electron transfer of a stepwise mechanism described in Eq. 3.

$$[C_7F_{15}COO]^- + e^- \rightarrow [C_7F_{15}COO]^{\bullet 2-} \quad (3)$$

For the computation of the reduction potentials compiled in Table 3 of the main manuscript, we employed the defining equation of the half-cell potential (Eq. 4) where $\Delta G^{0,sol}$ corresponds to the solution-state reaction Gibbs free energy of the redox event, n is the number of electrons transferred, and F is the Faraday constant (F = 96,485 C mol^{-1}).

$$E_{1/2} = \frac{-\Delta G^{0,sol}}{nF} \quad (4)$$

The standard reduction potential (E^0) was calculated according to Eq. 5, where $E_{1/2}{}^{0,ref}$ is the reference potential, which in our case is the standard hydrogen electrode (SHE), whose empirical value is 4.44 V[10].

$$E^0 = E_{1/2} - E_{1/2}{}^{0,ref} \quad (5)$$

As an illustration, Eq. 6 – 8 shows the calculation of E_0 for the redox process described in Eq. 1 at the C_4 dissociation site (energies are reported in Table S1):

$$\Delta G^{0,sol} = G^{0,sol}(F^-) + G^{0,sol}([C_7F_{14}COO]^{\bullet -}) - G^{0,sol}([C_7F_{15}COO]^-) \quad (6)$$

$$\Delta G^{0,sol} = (-62767.80) + (-1163347.64) - (-1226055.64) = -59.80 \text{ kcal mol}^{-1} \quad (7)$$

$$E^0 = 2.59 \text{ V} - (4.44 \text{ V}) = -1.85 \text{ V vs. SHE} \quad (8)$$

Construction of Gibbs free energy potential energy surfaces for the electroreduction of PFOA

Relative solution state Gibbs free energies were computed for each step of the proposed PFOA reduction mechanism to build the Gibbs free energy potential energy surface (e.g., Figure 6 in the

main manuscript). To provide a realistic representation of the reaction profile, an overpotential of U = −2.84 V vs. SHE was considered. Therefore, G(e^-) was determined to be − 36.94 kcal mol^{-1}. For building the PES, the number of electrons should remain constant throughout all steps for a valid comparison at different reaction stages. This implies that the solution state Gibbs free energies (see Table S1) of the species present in each step (even if they are not reacting yet) must be considered (see Table S2). The relative Gibbs free energies are calculated by subtracting the energy of the species in the corresponding step minus the energy of the reactants in the first step of the overall reaction.

Table S3. Calculated relative Gibbs free energies (kcal mol^{-1}) in each step of the proposed PFOA anion electroreduction mechanism. Values marked with (*) also correspond to the energy barriers computed as the energy of the transition state (TS) minus the energy of the reactants. Calculations were performed at the TPSSh-D3/def2-TZVP level of theory and the SMD solvation model.

Reaction step	**$G^{0,sol}$ (kcal/mol)**	**$\Delta G^{0,sol}$ (kcal/mol)**
C_2 dissociation site		
$H_2O + 2e^- + [C_7F_{15}COO]^-$	-1274111.49	0.00
$H_2O + [C_7F_{15}COO]\bullet^{2-} + e^-$	-1274111.48	0.00
H_2O + TS + e^-	-1274105.91	5.58*
$H_2O + [C_7F_{14}COO]\bullet^- + F^- + e^-$	-1274133.85	-22.37
$H_2O + [C_7F_{14}COO]^{-2} + F^-$	-1274180.95	-69.46
$[C_7HF_{14}COO]^- + F- + OH^-$	-1274190.20	-78.71
C_3 dissociation site		
$H_2O + 2e^- + [C_7F_{15}COO]^-$	-1274111.49	0.00
$H_2O + [C_7F_{15}COO]\bullet^{2-} + e^-$	-1274111.48	0.00
H_2O + TS + e^-	-1274108.43	3.05*
$H_2O +[C_7F_{14}COO]\bullet^- + F^- + e^-$	-1274132.89	-21.41
$H_2O + [C_7F_{14}COO]^{-2} + F^-$	-1274187.81	-76.32
$[C_7HF_{14}COO]^- + F- + OH^-$	-1274192.76	-81.27
C_4 dissociation site		
$H_2O + 2e^- + [C_7F_{15}COO]^-$	-1274111.49	0.00
$H_2O + [C_7F_{15}COO]\bullet^{2-} + e^-$	-1274111.48	0.00
H_2O + TS + e^-	-1274109.64	1.85*
$H_2O +[C_7F_{14}COO]\bullet^- + F^- + e^-$	-1274134.34	-22.86
$H_2O + [C_7F_{14}COO]^{-2} + F^-$	-1274191.03	-79.54
$[C_7HF_{14}COO]^- + F- + OH^-$	-1274194.11	-82.62
C_5 dissociation site		
$H_2O + 2e^- + [C_7F_{15}COO]^-$	-1274111.49	0.00
$H_2O + [C_7F_{15}COO]\bullet^{2-} + e^-$	-1274111.48	0.00

H_2O + TS + e^-	-1274110.42	1.06*
H_2O +[$C_7F_{14}COO$]$\bullet^-$ + F^- + e^-	-1274134.19	-22.71
H_2O + [$C_7F_{14}COO$]$^{-2}$ + F^-	-1274196.37	-84.88
[$C_7HF_{14}COO$]$^-$ + F− + OH^-	-1274194.61	-83.12
C_6 dissociation site		
H_2O + 2e^- + [$C_7F_{15}COO$]$^-$	-1274111.49	0.00
H_2O + [$C_7F_{15}COO$]$\bullet^{2-}$ + e^-	-1274111.48	0.00
H_2O + TS + e^-	-1274110.35	1.13*
H_2O +[$C_7F_{14}COO$]$\bullet^-$ + F^- + e^-	-1274134.47	-22.99
H_2O + [$C_7F_{14}COO$]$^{-2}$ + F^-	-1274198.41	-86.92
[$C_7HF_{14}COO$]$^-$ + F− + OH^-	-1274194.96	-83.47
C_7 dissociation site		
H_2O + 2e^- + [$C_7F_{15}COO$]$^-$	-1274111.49	0.00
H_2O + [$C_7F_{15}COO$]$\bullet^{2-}$ + e^-	-1274111.48	0.00
H_2O + TS + e^-	-1274109.71	1.77*
H_2O +[$C_7F_{14}COO$]$\bullet^-$ + F^- + e^-	-1274131.51	-20.03
H_2O + [$C_7F_{14}COO$]$^{-2}$ + F^-	-1274196.70	-85.21
[$C_7HF_{14}COO$]$^-$ (7-H) + F− + OH^-	-1274194.73	-83.24
C_8 dissociation site		
H_2O + 2e^- + [$C_7F_{15}COO$]$^-$	-1274111.49	0.00
H_2O + [$C_7F_{15}COO$]$\bullet^{2-}$ + e^-	-1274111.48	0.00
H_2O + TS + e^-	-1274108.45	3.03*
H_2O +[$C_7F_{14}COO$]$\bullet^-$ + F^- + e^-	-1274123.19	-11.71
H_2O + [$C_7F_{14}COO$]$^{-2}$ + F^-	-1274178.66	-67.17
[$C_7HF_{14}COO$]$^-$ + F− + OH^-	-1274186.65	-75.16

Figure S6 shows the resulting Gibbs free energy potential energy surfaces for the electroreduction of PFOA at U = −2.84 V vs. SHE for C_2 – C_8 dissociation sites.

Figure S10 Energy profile of the proposed pathway for the reduction of PFOA on gold electrode, at different dissociation sites.

