

Electronic Supplementary Information: Anti-Kasha emission in DCM-IFC: Computational evaluation of the Type III separated wave function hypothesis

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1 Natural transition orbitals (NTOs) for DCM-IFC (open)

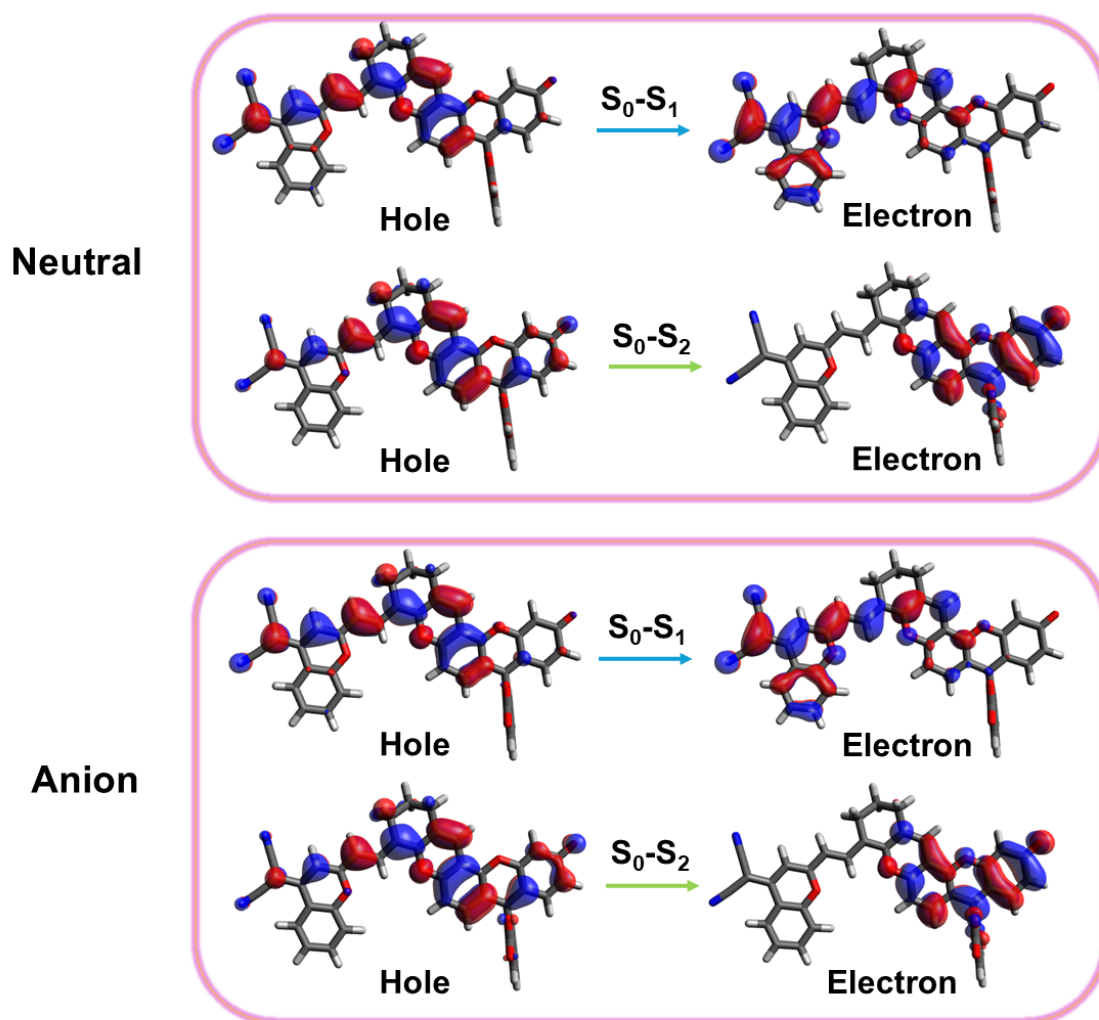


Figure S1: NTOs associated with $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for neutral and anion DCM-IFC (open) at the Franck-Condon (FC) region at M06-2X/def2-SVP/SMD(water) level.

