

Table S2. Vibrational frequencies [ $\text{cm}^{-1}$ ] calculated for the isolated and ion paired H-maleate anion.

isolated anion		paired anion
Frequency	PED <sup>[a]</sup>	Frequency
56	$\tau\text{C1C2}$ , $\tau\text{C3C4}$ ; 71, 18	
102	$\tau\text{C3C4}$ , $\tau\text{C1C2}$ ; 57, 24	
279	$\tau\text{C2C3}$ ; 69	295
281	$\delta\text{C2C3C4}$ , $\delta\text{C1C2C3}$ , $\delta\text{O1C1O1'}$ ; 38, 15, 12	292
309	$\delta\text{C1C2C3}$ , $\delta\text{O1C1C2}$ , $\delta\text{O4C4C3}$ ; 35, 29, 17	317
402	$\delta\text{O4C4C3}$ , $\delta\text{O1C1C2}$ , $\nu\text{C2C3}$ , $\nu\text{C1C2}$ ; 23, 20, 12, 12	423
569	$\delta\text{O4C4O4'}$ ; 60	610
592	$\tau\text{C3C4}$ , $\omega\text{O1C1O1'}$ , $\omega\text{O4'C4O4}$ , $\tau\text{C2C3}$ ; 29, 25, 23, 18	594
637	$\nu\text{C1C2}$ , $\delta\text{O1C1O1'}$ , $\delta\text{O4C4C3}$ ; 36, 28, 23	641
777	$\nu\text{C3C4}$ , $\delta\text{O1C1C2}$ , $\delta\text{C2C3C4}$ ; 26, 25, 19	791
802	$\omega\text{O4'C4O4}$ , $\omega\text{O1C1O1'}$ , $\tau\text{C2C3}$ ; 37, 35, 16	811
873	$\omega\text{O1C1O1'}$ , $\gamma\text{C2H}$ , $\omega\text{O4'C4O4}$ , $\gamma\text{C3H}$ ; 28, 25, 24, 18	886
875	$\delta\text{O1'C1O1}$ , $\nu\text{C3C4}$ , $\delta\text{C2C3C4}$ ; 30, 12, 11	875
945	$\nu\text{C1C2}$ , $\delta\text{C1C2C3}$ , $\nu\text{C4O4}$ , $\nu\text{C3C4}$ , $\nu\text{C1O1}$ ; 20, 16, 15, 15,12	950
1012	$\gamma\text{C3H}$ , $\gamma\text{C2H}$ ; 46, 44	1035
1197	$\nu\text{C4O4}$ , $\nu\text{C1O1}$ , $\nu\text{O4H}$ ; 27, 21, 14	1216
1210	$\tau\text{C4O4}$ ; 98	1039
1214	$\delta\text{HC2C3}$ , $\delta\text{HC3C4}$ ; 42, 35	1218
1367	$\nu\text{O4H}$ , $\nu\text{C1O1}$ , $\nu\text{C1O1'}$ ; 27, 16	1367
1387	$\delta\text{HC3C4}$ , $\delta\text{HC2C3}$ ; 44, 36	1415
1555	$\nu\text{C1O1'}$ , $\nu\text{O4H}$ ; 39, 25	1606
1639	$\delta\text{HO4C4}$ , $\nu\text{C4O4'}$ , $\nu\text{C2C3}$ ; 35, 31, 14	1561
1655	$\nu\text{C2C3}$ , $\delta\text{HO4C4}$ ; 58, 20	1668
1741	$\delta\text{HO4C4}$ , $\nu\text{C4O4'}$ , $\nu\text{C1O1'}$ ; 29, 21, 20	1772
1814	$\nu\text{O4H}$ , $\nu\text{C4O4'}$ , $\nu\text{C1O1}$ ; 40, 17, 13	2805
3128	$\nu\text{C2H}$ , $\nu\text{C3H}$ ; 60, 40	3154
3154	$\nu\text{C3H}$ , $\nu\text{C2H}$ ; 60, 40	3175

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