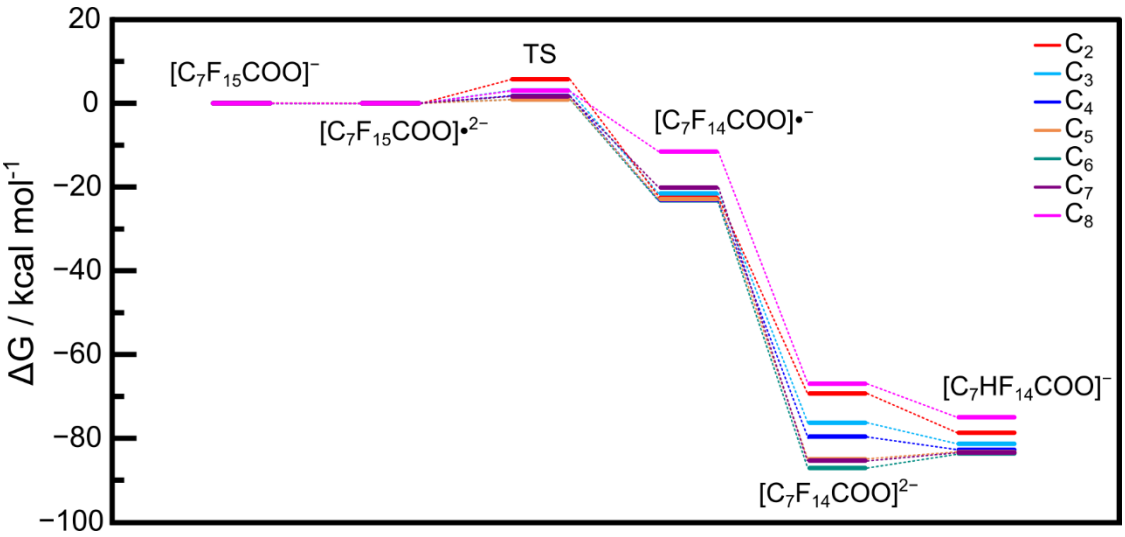

Figure S10. Calculated Gibbs free energy potential energy surface for the electroreduction of PFOA at U = –2.84 V vs. SHE for C_2 – C_8 dissociation sites. Calculations were performed at the TPSSh-D3/def2-TZVP/SMD level of theory.

Table S4. Cartesian coordinates of optimized structures (in Å) at TPSSh-D3/def2-TZVP/ defgrid2 level of theory. S is the spin multiplicity (M = 2S+1).

$[C_7F_{15}COO]^-$ S = 0

C	4.77538277376480	0.11873616680479	-0.46929380290674
O	5.20383245499588	-0.68487664120306	-1.31862708292012
O	5.16608397059546	1.26484859907359	-0.16723997896891
C	3.52092133530270	-0.36316113866069	0.34670977091429
C	2.21155685385340	0.30535931623378	-0.16221580883324
C	0.89215822324928	-0.42467936252897	0.24486045537788
C	-0.39274607384154	0.45894753906489	0.08050600553519
C	-1.71136940067184	-0.37756785856172	-0.00907232920367
C	-3.00246509867185	0.46684515549765	0.25578039837366
C	-4.30746507754347	-0.17596082846492	-0.31099739568869
F	3.35986013699923	-1.71569621230412	0.26135742501419
F	3.65861959288203	-0.06367903180395	1.67132034902390
F	2.15476633479832	1.57583544789216	0.30618185962511
F	2.25624573203980	0.35497817671942	-1.51749707968343
F	0.75335062706161	-1.53084679271452	-0.52028021522535
F	0.97736956449082	-0.80063211287722	1.53959236090093
F	-0.48400218941543	1.28760618929177	1.14378305695689
F	-0.28553210933389	1.19996392616004	-1.04237655557554
F	-1.66361627960115	-1.37203528036845	0.90273498028223
F	-1.79686745194423	-0.92132691669923	-1.24243882317764
F	-2.87239980875891	1.68659996165820	-0.30891480876494
F	-3.16060910215997	0.61611907941052	1.58509994162858
F	-4.38828359605369	-1.46348860060251	0.04072300039110
F	-5.36181710598542	0.47341227135877	0.19022988839356
F	-4.34503430605195	-0.08397405237622	-1.64129011146921

$[C_7F_{15}COO]^{\bullet 2-}$ S = 1/2

C	4.98240654919619	0.33606999726013	-0.09025273499764
O	5.41906685476932	0.43082180533967	-1.26198178146718
O	5.41320944826583	0.87907155330895	0.95515631988727
C	3.70340706836179	-0.53008847518481	0.08365238288953
C	2.37228445034393	0.26626352683095	-0.05260990160069
C	0.97931039396825	-0.42259921349573	0.08124732108794
C	-0.39016861296885	0.32900269350083	-0.05075550322317
C	-1.83696299429867	-0.27240899708435	0.05924448986933
C	-3.17745055379732	0.51344137727485	-0.06911957362618
C	-4.55558387294689	-0.18753498777266	-0.00263638077809
F	3.67555327233632	-1.53928840477058	-0.84702381030609
F	3.69758468355980	-1.13500138756548	1.31703218325885
F	2.41663488711946	1.26000290921710	0.89278008838062
F	2.40407110933920	0.86008155977022	-1.29022987491427
F	0.95160974987968	-1.41645256783701	-0.87649663903933
F	0.96360985424838	-1.01202875360372	1.32923879864296
F	-0.35050415905570	1.32000171461844	0.92423492937248
F	-0.35431554439262	0.92225656418131	-1.30706228008060
F	-1.89507303894787	-0.87188748048780	1.30805824193448

F	-1.90623159132995	-1.25374729671384	-0.91872661106137
F	-3.16277644407801	1.15753581868390	-1.28259202028058
F	-3.19878491050018	1.45391072249657	0.92981795204479
F	-4.69214176516064	-0.87259308060991	1.14508809244243
F	-5.59213561078817	0.69248847153194	-0.06056281934469
F	-4.70946078712325	-1.04133221988897	-1.02658546409079

TS (C_2) S = 1/2

C	4.86002575385927	0.25344867528303	0.15200833920172
O	5.63408284582650	0.62898078042371	-0.79078243206858
O	5.06955894620103	0.40255758869313	1.39812903250793
C	3.56253377897023	-0.37350597299424	-0.25249130383063
C	2.25341493556538	0.31721420971133	0.10206004546480
C	0.87940644963069	-0.42797846726059	0.02329798563597
C	-0.45208905433663	0.37767342298462	-0.08517993411003
C	-1.82255818556865	-0.33415719524037	0.14555533967729
C	-3.10742432518415	0.41554835230059	-0.32353675886590
C	-4.46776865269267	-0.11366065161597	0.21372423568018
F	3.51539930958558	-0.69240355513861	-1.58167818089621
F	2.32275178094594	0.88218517584550	1.33779046998661
F	2.12351984143167	1.38261611016182	-0.82827180584491
F	0.91099312185581	-1.27107103899275	-1.05289344694470
F	0.77150607866493	-1.18383830720014	1.17024486243290
F	-0.38803690114456	1.39371392472944	0.83243959815082
F	-0.50647222668913	0.91539275257560	-1.34352275547176
F	-1.95293005425400	-0.59105051874682	1.47495385296447
F	-1.79976998332616	-1.52552055727479	-0.52585198841599
F	-3.17155169880489	0.37018594838476	-1.67507003033639
F	-3.02439285801743	1.71926297639132	0.06398915840260
F	-4.58813409533043	0.10748125164760	1.52632956062956
F	-5.48095593975067	0.51359578649610	-0.40942278664504
F	-4.59203919923211	-1.42767151207455	-0.01605360573954
F	3.45093033179444	-1.73899917908972	0.44423254843482