2 Active space orbitals employed for neutral DCM-IFC (open)

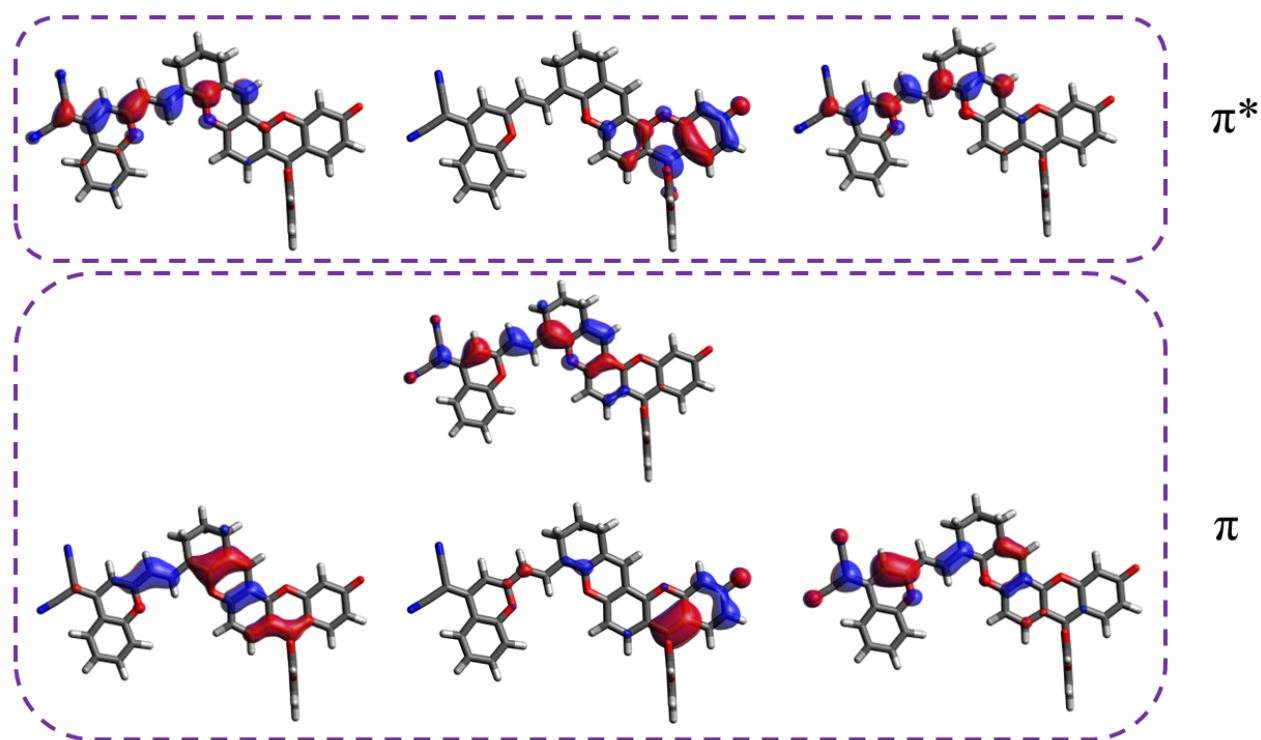


Figure S2: An active space of 8 electrons in 7 orbitals were used for the NEVPT2 single point calculations relevant to the neutral form of DCM-IFC (open). All of these orbitals (in addition to the three dominant orbitals) have contributions to the excitations and were required to reproduce the energy gap at the Franck-Condon region. A similar active space did not converge for the anionic form and no NEVPT2 single point calculations were performed for the anionic form.

3 Vertical excitation energies (VEEs) at the FC region between TDA and TD-DFT methods

Table S1: **DCM-IFC (open) neutral:** VEEs and oscillator strengths (f) associated with the lowest two excited states using M06-2X/def2-SVP/SMD (water) at the TDA and TD-DFT level. S_0 minimum geometry at TD-DFT-M06-2X/def2-SVP/SMD (water) was used. VEEs at TDA level are blue-shifted by ~ 0.1 eV compared to TD-DFT level, but the states retain the same energetic ordering.

| Method | State | Energy (eV) | f |
|--------|-------|-------------|------|
| TD-DFT | S_1 | 2.552 | 2.06 |
| | S_2 | 3.050 | 0.17 |
| TDA | S_1 | 2.659 | 2.47 |
| | S_2 | 3.124 | 0.09 |

Table S2: **DCM-IFC (open) anion:** VEEs and oscillator strengths (f) associated with the lowest two excited states using M06-2X/def2-SVP/SMD (water) at the TDA and TD-DFT level. S_0 minimum geometry at TD-DFT-M06-2X/def2-SVP/SMD (water) was used. VEEs at TDA level are blue-shifted by ~ 0.1 eV compared to TD-DFT level, but the states retain the same energetic ordering.

| Method | State | Energy (eV) | f |
|--------|-------|-------------|------|
| TD-DFT | S_1 | 2.539 | 2.01 |
| | S_2 | 3.119 | 0.23 |
| TDA | S_1 | 2.646 | 2.41 |
| | S_2 | 3.201 | 0.13 |

