

Table S1. Vibrational frequencies [ $\text{cm}^{-1}$ ] calculated for the isolated and ion paired H-fumarate anion.

isolated anion		paired anion
Frequency	PED <sup>[a]</sup>	Frequency
30	$\tau\text{C1C2}$ , 83	
108	$\tau\text{C2C3}$ , $\delta\text{O1C1C2}$ ; 70, 17	
125	$\tau\text{C3C4}$ , $\delta\text{C1C2C3}$ , $\delta\text{C2C3C4}$ ; 41, 23, 16	
166	$\tau\text{C3C4}$ , $\delta\text{C2C3C4}$ , $\delta\text{C1C2C3}$ ; 34, 20, 15	
261	$\delta\text{C1C2C3}$ , $\delta\text{C2C3C4}$ , $\nu\text{C1C2}$ ; 24, 22, 17	304
388	$\delta\text{O1C1C2}$ , $\delta\text{O4C4C3}$ ; 41, 13	394
455	$\delta\text{O4C4C3}$ , $\delta\text{O1C1C2}$ ; 47, 11	561
550	$\tau\text{C4O4}$ ; 86	572
606	$\delta\text{O4'C4O4}$ , $\delta\text{O1'C1O1}$ ; 56, 17	620
664	$\omega\text{O1'C1O1}$ , $\delta\text{O1'C1O1}$ , $\delta\text{C4C3C2}$ ; 22, 21, 13	723
740	$\omega\text{O4'C4O4}$ , $\delta\text{O1'C1O1}$ ; 29, 17	681
781	$\omega\text{O4'C4O4}$ , $\omega\text{O1'C1O1}$ ; 41, 28	802
882	$\gamma\text{C2H}$ , $\tau\text{C3H}$ ; 59, 11	936
910	$\nu\text{C1C2}$ , $\nu\text{C4O4}$ , $\delta\text{O1'C1O1}$ ; 39, 18, 14	935
974	$\nu\text{C3C4}$ , $\delta\text{C1C2C3}$ ; 25, 17	970
994	$\gamma\text{C3H}$ , $\gamma\text{C2H}$ ; 68, 20	1026
1107	$\nu\text{C4O4}$ , $\delta\text{HO4C4}$ , $\nu\text{C3C4}$ , $\delta\text{HC3C4}$ ; 37, 23, 17, 11	1129
1245	$\delta\text{HC2C3}$ , $\delta\text{HC3C4}$ , $\delta\text{HO4C4}$ ; 42, 24, 20	1236
1284	$\delta\text{HC2C3}$ , $\delta\text{HO4C4}$ , $\delta\text{HC3C4}$ ; 34, 19, 15	1288
1343	$\delta\text{HC3C4}$ , $\delta\text{HO4C4}$ , $\nu\text{C2C3}$ ; 24, 20, 13	1356
1365	$\nu\text{C1O1'}$ , $\nu\text{C1O1}$ , $\delta\text{O1'C1O1}$ ; 40, 32, 10	1387
1627	$\nu\text{C2C3}$ , $\delta\text{HC3C4}$ ; 65, 10	1698
1662	$\nu\text{C1O1}$ , $\nu\text{C1O1'}$ ; 53, 43	1615
1748	$\nu\text{C4O4'}$ ; 76	1780
3146	$\nu\text{C2H}$ ; 99	3181
3181	$\nu\text{C3H}$ ; 99	3200
3778	$\nu\text{O4H}$ ; 100	3768

<sup>[a]</sup> PED calculated for the isolated anion.  $\nu$ , stretching;  $\delta$ , bending;  $\tau$ , torsion;  $\omega$ , wagging,  $\gamma$ , out of plane bending.