TS (C_3) S = 1/2

C	4.83426542479384	0.37692302074982	0.08701200864986
O	5.37851537757032	0.92164106601405	-0.90504345605084
O	5.17393094997599	0.44630064708501	1.29522441567996
C	3.56350856175769	-0.46073888307750	-0.20055101839449
C	2.23956339487364	0.20369039463910	0.18693431325810
C	0.90887495611914	-0.47797647545357	0.03773482337385
C	-0.42967195200673	0.32173376457173	-0.09358694909584
C	-1.83227431683827	-0.31880564195689	0.14270636092605
C	-3.11385025909281	0.43123658339804	-0.32648861367844
C	-4.49192041413285	-0.08161586540399	0.17363421330588
F	3.50495199825502	-0.83080945557696	-1.51679946845878
F	2.33123225061055	0.77903194196253	1.41337968928297
F	0.95019872120173	-1.36025525834069	-1.00483401736208
F	0.71106822909395	-1.23198130904521	1.24431173776905

F	-0.34369172319866	1.38138643264732	0.77693207370710
F	-0.46458625366197	0.80647759016190	-1.38690549005867
F	-1.97281955487516	-0.54244268784916	1.48328012971169
F	-1.84116149656752	-1.52950418551549	-0.50878256692674
F	-3.16129254151839	0.40918848262194	-1.68296818095398
F	-3.02687052369282	1.73248162090849	0.08527394663778
F	-4.62934035695619	0.10439297559252	1.49122593540858
F	-5.49494002399825	0.57743955099211	-0.44230897773979
F	-4.64116439481406	-1.38742260801056	-0.09350930390781
F	3.64135254099225	-1.66476549170565	0.51794663617200
F	2.20612140610954	1.39439379059114	-0.77381824125539

TS (C_4) S = 1/2

C	4.88428804585299	0.24766471377375	0.00436480832706
O	5.42055862042748	0.23811842717816	-1.12962643109552
O	5.25215862829471	0.85703491193168	1.03972169579138
C	3.56189666179825	-0.55048140307916	0.14616123609326
C	2.27383883702161	0.32532694908448	0.01977924806866
C	0.88358380288403	-0.27957453054671	-0.20578081922479
C	-0.44246054771244	0.43062571237051	-0.06459800616013
C	-1.82944710232515	-0.30183913330376	-0.00701555079209
C	-3.16333149246362	0.47444662310804	-0.21815612244207
C	-4.48866146208791	-0.20922909446472	0.21412982142735
F	3.48289833506684	-1.53882921827864	-0.80473094333027
F	2.23341080518229	1.11908580050233	1.13280346304755
F	2.50685063788761	1.15326479824133	-1.07541294059506
F	0.89384773669301	-0.93925988685570	-1.40065021892868
F	-0.40487765504129	1.23456113360943	1.04603011700673
F	-0.56680317540775	1.24910433846286	-1.22061135768504
F	-1.92341539422901	-0.89027048442861	1.22938423036169
F	-1.80995480548195	-1.28995858350207	-0.95915041052147
F	-3.29439228503080	0.77358688738326	-1.53655151341197
F	-3.10153429576608	1.64451530808945	0.48913620150408
F	-4.55918403332585	-0.33514909611286	1.54470754521680
F	-5.55634469905961	0.51451452101195	-0.18459273091958
F	-4.59824888811333	-1.42761247911057	-0.33784564569028
F	3.52119069807249	-1.17979081127450	1.36628716042188
F	0.82413302686345	-1.31985540378991	0.91221716353048

TS (C_5) S = 1/2

C	4.91180929689932	0.37055367453346	-0.03129853763718
O	5.31705724450501	0.77577038372872	-1.14568049482577
O	5.35398976173508	0.62925007983209	1.11144636682602
C	3.65402888750786	-0.54658580777948	-0.08072208708415
C	2.31239466873114	0.23919195073252	-0.16012119764693
C	0.95570394935341	-0.49732909260396	0.10360462193277
C	-0.40337236723546	0.08719443829508	-0.29702815718932
C	-1.79954693728503	-0.36487254416658	0.11967195915207
C	-3.09419530151344	0.49586825281835	-0.07234211476996

C	-4.49446137400371	-0.15768823644805	0.04283001235081
F	3.71515792616740	-1.38550643308834	-1.16315300104190
F	2.40180918276545	1.26677946864823	0.73857897835476
F	2.24806947480279	0.78879799629003	-1.41327246111368
F	1.06182966010778	-1.70538773128998	-0.58569102892501
F	0.92188971070558	-0.77000435415459	1.44688195546741
F	-0.40892917134841	0.22519391136615	-1.66078386285585
F	-1.77108887747174	-0.68216016065093	1.45711979301308
F	-2.06042359110591	-1.53031965239624	-0.61528881059758
F	-3.04962524766188	1.04940523439608	-1.32614992889951
F	-3.07692148961984	1.50133973698811	0.84811533224110
F	-4.61218605576034	-0.82891652218112	1.20121881318074
F	-5.48404473541127	0.76909731177944	0.01808820593695
F	-4.72284271225611	-1.00827911917980	-0.96662576173360
F	3.59659291747306	-1.35135356968606	1.03110346197010
F	-0.33223282008076	1.45812678421684	0.34898594389463

TS (C_6) S = 1/2

C	4.94455966296419	0.20135365471252	-0.25899077406549
O	5.42156062970213	-0.30864053416473	-1.29608066994439
O	5.35623919689753	1.17626955829034	0.40942453305349
C	3.62329264594567	-0.44092817484574	0.26919516819918
C	2.34512481030025	0.33121993018189	-0.16647684436617
C	0.95846608039735	-0.35871301287965	0.01762360189117
C	-0.36976735285597	0.47605905412048	-0.05283508493476
C	-1.76551465512435	-0.11855303624702	-0.21515978648253
C	-3.12545467921830	0.54601512511756	0.01584374528834
C	-4.46215801640992	-0.23978537653075	0.00498555054419
F	3.49729690563702	-1.73323369579224	-0.17253820601310
F	2.32553209582838	1.50641373334487	0.53437216795338
F	2.48624375106333	0.64142476316695	-1.48870955264390
F	0.86924006683476	-1.32417383376488	-0.95512120412147
F	0.97993400981140	-0.97975957774300	1.23725002514795
F	-0.37899764486878	1.25159362584781	1.08595332577347
F	-0.18665193872300	1.30698643188031	-1.16873108482098
F	-1.82182464137590	-0.72066559878918	-1.44780336411551
F	-3.28604294385830	1.48205148363837	-1.00482495570505
F	-3.10103745386669	1.20695706241060	1.21430910546887
F	-4.54964295288441	-1.06909700182815	1.05578429954131
F	-5.55568259470763	0.57376023618461	0.06025129845969
F	-4.57867393850534	-0.96797983689193	-1.11942638858854
F	3.63482649236378	-0.49744511769452	1.63801806556813
F	-1.78255853534717	-1.17069886172455	0.86931502891273

TS (C_7) S = 1/2

C	4.93297671620382	0.30417599365959	-0.20243141341804
O	5.39954388623378	0.10133419045110	-1.34440886405727

O	5.32736398060556	1.08782204357680	0.69051760405537
C	3.64771244725723	-0.50646062068650	0.15849338439854
C	2.33495062418827	0.30512319317339	-0.05138392092175
C	0.97397424644535	-0.46143595807329	-0.06677682063617
C	-0.37997941887617	0.30964857010847	0.01434208086407
C	-1.80650778202255	-0.37274806448851	-0.04268482840907
C	-3.10154156023192	0.37216778639207	-0.25882123060500
C	-4.48004873107144	-0.15474685660570	0.12203596084399
F	3.56445147515081	-1.64884240947006	-0.59343915066828
F	2.28877549229412	1.25036157543308	0.93259148147303
F	2.44247982776578	0.95861489233688	-1.24673165893054
F	0.96328321822623	-1.19256866015502	-1.22273442107711
F	0.99120696572601	-1.32961085661368	0.99813742539292
F	-0.35085716699141	1.01296510021742	1.19393103103895
F	-0.36270538776244	1.20644234547528	-1.03963410328925
F	-1.91667897236245	-1.09185299893744	1.12732205994604
F	-1.70519851690584	-1.27016709473408	-1.12598855382320
F	-3.17565689190968	0.82285728527391	-1.53870029122030
F	-4.54711887153507	-0.53087413817236	1.40713152778461
F	-5.49164012639368	0.74181096730600	-0.08786422095132
F	-4.79502300654746	-1.23092399650137	-0.64394586753089
F	3.68393474860091	-0.90558063077482	1.46844764346453
F	-3.01326319608775	1.59270834180885	0.63600714627614