4 Simulated absorption spectra of DCM-IFC (open) with geometries sampled via classical thermostat AIMD

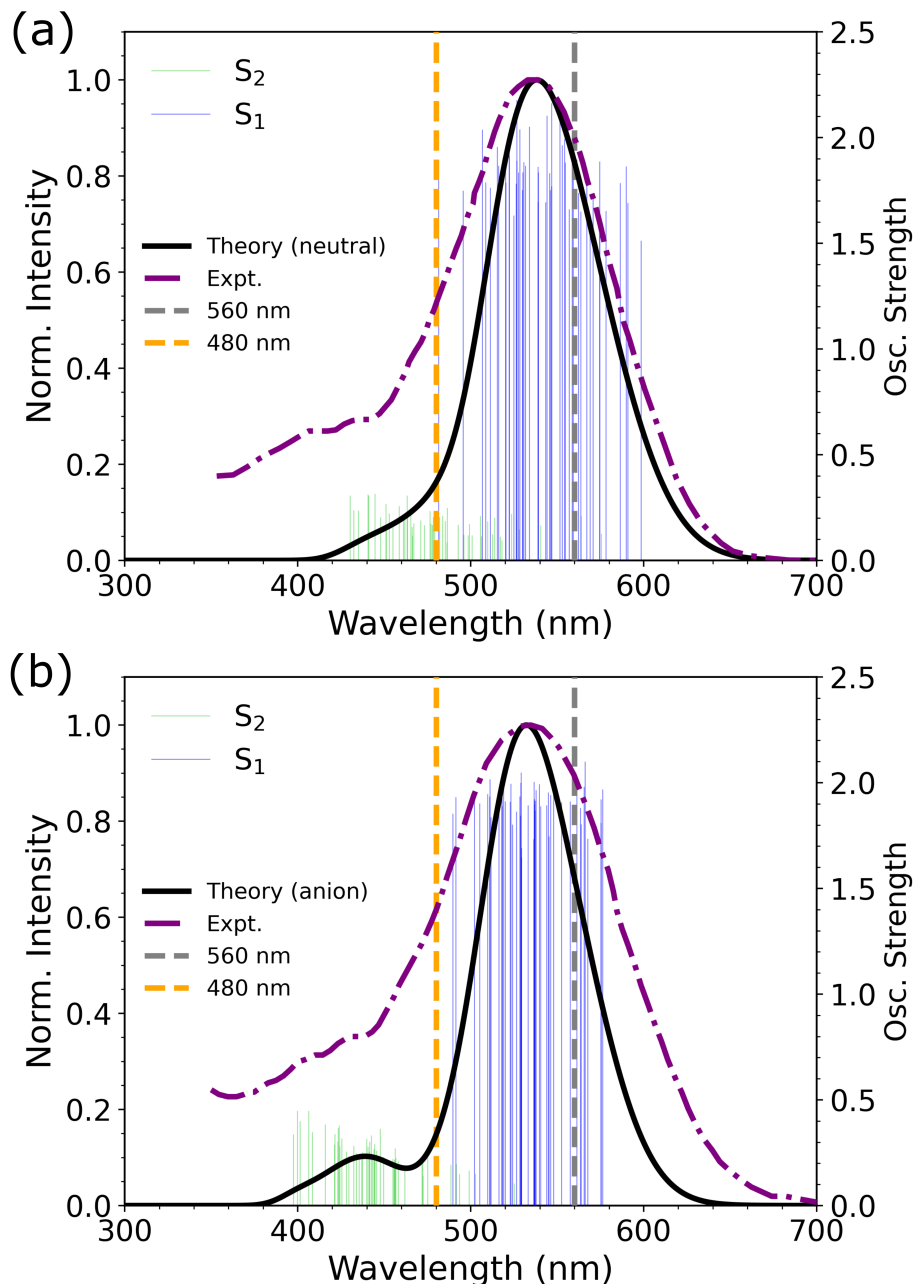


Figure S3: Absorption Spectra of the (a) neutral form and the (b) anion form of DCM-IFC (open) simulated from calculating VEEs and oscillator strengths at TD-M06-2X/def2-SVP/SMD (water) level with geometries sampled from classical thermostat AIMD. VEEs were updated using the cLR formalism. The resultant stick spectra were convolved with a gaussian with FWHM of 0.2 eV and redshifted by 0.29 and 0.25 eV for the neutral and the anion to match with the experimental absorption maximum of DCM-IFC-ester (open) (digitised and normalised from the SI of Ref 1) and anionic DCM-IFC (open) (digitised and normalised from Ref 2), respectively.

5 Linearly interpolated pathways in internal coordinate (LIIC) between S_2 optimised geometry and S_2/S_1 -intersection region

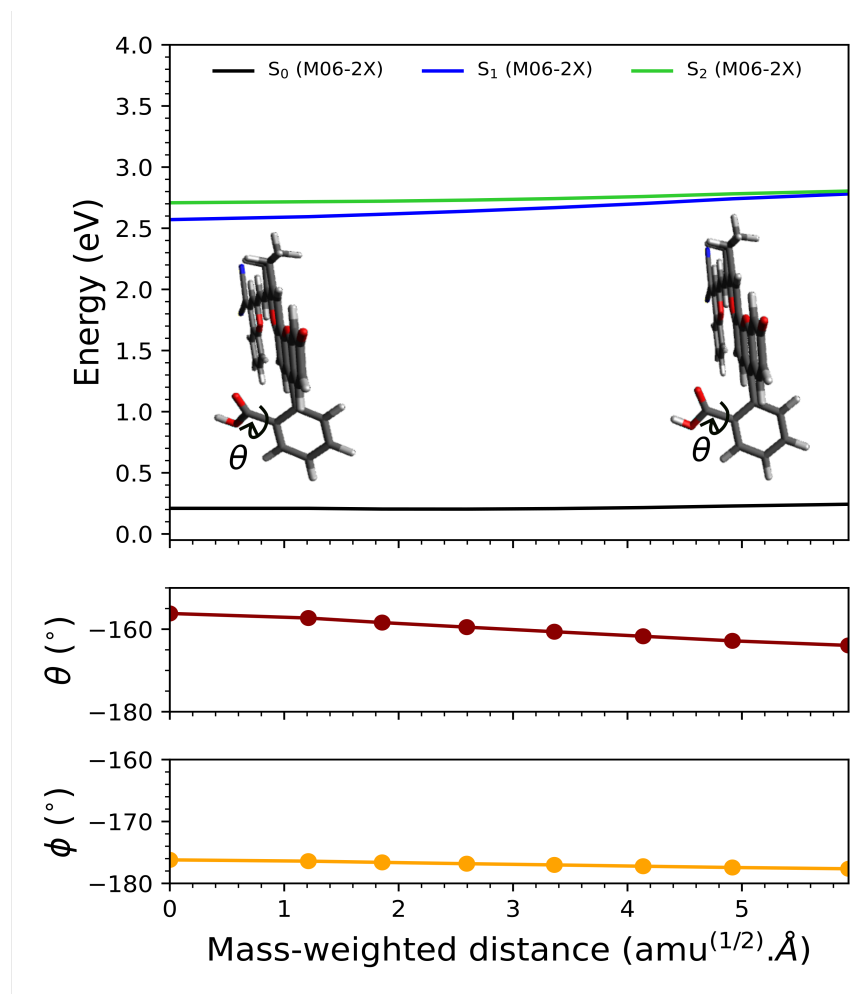


Figure S4: Relative energies (top panel) along LIIC pathways from the S_2 optimised geometry to S_2/S_1 -intersection region for the neutral DCM-IFC (open) with the important torsions (dihedral angles) θ (middle panel) and ϕ (bottom panel) along the same LIIC. Energies are calculated relative to the ground state energy at the same level of theory at the neutral FC geometry. Energy difference between S_2 and S_1 at the S_2 optimised geometry is 0.14 eV. The barrier to reach the S_2/S_1 -intersection region from the S_2 optimised geometry is ≤ 0.02 eV.

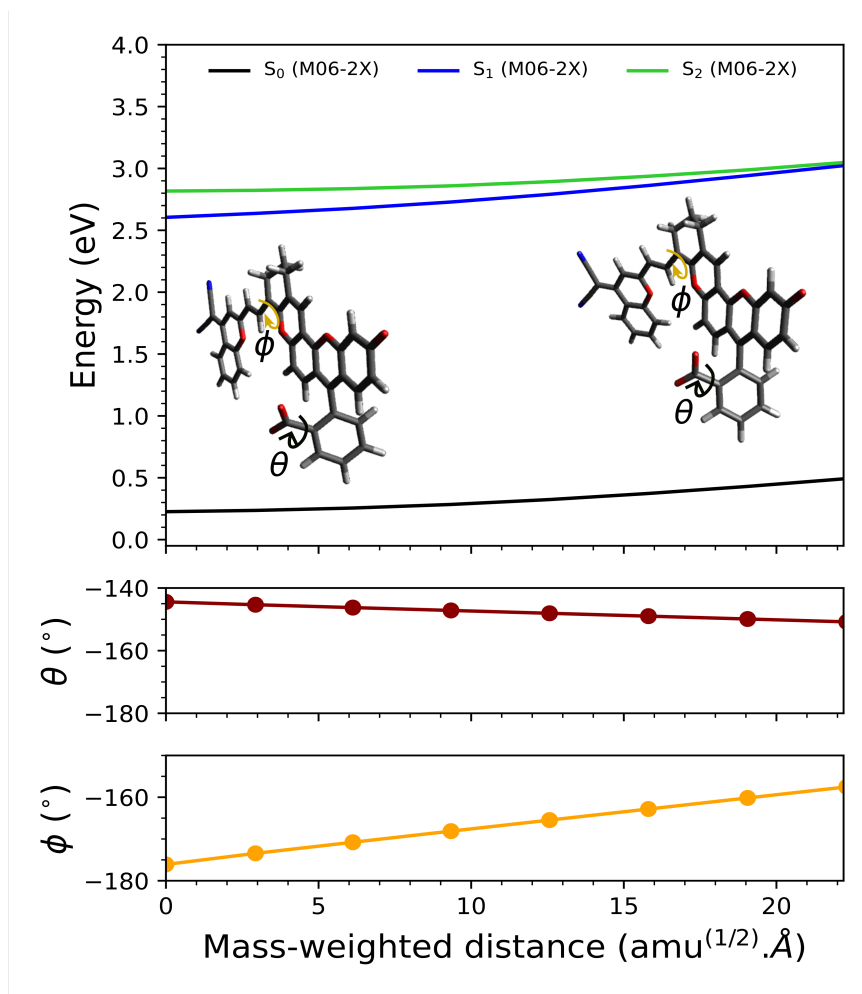


Figure S5: Relative energies (top panel) along LIIC pathways from the S_2 optimised geometry to S_2/S_1 -intersection region for the anionic DCM-IFC (open) with the important torsions (dihedral angles) θ (middle panel) and ϕ (bottom panel) along the same LIIC. Energies are calculated relative to the ground state energy at the same level of theory at the anionic FC geometry. Energy difference between S_2 and S_1 at the S_2 optimised geometry is 0.22 eV. The barrier to reach the S_2/S_1 -intersection region from the S_2 optimised geometry is ≤ 0.23 eV.

6 Linearly interpolated pathways in internal coordinate (LIIC) between S_2/S_1 -intersection region and S_1 optimised geometry