TS (C_8) S = 1/2

C	4.93844261490970	0.31141901060254	-0.13134780296646
O	5.38166339323941	0.33459166593807	-1.29866232533136
O	5.35975886795342	0.88294783791281	0.89627341817187
C	3.64180347777849	-0.54851489829218	0.07413939079135
C	2.33949105384555	0.28688694947620	-0.08578557793208
C	0.96563177055200	-0.43994478352631	0.06209185714351
C	-0.34657480754658	0.39847466542185	-0.07889793010216
C	-1.75052405161578	-0.27153700163514	0.04482121771569
C	-3.13618376625515	0.48970013351251	-0.07565237518596
C	-4.48681049370537	-0.15890856343174	0.01847677458851
F	3.59888754091144	-1.57726764775725	-0.82479528268800
F	2.38486393597901	1.28506783291273	0.83982933349218
F	2.37955902757502	0.85643110485783	-1.32342705863439
F	0.92037390233521	-1.42281153187186	-0.88198622285445
F	0.94499501289761	-1.02153531649366	1.29540759167837
F	-0.29451424305197	1.37601681051469	0.88092245826731
F	-0.30447104859933	0.99116313012277	-1.31406829597943
F	-1.78161065306252	-0.87787723604986	1.28286485757948
F	-1.79727812860272	-1.25042992616056	-0.92696492952752
F	-3.09829081981248	1.10644361487128	-1.31866368779480
F	-3.10123474597202	1.44558800780731	0.93286200605714
F	-4.66099043782653	-0.78319446181427	1.19843806190015
F	-4.69057078571779	-1.03453703313300	-0.98234470455848
F	3.63588608933673	-1.11322113387873	1.31994186259132
F	-5.77594070554538	0.69772577009399	-0.05776063642178

$[C_7F_{14}COO]^{\bullet-}$ (C_2) S = 1/2

C	4.84689165561349	0.11744281703011	-0.12987700646041
O	5.75931342181797	-0.66960761581665	0.22364238410472
O	4.94349449007860	1.30345962600470	-0.54285397858611
C	3.45846775150746	-0.41572685866437	-0.06460211310399
C	2.21316882933756	0.31737546137847	-0.44905213557759
C	0.89876640462228	-0.40917307040770	-0.02283920706796
C	-0.39124569772647	0.47486638578364	-0.11513297231141
C	-1.71520986161150	-0.36513222641345	-0.09709221013551
C	-2.97228520990065	0.47274009779482	0.30737446448014
C	-4.33426744308303	-0.19118681596314	-0.06704456965878
F	3.28527668458810	-1.72783279096755	0.14578974552727
F	2.18734915195352	1.55852136095416	0.11601690547562
F	2.15509320876182	0.50665009658931	-1.81014557855236
F	0.72508750121916	-1.50144144111880	-0.80383521602355
F	1.02453101442462	-0.80662792612981	1.26475245626695
F	-0.40788792997423	1.32381835575468	0.93585249976095
F	-0.37126970113307	1.19751538781310	-1.25388389840429
F	-1.58925017673158	-1.38150764132854	0.78293798512941
F	-1.91447453356483	-0.88242077829005	-1.32830009589884
F	-2.92727024574055	1.67813697015703	-0.30048324681247
F	-2.96124357837616	0.65510557057553	1.64289196598600
F	-4.37135880850359	-1.45875006012247	0.35543849864186
F	-5.32091386868448	0.48736903650571	0.52618912977821
F	-4.53349575989444	-0.16505746711875	-1.38583647955787

$[C_7F_{14}COO]^{\bullet-}$ (C_3) S = 1/2

C	3.86161266876965	1.05489552758341	-0.11549452650615
O	5.09248549145235	1.21431870421592	-0.20176462779537
O	2.92066703768761	1.84548798346639	-0.34290208885202
C	3.35486621448397	-0.34563671874293	0.38441086758577
C	2.28392072655935	-0.90242139728916	-0.49226819156641
C	0.87863867340765	-1.28052798488218	-0.15248103849617
C	-0.13655848259112	-0.08786248545661	-0.15401756092018
C	-1.64445353834633	-0.50447673731887	-0.12419813239029
C	-2.59933501303495	0.65097564363820	0.31967419284128
C	-4.10216312497457	0.41945521257879	-0.02990760152147
F	4.38646133342553	-1.25546071360905	0.47219503192465
F	2.54126387433564	-0.82782604869684	-1.79961678376147
F	0.43068880041850	-2.18322943811435	-1.07480242667056
F	0.84335067991414	-1.86308717535428	1.07151765575622
F	0.12193818900767	0.68526030752707	0.92361716254733
F	0.07295596930801	0.63806639684051	-1.27436261218296
F	-1.80982656554175	-1.53572546787736	0.73239194869245
F	-2.00651678521112	-0.91298755386460	-1.36006847053498
F	-2.21960443508350	1.80453281260497	-0.27232682827045
F	-2.51318181372678	0.79778232843349	1.65719744830180
F	-4.50882016720825	-0.77796020493491	0.40390481106042
F	-4.83085517184693	1.36430535542124	0.57270981393871

F	-4.30926986534247	0.49956302968733	-1.34532795983779
F	2.87132668813770	-0.20089265985617	1.66234292465764

$[C_7F_{14}COO]^{\bullet-}$ (C_4) S = 1/2

C	4.53029859088469	0.00158846952829	0.52939718690881
O	5.30365479145781	-0.86611772605478	0.07995359314070
O	4.77064090519327	1.11681661450228	1.03510526563184
C	3.00356231008701	-0.34393529878104	0.42682212387225
C	2.29671744782286	0.29653236647982	-0.79774370497514
C	0.87042151349011	-0.13601383680985	-0.98079604212819
C	-0.35609218434239	0.64158334344296	-0.62995068755309
C	-1.57451526210043	-0.28055899464915	-0.29995707079355
C	-2.76268087893080	0.44642679994073	0.40819489612892
C	-4.10927862510526	-0.34320117630348	0.36162867049893
F	2.79480602594440	-1.69201084592891	0.32464444313881
F	2.34245328255758	1.64996770899306	-0.67999681795739
F	3.00203902925142	-0.05574619779613	-1.91219211932427
F	0.68261293792159	-1.23809063756496	-1.69639529244900
F	-0.10877876497837	1.42420922556663	0.45029296863572
F	-0.72409724655873	1.46814705915077	-1.65728833698075
F	-1.14218205190497	-1.26787426308421	0.51727031644404
F	-2.02656552481931	-0.83334103304478	-1.44734929051362
F	-2.97755860759621	1.64568267292481	-0.17293232872170
F	-2.44520930708730	0.64111934311049	1.70385110664294
F	-3.92777065033795	-1.61125701908395	0.74452179523191
F	-4.97865783116990	0.23581090939730	1.19486608222701
F	-4.62678463894309	-0.32929794065148	-0.86818086255823
F	2.32657778026399	0.06922525171559	1.54069005045304

$[C_7F_{14}COO]^{\bullet-}$ (C_5) S = 1/2

C	4.56863907560158	0.54995433690236	0.16542562496439
O	5.46351207381240	-0.18690474631262	-0.28924498428397
O	4.54319688704934	1.78641979046931	0.33314248827833
C	3.24081225194858	-0.17246677261979	0.59628332944106
C	2.06264156045467	0.15681838391462	-0.36151397420101
C	0.83769181259996	-0.80928214500104	-0.29666396424258
C	-0.38191457849798	-0.24007337628743	-0.95501286050282
C	-1.80714389625452	-0.63240231020203	-0.67877531603536
C	-2.55842414071868	0.41214502506876	0.20275473035658
C	-4.07625866644760	0.16399273562683	0.43737387786329
F	3.39109585648098	-1.52791834817008	0.62489083810753
F	1.60439525801961	1.40461464785264	-0.08966608545188
F	2.53544909548403	0.14595022139049	-1.63514268960486
F	1.18537136587711	-1.99674481047816	-0.87992192689853
F	0.55196195324681	-1.06827488310405	1.00620698366265
F	-0.19443876162887	0.48497947927018	-2.04744731436742

F	-1.84158624066245	-1.83316291339430	-0.05102920598875
F	-2.47380346876685	-0.73754914098746	-1.85723410081484
F	-2.42539036290186	1.62120192202011	-0.39014216628128
F	-1.95739679229493	0.45420133034497	1.41155407049955
F	-4.27825957445631	-1.03144267487938	0.99827187768918
F	-4.54592581987478	1.10735953597323	1.26145241927529
F	-4.75529437384676	0.22607171191597	-0.71022637823965
F	2.88193468677651	0.21140666468687	1.85760571577510

$[C_7F_{14}COO]^{\bullet-}$ (C_6) S = 1/2

C	4.69303524769469	-0.25315997642706	0.01971355201867
O	5.22031246755956	-1.21248483425062	-0.57380945447706
O	5.13826426402955	0.88262024077653	0.28251876961498
C	3.22206941366885	-0.48530371596816	0.52313316136651
C	2.18787494460387	0.34835925671987	-0.28308858168308
C	0.70502594997403	-0.11628508148283	-0.14312317413565
C	-0.37174897459034	0.92231928076068	-0.59957221241902
C	-1.74347891169124	0.31790905664582	-0.71109602098463
C	-2.86622752378760	0.50829676356240	0.25523120282260
C	-3.95362739554605	-0.60347081774852	0.18001391243686
F	2.85617328780639	-1.79681006438894	0.42744775757764
F	2.26338232846758	1.64504845835049	0.09857308349531
F	2.52124496962798	0.27445416442527	-1.59798227490821
F	0.51973969219061	-1.23214469961959	-0.88908598517531
F	0.44447828799091	-0.41967990375112	1.14969780086912
F	-0.40906380577975	1.94209116795360	0.29054345183255
F	-0.00217855674480	1.40976611865708	-1.81322270038040
F	-2.03475007323664	-0.25321835078440	-1.86952140111601
F	-3.50487273469047	1.70203254240863	0.05999925845027
F	-2.37851564589682	0.51603034037728	1.52060868665861
F	-3.38288854726554	-1.80854859156576	0.29848103706299
F	-4.82211582473691	-0.43952921282609	1.18079378633536
F	-4.61904646223299	-0.54927380374240	-0.97651345257034
F	3.11302896058512	-0.13978566108216	1.84074409130820

$[C_7F_{14}COO]^{\bullet-}$ (C_7) S = 1/2

C	4.81047929337783	0.17973847931883	-0.29403848086256
O	5.42564730912020	-0.63806753490917	-1.00295965897224
O	5.05662116964169	1.37518884685886	-0.03358411810715
C	3.50076107105260	-0.35602672098252	0.38978424645998
C	2.22186242824216	0.29413237210965	-0.20846627527028
C	0.89069412521315	-0.47305382461378	0.08328498526138
C	-0.39277257534339	0.39673691956043	-0.13298449690942
C	-1.71033075077879	-0.43474159946333	-0.26333096663445
C	-2.93917099463076	0.41030326528212	-0.09127009472668
C	-4.34317177133634	-0.12102615164856	-0.02723720747599
F	3.37762590025355	-1.70839123966206	0.25420015945417
F	2.09660214270350	1.55565749831508	0.26699781416740
F	2.37559872912599	0.35965718343390	-1.55624926002531

F	0.82336313814522	-1.55341286411445	-0.72596648841852
F	0.89848488022513	-0.89417694377478	1.36742867986016
F	-0.52961309724080	1.22720818208599	0.92536545555308
F	-0.24350878132537	1.13654987206441	-1.25418496676090
F	-1.70015257692903	-1.41555757395598	0.67251617500938
F	-1.71807650924147	-1.04112181970112	-1.48930635175777
F	-2.86677398693674	1.65031345773887	-0.55829498520056
F	-4.38160309772102	-1.33981894145252	0.52036879737642
F	-5.11871842449813	0.70258936173645	0.69708353124918
F	-4.89368664317686	-0.20198928200437	-1.25954205866385
F	3.52607002205767	-0.09309644222195	1.73047306539453

$[C_7F_{14}COO]^{\bullet -}$ (C_8) S = 1/2

C	4.81256819780283	0.15904991792840	-0.39131312418069
O	5.34451353470945	-0.62597514901847	-1.19786620744523
O	5.12593933664985	1.32170336291699	-0.06276701211548
C	3.52554420611369	-0.37801166565840	0.33478901872272
C	2.23185638662750	0.30004507567091	-0.19598794811114
C	0.90124951911123	-0.44052027974769	0.15683150983125
C	-0.37749406708576	0.44737978283941	-0.01137627766154
C	-1.70725622268834	-0.37480203710500	-0.07187695829719
C	-3.00107648018368	0.46775005542233	0.19722754853806
C	-4.29788110808608	-0.20450105091303	-0.21599260644813
F	3.38187403341960	-1.72510702547640	0.17253055329146
F	2.15767622964336	1.56059693105252	0.29438630354215
F	2.31947157288184	0.37464820046228	-1.54871258081347
F	0.77738138004017	-1.52264871774878	-0.64498979982579
F	0.95654157312602	-0.85701588567523	1.44094868665191
F	-0.44870907770170	1.30331002429239	1.03109136522403
F	-0.27177573336023	1.16091959133231	-1.15325667685323
F	-1.66086983498081	-1.36886520227782	0.84241042717733
F	-1.81981927411960	-0.92592448943306	-1.30175642549113
F	-2.90769968802930	1.63498377229611	-0.48111886169909
F	-3.07205365520440	0.72521562632384	1.52367694916024
F	-4.55008816141240	-1.36109687557236	0.37526818905277
F	-4.53830950911076	-0.24946684478468	-1.51455680749875
F	3.60628213483751	-0.14653663912659	1.67856325924897

$[C_7F_{14}COO]^{2-}$ (C_2) S = 0

C	4.28547667391378	-0.21885871131303	-0.44200011930530
O	4.13477869619218	-0.31516832037202	-1.71370445403864
O	5.09975469615268	-0.96358093843342	0.21548619113744
C	3.57570999761582	0.81942495611098	0.27463033026439
C	2.22975221138019	1.25431272181110	-0.05709188664398
C	1.03169205356893	0.26625303806724	0.20054317608613
C	-0.42655432134080	0.81208600460713	0.06123518814334
C	-1.52588645070486	-0.29493109426756	-0.07107590196273
C	-2.97686233111307	0.21542524454866	0.20645594011413
C	-4.10803044051251	-0.73896238849461	-0.28683689721566