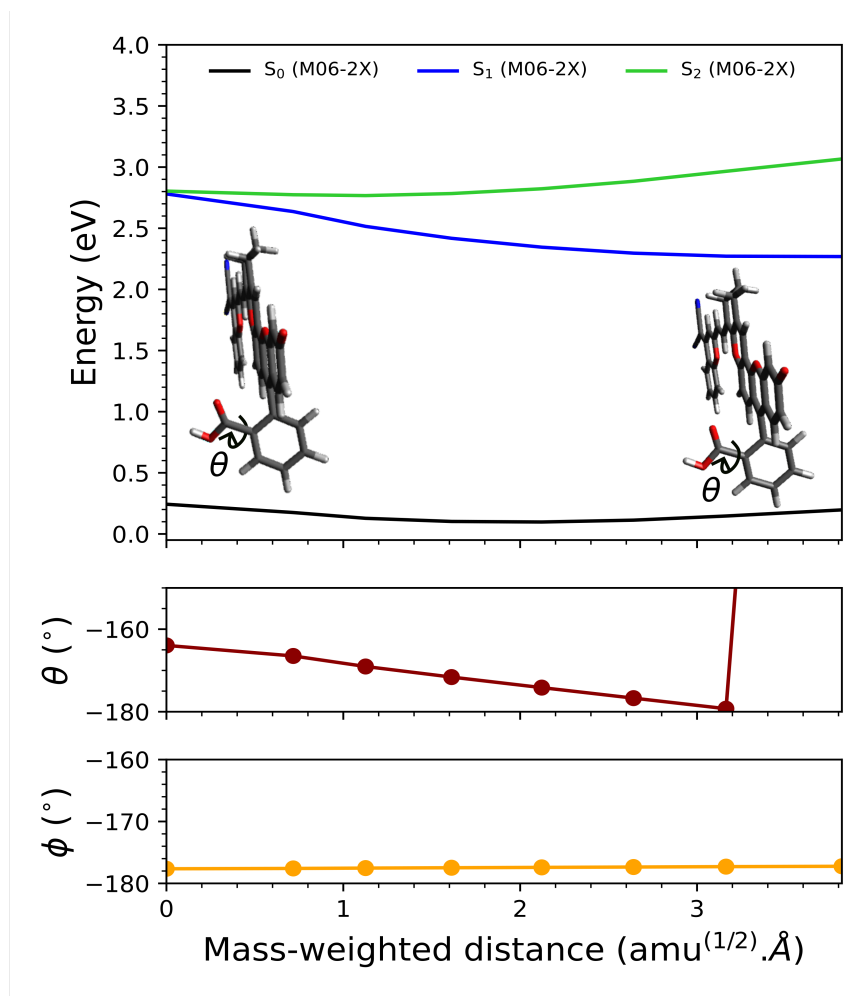


Figure S6: Relative energies (top panel) along LIIC pathways from the S_2/S_1 -intersection region to S_1 optimised geometry for the neutral DCM-IFC (open) with the important torsions (dihedral angles) θ (middle panel) and ϕ (bottom panel) along the same LIIC. Energies are calculated relative to the ground state energy at the same level of theory at the neutral FC geometry. Energy difference between S_2 and S_1 at the S_1 optimised geometry is 0.80 eV. The θ value for the last LIIC point falls on the positive side of 180° showing a jump in θ between the penultimate and the last point of the LIIC. However, the difference in θ between these two points is only 2.6° .

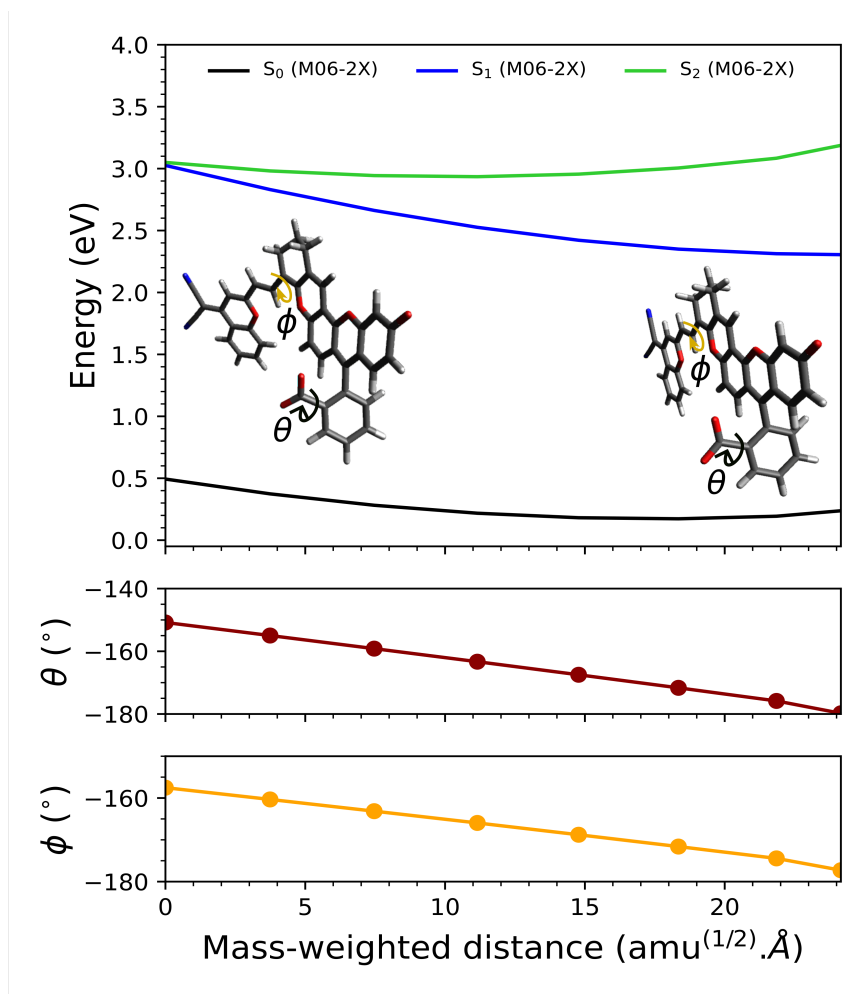


Figure S7: Relative energies (top panel) along LIIC pathways from the S₂/S₁-intersection region to the S₁ optimised geometry for the anionic DCM-IFC (open) with the important torsions (dihedral angles) θ (middle panel) and ϕ (bottom panel) along the same LIIC. Energies are calculated relative to the ground state energy at the same level of theory at the anionic FC geometry. Energy difference between S₂ and S₁ at the S₁ optimised geometry is 0.88 eV.