F	3.67426563947960	0.71685287389615	1.69819624834913
F	1.86035280080155	2.39026304299075	0.69910311385756
F	2.12001580785430	1.61185710181841	-1.37873104169294
F	1.15694029265569	-0.77806945849678	-0.66763444759099
F	1.14202471781514	-0.23428348406683	1.46064916484138
F	-0.72332919828854	1.56227378459039	1.15152757832309
F	-0.51697012247889	1.60141988235941	-1.03487484348300
F	-1.26914974174417	-1.29449183335513	0.80274555900126
F	-1.48641750961209	-0.80121315467626	-1.32496444288650
F	-3.16529759519184	1.40600267203647	-0.40447957388552
F	-3.13859288595538	0.37738078707646	1.53603120154744
F	-3.90934242364757	-1.98358141308843	0.15934788954584
F	-5.27871024397546	-0.29694178294678	0.18607418269411
F	-4.17223532286467	-0.75968753040228	-1.61969815519999

$[C_7F_{14}COO]^{2-}$ (C_3) S = 0

C	4.69666432462711	0.23026132080907	-0.35970018351845
O	5.25252735754971	-0.47348321800070	-1.23389367233624
O	5.02726235910223	1.37873645444968	0.02664506219802
C	3.43929011872268	-0.36192191557260	0.34861653299034
C	2.18799964589967	0.22812211120593	-0.13805807493829
C	0.94680017275595	-0.47291535955969	0.12161404929008
C	-0.34463576955671	0.38023516234467	-0.06789300790923
C	-1.70144600459616	-0.39749277244274	-0.05637023728828
C	-2.94688205061409	0.50281638738000	0.23450040756822
C	-4.31273249080891	-0.13449646389383	-0.17106893082368
F	3.52424468570568	-1.79361202214647	0.25962806737116
F	2.30655515581873	0.46735165328335	-1.55133997120257
F	0.67687974800416	-1.64369627073337	-0.68763437358200
F	0.92821178567462	-0.93902801856310	1.40946113799944
F	-0.40020705725434	1.29570044423782	0.94079045909820
F	-0.28792950565069	1.06001298536333	-1.23895143530955
F	-1.67561596319466	-1.36379593535115	0.88985765789072
F	-1.88980807650774	-0.98473800212654	-1.26198364436133
F	-2.84142821773691	1.67105408272730	-0.43795063358288
F	-3.00214456823939	0.76706632132303	1.55723056570437
F	-4.42034440097230	-1.37937544200566	0.30551130165066
F	-5.30485562043607	0.60352567378248	0.34069587380502
F	-4.45368180172839	-0.16377172161245	-1.49839246894622
F	3.57486755743584	-0.18000673889835	1.72910852623248

$[C_7F_{14}COO]^{2-}$ (C_4) S = 0

C	4.73691280239335	-0.01526321268190	-0.24549409054344
O	5.35935791493159	-0.70311621493274	-1.08509220278915
O	5.04677808387067	1.09277321699232	0.24665132686295
C	3.38125316596019	-0.60189799909317	0.26046361541244
C	2.12275052722476	0.11275059326488	-0.29569012871739
C	0.82770281431491	-0.51545367108821	-0.01648932488237
C	-0.36606873798766	0.28696411351218	-0.18765561528635

C	-1.69022815977244	-0.53675406153765	-0.15594224283975
C	-2.96936541774198	0.29788843555970	0.18911802207588
C	-4.31432713004809	-0.40871504065293	-0.17126665237212
F	3.29000069024049	-1.93568805519021	-0.03382273877449
F	3.33163005444177	-0.51809168875957	1.63377165164188
F	2.13371693615703	1.39284019638387	0.19453429640755
F	2.41685099962311	0.26097516860487	-1.69068962299683
F	0.70725999888232	-1.70739902550325	-0.79857923986797
F	-0.46532635484897	1.27690364349175	0.77086712636937
F	-0.50473936139800	1.05392264500216	-1.41339123447963
F	-1.61709440599523	-1.51766374850454	0.77929743606328
F	-1.90392864357874	-1.13374743343208	-1.35821539943648
F	-2.97551207567328	1.48335880262087	-0.45890918935668
F	-2.99211251816085	0.53829029026973	1.52044677980866
F	-4.34514371550879	-1.66325632303579	0.29073929689777
F	-5.32453604587600	0.27111531220819	0.38857881402617
F	-4.50982246945017	-0.42999999549847	-1.49294749322331

$[C_7F_{14}COO]^{2-}$ (C_5) S = 0

C	4.74487778607340	0.27923118943797	-0.28054793442757
O	5.33572756587528	-0.43116929643989	-1.11901668715630
O	5.01715876639835	1.42949580610677	0.12495714360975
C	3.45840519803981	-0.35111326398576	0.36273023764236
C	2.15150662692066	0.24763095106212	-0.23375244978936
C	0.82897215155593	-0.52957693177857	0.05544471790056
C	-0.37729571682716	0.28000092757244	-0.08092732363209
C	-1.66080312715525	-0.41119965405563	-0.08597844910189
C	-2.88990062694046	0.50628073050073	0.18794598432672
C	-4.29710457383509	-0.09468612423102	-0.10021437469413
F	3.44845859934656	-1.70492861178692	0.19363372646171
F	2.04545394813120	1.51847752382728	0.23954624981988
F	2.33535580290771	0.33386654631507	-1.58491908358803
F	0.92749728204429	-1.69183823512861	-0.78368328168732
F	0.92087555180742	-1.07367603312278	1.32060457043044
F	-0.28412676148954	1.07669823167143	-1.26404803347934
F	-1.69167270199401	-1.39459534985139	0.86563467423013
F	-2.00453651731640	-1.07994080273652	-1.30650458369942
F	-2.80898337181185	1.64916584167145	-0.53713932680460
F	-2.87817447506744	0.84808339486658	1.50354202427575
F	-4.42747146875695	-1.31738643184309	0.43010581315921
F	-5.24033665107157	0.69446173007300	0.44424799991789
F	-4.54119365229793	-0.16788152616361	-1.41321802641127
F	3.45817556646303	-0.12650694798104	1.71449740169693

$[C_7F_{14}COO]^{2-}$ (C_6) S = 0

C	4.78945333425611	0.08275610413701	-0.29212485515962
O	5.30942354603374	-0.68886215765121	-1.12143877200318
O	5.15959379060396	1.20902253053373	0.10158081422660
C	3.45125358532771	-0.41690408081705	0.35975122963072

C	2.20572260977710	0.30875537897962	-0.22381153721123
C	0.83044496033348	-0.37893301706203	0.04831813599752
C	-0.44267361701510	0.50977739628584	-0.11106096168661
C	-1.70227979974613	-0.23324401546081	-0.10256043755363
C	-2.91718907324446	0.49179794088639	0.20768328923085
C	-4.22757996249175	-0.27844565631175	-0.10434478907176
F	3.28312232772692	-1.75927520310144	0.17390147677164
F	2.17997909204903	1.57131139434312	0.27180971286018
F	2.38138664884555	0.39330204341861	-1.57160190293013
F	0.73609306946112	-1.44885316657347	-0.78125434019259
F	0.84437427365091	-0.84753488799913	1.32693499386954
F	-0.42608079549672	1.42182270564507	0.90929342278464
F	-0.19710046552262	1.26612199514657	-1.29113059521685
F	-1.85248650356514	-0.92468656375383	-1.34153067900304
F	-3.15572933970123	1.75747796006490	-0.46125762663372
F	-2.97507042586742	0.86299734975223	1.53310521624990
F	-4.19913416884981	-1.53324134401370	0.37541068235313
F	-5.27350350180866	0.34558390393866	0.47393263369939
F	-4.48398678486893	-0.34471652629208	-1.42008998680381
F	3.47808255811235	-0.20679740709525	1.71096916979205