7 Excited state sampling via QT-AIMD

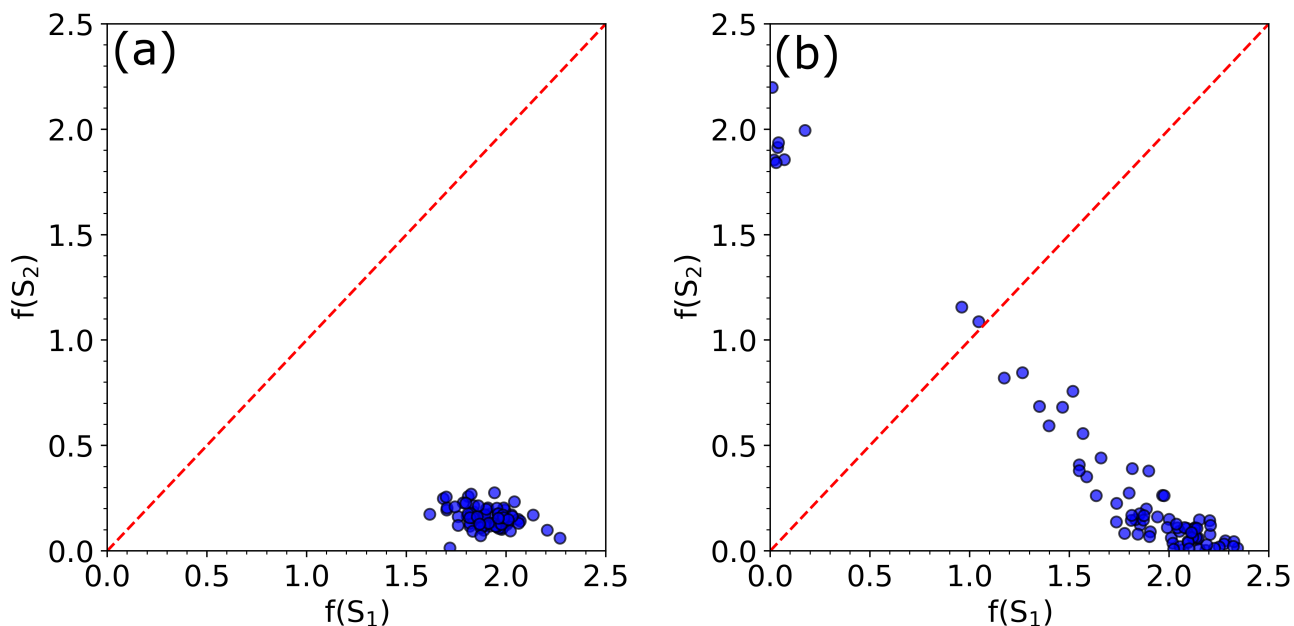


Figure S8: Scatter plot of oscillator strengths of S_2 ($f(S_2)$) and S_1 ($f(S_1)$) states at geometries sampled at the (a) S_1 minimum, and (b) S_2 minimum of the neutral form of DCM-IFC (open). All geometries sampled on the S_1 minimum illustrate that S_1 is always the brighter of the two states, whilst in 11% (9 out of 79 sampled geometries) of the sampled geometries on the S_2 minimum, the S_2 state is brighter representing a switching of states.

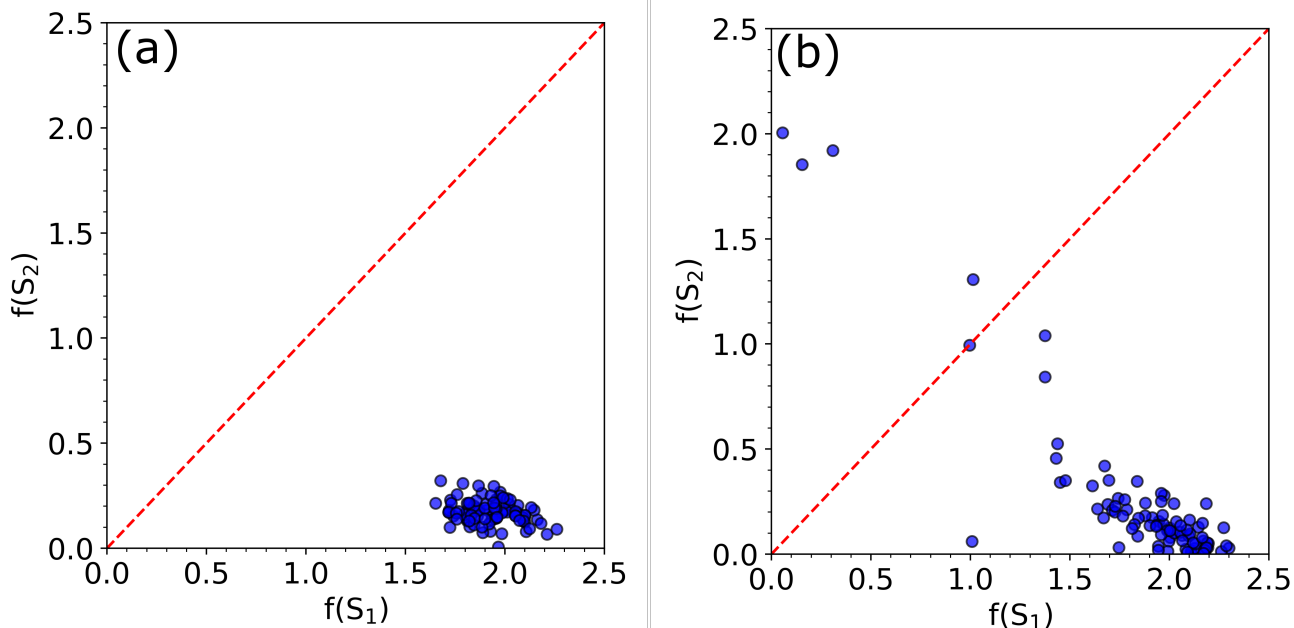


Figure S9: Scatter plot of oscillator strengths of S_2 ($f(S_2)$) and S_1 ($f(S_1)$) states at geometries sampled at the (a) S_1 minimum, and (b) S_2 minimum of the anion form of DCM-IFC (open). All geometries sampled on the S_1 minimum illustrate that S_1 is always the brighter of the two states, whilst in 5% (4 out of 87 sampled geometries) of the sampled geometries on the S_2 minimum, the S_2 state is brighter representing a switching of states.

8 Cartesian Coordinates (in Å) of S₀ minimum geometry of DCM-IFC (open)

Neutral (M06-2X/def2-SVP/SMD(water)):

C 0.00000000 0.00000000 0.00000000
C -0.46032200 1.43865300 -0.04494100
C 0.49932800 2.51018900 -0.07874000
C 1.84657100 2.34416400 -0.01902800
C 2.77042100 3.45008300 -0.03850600
C 4.13111500 3.29984600 0.04457400
C 5.02399200 4.40712800 0.03036900
C 4.39574600 5.72540500 -0.09986000
C 2.98978100 5.78152300 -0.17863500
C 2.29454200 6.98758400 -0.30154200
C 3.00324800 8.17441800 -0.35176800
C 4.40379300 8.15710600 -0.28129600
C 5.08322800 6.95771900 -0.15844900
H 6.16776400 6.98360700 -0.10968800
H 4.96539600 9.09026500 -0.32388400
H 2.46924900 9.12044400 -0.44821500
H 1.20626900 6.95739500 -0.35599100
O 2.21508300 4.66644600 -0.14206300
C 6.39952300 4.16504000 0.14001200
C 7.44793300 5.12711400 0.16495200
N 8.35495300 5.85074900 0.19501600
C 6.87118600 2.82261100 0.25320800
N 7.26176800 1.73396900 0.34467100
H 4.51149100 2.28314300 0.13038400
H 2.30635900 1.35804800 0.05759200
H 0.10835700 3.52776800 -0.13890800
C -1.80083300 1.72545500 -0.03642500
C -2.84102600 0.71640100 0.09557000
C -2.38567100 -0.69801400 0.32187300
C -1.08942300 -0.97701600 -0.43037400
H -1.26761700 -0.87331700 -1.51262900
H -0.76085400 -2.00897500 -0.24907600
H -3.18801700 -1.38981200 0.03297700
H -2.20892200 -0.83516200 1.40276200
C -4.14121000 1.08647100 0.04863300
C -4.49629300 2.48160200 -0.10081200
C -3.46998800 3.42746200 -0.18074400
O -2.17770200 3.03765700 -0.14192700
C -3.72256000 4.80157600 -0.30349500
C -5.03026700 5.23809600 -0.35134700
C -6.10701700 4.32634500 -0.27496500
C -5.81619300 2.95949400 -0.15079200
O -6.79464400 2.03284900 -0.07175800
C -8.10839400 2.37249500 -0.10237900
C -8.47533400 3.76948500 -0.22514100
C -7.49377800 4.72665300 -0.30673500
C -7.83383900 6.16292500 -0.51939200
C -7.83994900 7.12274000 0.50986400
C -8.15485000 8.45439700 0.21562700
C -8.45748400 8.83914900 -1.08698200
C -8.45196900 7.88955500 -2.10697300
C -8.14314500 6.55998300 -1.82355300

H -8.13908000 5.81533600 -2.62150300
H -8.69037700 8.18068900 -3.13084300
H -8.69986400 9.87985800 -1.30389700
H -8.16302100 9.18963800 1.01938900
C -7.52578700 6.72076500 1.91283000
O -7.24212200 5.59480400 2.25248600
O -7.58814500 7.73386500 2.77348200
H -7.38183800 7.39829800 3.66392200
C -9.89144800 4.06901700 -0.23844200
C -10.8180430 3.08988300 -0.15130500
C -10.4463130 1.66973500 -0.04294100
C -9.02755600 1.37245900 -0.01790700
H -8.70480700 0.33496300 0.06863200
O -11.3111630 0.78683000 0.02287000
H -11.8856210 3.31607200 -0.15931300
H -10.1944020 5.11448100 -0.31752900
H -5.24262500 6.30355200 -0.44990600
H -2.88248700 5.49274200 -0.36112400
H -4.93312300 0.34249700 0.14268200
H 0.87631600 -0.11241400 -0.65526600
H 0.34556100 -0.24370000 1.01981000

Anion (M06-2X/def2-SVP/SMD(water)):

C 0.00000000 0.00000000 0.00000000
C -0.46288200 1.43781400 -0.04817400
C 0.49430400 2.51087400 -0.07441100
C 1.84182000 2.34813900 -0.00314500
C 2.76323600 3.45545000 -0.02116900
C 4.12387400 3.30867900 0.07459000
C 5.01459500 4.41717400 0.05826200
C 4.38506800 5.73333100 -0.08666300
C 2.97970700 5.78633800 -0.17712300
C 2.28333800 6.99013300 -0.31483300
C 2.99033500 8.17787300 -0.36816700
C 4.39023500 8.16368000 -0.28550700
C 5.07074800 6.96648600 -0.14792500
H 6.15472900 6.99481700 -0.08942900
H 4.95048800 9.09756500 -0.33000900
H 2.45545600 9.12213700 -0.47630500
H 1.19561000 6.95752300 -0.37802500
O 2.20679500 4.67009000 -0.13854500
C 6.39015100 4.17882400 0.17927600
C 7.43686200 5.14272400 0.19870800
N 8.34280400 5.86794700 0.22458200
C 6.86350100 2.83869900 0.31010300
N 7.25551800 1.75187200 0.41635100
H 4.50538400 2.29333700 0.17088500
H 2.30290000 1.36328800 0.08127000
H 0.10174900 3.52751500 -0.14039600
C -1.80459900 1.72194100 -0.05121900
C -2.84331400 0.70986700 0.06609200
C -2.38751300 -0.70448700 0.29251000
C -1.08201700 -0.97856800 -0.44536500
H -1.24787300 -0.87264300 -1.52937000
H -0.75310200 -2.01021200 -0.26273000
H -3.18499700 -1.39695600 -0.00809900