$[C_7F_{14}COO]^{2-}$ (C_7) S = 0

C	4.79162822090311	0.15913583044402	-0.29746982094251
O	5.33783927833145	-0.60741464520579	-1.11341827012877
O	5.11466903548741	1.30602247103536	0.07566113768758
C	3.47664886746115	-0.38180612441753	0.37087038364359
C	2.20473376292047	0.30194337035431	-0.20586097715192
C	0.85829113180976	-0.44094858723920	0.08366878662902
C	-0.41603082680429	0.44943098524744	-0.09527954274749
C	-1.76226271550171	-0.34608852544322	-0.17963642837995
C	-2.92961023021203	0.44865928305685	0.17611865474010
C	-4.24361428362895	-0.15929780322452	-0.02488423875669
F	3.34566583836015	-1.72870713277324	0.19268688253709
F	2.12998942889561	1.56183338096286	0.28684346142185
F	2.35480539843034	0.38670339544814	-1.55466246522983
F	0.78900785167897	-1.51025315089002	-0.74155633792768
F	0.88539498286167	-0.88967175959531	1.36320019080776
F	-0.45167100112676	1.30232643586759	0.95817582484575
F	-0.25178666311153	1.19236389320802	-1.22166018852000
F	-1.66513422801679	-1.45777296642532	0.62445060852051
F	-1.72103010516385	-0.90797994516368	-1.50196980635157
F	-2.90833431113078	1.66411211229136	-0.58347476746931
F	-4.37164722381442	-1.34180910049927	0.62677996762424
F	-5.25342942461354	0.65353529638685	0.41629193248537
F	-4.63670027532384	-0.44052018523241	-1.33855198250289
F	3.50600600130841	-0.16228883919328	1.71938813816577

$[C_7F_{14}COO]^{2-}$ (C_8) S = 0

C	4.79455659262829	0.15102966023947	-0.40287828598442

O	5.31556183284796	-0.64153717641476	-1.20989985355121
O	5.12025708109865	1.31311771574463	-0.08367580603007
C	3.50936269119245	-0.37307620591812	0.33465633819681
C	2.21362870831097	0.29616918359918	-0.20307247123407
C	0.88255400980782	-0.43680057332000	0.16345249374458
C	-0.40038460461887	0.44334589633303	-0.00912079501282
C	-1.73740319589841	-0.37115960583442	-0.05799189927963
C	-3.03864768487044	0.45121047801279	0.21035331409297
C	-4.41931500855871	-0.08886961079980	-0.15989900079008
F	3.36843665602143	-1.72338305075071	0.19558726760454
F	2.14824591567186	1.56561802185571	0.26618809957288
F	2.30159115449274	0.35013834849669	-1.55793685303208
F	0.76805838117560	-1.53322440308794	-0.62198383748475
F	0.95081963351514	-0.83735275078044	1.45443877005997
F	-0.44724847194288	1.31574318973993	1.02459519039895
F	-0.28439850117295	1.14926603754559	-1.15978111191051
F	-1.65128641084480	-1.36764996849181	0.86304101705036
F	-1.81143332845087	-0.94373018847053	-1.28566035279276
F	-2.87991895707486	1.65922840482928	-0.42493231365546
F	-3.04325347213853	0.69887163307105	1.56382844570019
F	-4.38216253232906	-1.45906424216031	0.26652989692073
F	-4.38497696335502	-0.22265556496602	-1.58435779349830
F	3.59522176749250	-0.12010475047249	1.67467206491418

$[C_7HF_{14}COO]^-$ (C_2) S = 0

C	4.77908262999401	0.20296629442861	-0.32253915041701
O	5.45761551864670	-0.54434976591068	-1.05595969375324
O	4.99310513068001	1.39420033828578	0.00616865376656
C	3.48904728443830	-0.40341373073659	0.29930512139432
C	2.23160393484318	0.26500100644180	-0.26112055059635
C	0.89931948796696	-0.44958137457533	0.13650891568796
C	-0.37799724525262	0.44008393599097	-0.02889959265986
C	-1.71323910228186	-0.37815013064522	-0.03123278632053
C	-2.97754519645690	0.50065837116469	0.24472220637409
C	-4.32444199804042	-0.16362023700815	-0.18050261489625
F	3.37850743487731	-1.76631365010097	0.02071816224890
F	2.15259369205295	1.54583941337583	0.19028308948553
F	2.28049203235489	0.30817667118123	-1.62313050573686
F	0.73931274462227	-1.55932300241328	-0.62048637869779
F	0.98368366973940	-0.81996357027572	1.43604480892726
F	-0.42733255848149	1.32986775310763	0.98690873178890
F	-0.29919056985339	1.11537826561485	-1.19578243136639
F	-1.65057022931521	-1.33480264565288	0.91985580780191
F	-1.85580453487640	-0.97304502630076	-1.23493823336055
F	-2.87361194243439	1.66728924540901	-0.42799937342626
F	-3.04727830995306	0.76201751772040	1.56503666859813
F	-4.41332262006709	-1.40543191836548	0.30622992063412
F	-5.33526082002628	0.56171286086767	0.30700805080034
F	-4.43601986502375	-0.20631881645928	-1.50932577192999
H	3.50297322084688	-0.28002371914415	1.38245585965309

$[C_7HF_{14}COO]^-$ (C_3) S = 0

C	4.75692553314596	0.27260115474485	-0.28548624710430
O	5.59191896350483	-0.47322015291192	-0.83139720041919
O	4.77335942531243	1.51284460506606	-0.11489470919469
C	3.47960095416216	-0.40764056369938	0.31062134048541
C	2.20193689803169	0.23827054508409	-0.23890982744246
C	0.90040642167886	-0.52563045127693	0.07733381776211
C	-0.36436711886871	0.37278434717396	-0.08142551737932
C	-1.72488701098939	-0.39848972545844	-0.05004747290877
C	-2.95473098447415	0.51722796160085	0.25409595530388
C	-4.33162296217755	-0.10922927331586	-0.13182462733107
F	3.46439150784678	-1.75608217682357	0.08521524300514
F	2.32465035812592	0.29112359918450	-1.61953794639326
F	0.76461246307660	-1.60017696279301	-0.73931627483481
F	0.93235782686850	-0.96849861485669	1.35880310568065
F	-0.34842615938196	1.28274497787498	0.92235065843455
F	-0.28558577223243	1.03624341977412	-1.25597554770879
F	-1.67537869360316	-1.36123515350499	0.89484487182208
F	-1.90978331339740	-0.98597914129572	-1.25261847823900
F	-2.83414317555187	1.67780026757165	-0.42629840570281
F	-2.97994997359562	0.78537900672313	1.57492486287592
F	-4.43775804994971	-1.35202356589823	0.34894547182984
F	-5.30777559403394	0.63763644081701	0.39243487647555
F	-4.48559496122412	-0.13933422235136	-1.45681839809804
F	3.49615552152268	-0.24410466732775	1.67771038625398
H	2.14391020220359	1.25511157889865	0.14967072082739

$[C_7HF_{14}COO]^-$ (C_4) S = 0

C	4.80126700978460	0.28139254026281	-0.09731022885450
O	5.31444716506347	-0.09913669999675	-1.16915110967653
O	5.18013170331534	1.14633298764171	0.71653153225091
C	3.45536610682291	-0.43748501594572	0.27102282492967
C	2.20467763572875	0.23063115851183	-0.35033861075989
C	0.87451947741774	-0.44284070715783	0.05681430380370
C	-0.36292829017091	0.44407938893311	-0.17506800435311
C	-1.69991479011559	-0.35827628334397	-0.05177797677400
C	-2.95291928404644	0.53339183365555	0.22365301574667
C	-4.31581504451178	-0.17451174302247	-0.05697124877677
F	3.47161637929541	-1.74365605594472	-0.13289473065746
F	2.18764412792670	1.53086328513876	0.05765846185864
F	2.32590599041321	0.22273667784625	-1.70190171341468
F	0.73117033033842	-1.59115224216701	-0.69748242227175
F	-0.37908609848248	1.42284001903858	0.76673929518771
F	-0.33652852040187	1.03002769928753	-1.39636965850933
F	-1.57920393786784	-1.23569951664907	0.97134036070918
F	-1.91013843210390	-1.05088112330182	-1.19216757026286
F	-2.90373412225879	1.63814695081530	-0.55248218235996
F	-2.94828326771098	0.90884048664102	1.51823449797925
F	-4.35198680951895	-1.37899077598051	0.52282361210070

F	-5.30239960524729	0.57301830788351	0.44717313778567
F	-4.51990305645697	-0.31621191893007	-1.36773413404173
F	3.25453820783076	-0.45348543408489	1.62524669651393
H	0.90654561595647	-0.71189261813114	1.11263004284655

$[C_7HF_{14}COO]^-$ (C_5) S = 0

C	4.79327073053363	0.20479691578585	-0.22287262761920
O	5.41907146004988	-0.47757568111039	-1.05570802414197
O	5.03770817546331	1.33621883598501	0.24497367675429
C	3.47582541511412	-0.43957274058819	0.34057848651716
C	2.20222481295534	0.29758869487629	-0.16001412597590
C	0.86059123004830	-0.48576481742535	-0.00235591823684
C	-0.37770906231460	0.43099206391489	-0.08320066514592
C	-1.70292637106903	-0.35149751275855	-0.22138526838364
C	-2.95195646109456	0.53322194189356	0.06241127010388
C	-4.32216777395245	-0.21029410201620	0.07675708226674
F	3.36326641816289	-1.75139414867606	-0.01972759000747
F	2.07214773384786	1.46835565804451	0.51346602771376
F	2.37843748203121	0.58202932999032	-1.47674301641307
F	0.80855608683947	-1.45497551034568	-0.94929861274937
F	0.86195188810350	-1.08386774309806	1.21835371765214
F	-0.26203937753810	1.24213084408808	-1.19306273893511
F	-1.71987552720862	-1.38096173156221	0.66189058841255
F	-1.81901391846685	-0.85823267513590	-1.47059436907980
F	-3.02795931845895	1.50433116963242	-0.87289621488120
F	-2.79577590858877	1.11079130398373	1.27630003247843
F	-4.38087467642201	-1.09384770008921	1.07592720549465
F	-5.29434299709880	0.69223813084390	0.25008675776398
F	-4.53350554409982	-0.84788669642469	-1.07753296724003
F	3.48459760024734	-0.40531197616468	1.70702917821982
H	-0.40261172808430	1.05116224635662	0.81311104543212

$[C_7HF_{14}COO]^-$ (C_6) S = 0

C	4.80668448458304	0.09851816686800	-0.28118336811318
O	5.35035848015623	-0.69855909343803	-1.06806325847296
O	5.14451147495574	1.24712637379802	0.07247924672336
C	3.46793747372697	-0.39792777275852	0.37563913475647
C	2.22321411841350	0.31612193203937	-0.22036704233545
C	0.85679891669247	-0.38615230349105	0.05828699037947
C	-0.40373798334694	0.50947477640835	-0.13732274137419
C	-1.70567272530921	-0.32896048073521	-0.11892105849751
C	-2.95295555057765	0.50373939541774	0.22532785242588
C	-4.28975502652060	-0.23617950751416	-0.08093305731868
F	3.29276757119769	-1.74065416077786	0.20516619073629
F	2.16375167135277	1.58039220328252	0.26040826874344
F	2.38155261718304	0.38535536553327	-1.56797941875189
F	0.74270864376491	-1.45705259369009	-0.76166893632682
F	0.82770145225610	-0.83019078124414	1.33863806424631
F	-0.44059280189918	1.41972365096762	0.86626982766999

F	-0.29906477709343	1.17359492090267	-1.31171400778777
F	-1.87727267594681	-0.87996055051079	-1.37067575476973
F	-2.98001926489203	1.68003808606433	-0.44818604730846
F	-2.94418045416330	0.77372743730957	1.55347587426341
F	-4.24064282722250	-1.48713256858931	0.39650182864391
F	-5.30098769524924	0.40718456898238	0.51288991130981
F	-4.53304354875699	-0.28214888513010	-1.39246653914152
F	3.48436408425698	-0.16800307637676	1.72227572382232
H	-1.62061964556154	-1.13140378431779	0.61534389847750

$[C_7HF_{14}COO]^-$ (C_7) S = 0

C	4.80039181263070	0.17441438165246	-0.31884513663830
O	5.35030448380835	-0.56504878830845	-1.15595884739397
O	5.10723750238294	1.31650152003512	0.08080123043772
C	3.49697981890217	-0.39928724759887	0.34582733192253
C	2.21613726884532	0.29867133497425	-0.19054845576925
C	0.87732494615048	-0.45425447826942	0.09983456719141
C	-0.39560944421125	0.44068284679976	-0.05965861022192
C	-1.73183058536995	-0.36648649280308	-0.16527532966699
C	-2.95874372943654	0.49940580783363	0.16847783111193
C	-4.30743861037030	-0.19909450447140	-0.06045057574483
F	3.36333706690875	-1.73838277752320	0.11804725781148
F	2.13034843034092	1.53958085209852	0.34683304265837
F	2.33927963378375	0.42684606996332	-1.53636712511125
F	0.77198938647328	-1.50099976283434	-0.75000757645340
F	0.90678951726393	-0.92569969127920	1.36617366247742
F	-0.48404207363693	1.25818443347806	1.01538361515684
F	-0.26180800567407	1.19861944989102	-1.17011583730584
F	-1.68324993635743	-1.39756807685526	0.71596662710986
F	-1.82115634555602	-0.88015025085956	-1.41468200045754
F	-2.94123303194677	1.61785646365138	-0.63825616213078
F	-4.39425771481083	-1.33470831155181	0.64660977480085
F	-5.29401693292840	0.62020491502653	0.34153115818594
F	-4.52386527740634	-0.48828083280281	-1.35164044244425
F	3.53928447812150	-0.22942959662289	1.70016476634923
H	-2.90940425190726	0.80358589737626	1.21454223012473

$[C_7HF_{14}COO]^-$ (C_8) S = 0

C	4.79539574745791	0.13374424271009	-0.43254141239872
O	5.36652013610750	-0.70008336321289	-1.15959273034141
O	5.06683118749268	1.32956808945061	-0.20032595996916
C	3.51636312803687	-0.37897426566046	0.32327213855370
C	2.21621257337487	0.28573190305547	-0.20872755711923
C	0.89132813576388	-0.45235044860079	0.17002305046299
C	-0.39142394268038	0.42848976801719	-0.00496901270940
C	-1.71937174849686	-0.39974524931482	-0.04102832486550
C	-2.99782383383504	0.45664428531724	0.22601672574034
C	-4.33605663302052	-0.17839124096744	-0.21194574668924
F	3.36647436313283	-1.73013256458450	0.20397085686496

F	2.13894182821240	1.55467667632256	0.25673466327763
F	2.29327935278767	0.33206805573675	-1.56397006392133
F	0.76458548001844	-1.55157212016822	-0.60768960538933
F	0.96035428499014	-0.84121435742633	1.46256004616670
F	-0.45719103752119	1.30234424647389	1.02353442000529
F	-0.29355599010203	1.12238896203278	-1.15996365848653
F	-1.65349543147976	-1.37262282552348	0.89554452579735
F	-1.83026863272304	-0.97879556690877	-1.25677508042993
F	-2.87799662267976	1.64462564779498	-0.41637734206731
F	-3.08227579730681	0.69629287184347	1.55663196285104
F	-4.39870818619826	-1.45846349752653	0.24193714376479
F	-4.41838986832087	-0.20265000580634	-1.56564189416990
F	3.61864315530227	-0.10860545347542	1.65892540684348
H	-5.16816464831294	0.39717521042095	0.19611194822871

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