H -2.22315100 -0.84528900 1.37488800
C -4.14396300 1.07728700 0.00646100
C -4.50143400 2.47212100 -0.13684500
C -3.47713100 3.42052600 -0.19934600
O -2.18329100 3.03286600 -0.15519500
C -3.73275100 4.79513800 -0.30836200
C -5.04162800 5.22822200 -0.35648800
C -6.11712300 4.31395800 -0.29840000
C -5.82307500 2.94764200 -0.19147300
O -6.79807800 2.01554600 -0.13084700
C -8.11231900 2.35420100 -0.16634200
C -8.48210100 3.74922200 -0.26881700
C -7.50482300 4.71735900 -0.32262700
C -7.84756900 6.15177400 -0.53800700
C -7.79814500 7.12098300 0.47899000
C -8.10918700 8.44644000 0.16025700
C -8.46119000 8.81732600 -1.13514500
C -8.51184700 7.85137700 -2.13963000
C -8.20693200 6.52527300 -1.84014300
H -8.24392500 5.76476300 -2.62293800
H -8.78946600 8.12648300 -3.15823500
H -8.69960200 9.85784000 -1.36074400
H -8.07215800 9.18662400 0.95973000
C -7.44002900 6.76341400 1.92569300
O -7.21182000 5.55747700 2.16897600
O -7.40796200 7.70274400 2.74895900
C -9.89831500 4.04063600 -0.28499600
C -10.8228420 3.05602100 -0.22112600
C -10.4473690 1.63713700 -0.13496400
C -9.02865400 1.34746200 -0.10548000
H -8.70039500 0.31051800 -0.03354400
O -11.3098720 0.74789000 -0.08920500
H -11.8910590 3.27947600 -0.23059400
H -10.2055580 5.08595300 -0.34518200
H -5.25735000 6.29414800 -0.43905500
H -2.89429800 5.48933400 -0.35218100
H -4.93470800 0.33061600 0.08864800
H 0.88472400 -0.10968100 -0.64433700
H 0.33317500 -0.24502700 1.02363600

9 Cartesian Coordinates (in Å) of S₂ minimum geometry of DCM-IFC (open)

Neutral (TD-M06-2X/def2-SVP/SMD(water)):

C 0.00000000 0.00000000 0.00000000
C -0.42994800 1.43727400 -0.08180400
C 0.51506900 2.51118400 -0.11393700
C 1.86176200 2.33347600 -0.03296500
C 2.79380600 3.43625600 -0.04705600
C 4.14532700 3.26365700 0.05067000
C 5.05523500 4.36726000 0.03854900
C 4.43977500 5.68871500 -0.10251000
C 3.03428100 5.75991400 -0.19575800
C 2.35397900 6.97299200 -0.33025100

C 3.07671700 8.15112300 -0.37712100
C 4.47663200 8.11903700 -0.29143700
C 5.14169600 6.91347800 -0.15739900
H 6.22585000 6.92778800 -0.09655000
H 5.04845000 9.04603300 -0.33075800
H 2.55445200 9.10268300 -0.48254100
H 1.26612500 6.95471300 -0.39593900
O 2.24610200 4.65379700 -0.16248700
C 6.41947800 4.10249000 0.15992000
C 7.48267600 5.05128700 0.18576200
N 8.39913000 5.76138200 0.21713200
C 6.87444700 2.75298800 0.28357900
N 7.25483100 1.66239100 0.38342400
H 4.51184400 2.24231000 0.14348100
H 2.31351300 1.34465700 0.05675000
H 0.12551500 3.52709700 -0.18665700
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C -2.81552600 0.74282100 0.03595400
C -2.39987500 -0.68986600 0.21141900
C -1.07565000 -0.96445300 -0.48864200
H -1.20462400 -0.84645600 -1.57590600
H -0.75596600 -1.99767800 -0.30319000
H -3.20076700 -1.34427400 -0.15702300
H -2.29132400 -0.88914000 1.29185400
C -4.13487200 1.14265100 0.02472300
C -4.46868800 2.51531300 -0.10245700
C -3.40375200 3.46151100 -0.22046700
O -2.12865300 3.03539300 -0.20819800
C -3.65030700 4.82901500 -0.35642800
C -4.95441200 5.27549400 -0.36520400
C -6.07577700 4.38146900 -0.23485500
C -5.78636100 3.00180700 -0.11921300
O -6.75807400 2.07594900 -0.02598400
C -8.08587000 2.42572200 -0.00679600
C -8.45001200 3.79953700 -0.10136500
C -7.43460700 4.79160000 -0.22974100
C -7.80183600 6.21617100 -0.41650900
C -7.40826800 7.24796800 0.46298000
C -7.73073700 8.58043600 0.17874800
C -8.46436800 8.90574500 -0.95770900
C -8.87092200 7.89274600 -1.82584600
C -8.53859500 6.56725600 -1.55771300
H -8.84018000 5.77987300 -2.25095200
H -9.44212600 8.13482900 -2.72330200
H -8.71777000 9.94608300 -1.16390200
H -7.41571500 9.36280900 0.86895300
C -6.68693500 6.93850300 1.73453800
O -6.74538400 5.88450900 2.32426500
O -5.96316800 7.96618200 2.17947600
H -5.55452800 7.71339700 3.02681800
C -9.84785200 4.07125800 -0.02784300
C -10.7775610 3.06992600 0.09030400
C -10.4089500 1.66690600 0.15175400
C -8.99441600 1.40165200 0.10924700
H -8.64148000 0.37151900 0.17204400
O -11.2703160 0.75357300 0.24296900

H -11.8423010 3.30581800 0.14597600
H -10.1795860 5.11002800 -0.06006300
H -5.14386600 6.34202900 -0.48884000
H -2.81027500 5.51595000 -0.45701100
H -4.92865400 0.40043700 0.11890300
H 0.92525800 -0.13556500 -0.57598700
H 0.25351500 -0.21965400 1.05299400

Anion (TD-M06-2X/def2-SVP/SMD(water)):

C 0.00000000 0.00000000 0.00000000
C -0.44849300 1.43326300 -0.07008900
C 0.48735100 2.51720600 -0.07342000
C 1.83404600 2.35193500 0.02582200
C 2.75501600 3.46327200 0.05291900
C 4.10662900 3.30309100 0.17709400
C 5.00410400 4.41480800 0.21418200
C 4.37799400 5.73333600 0.09357500
C 2.97461700 5.79233700 -0.03285400
C 2.28455700 7.00153200 -0.15217300
C 2.99505900 8.18806400 -0.14892700
C 4.39250000 8.16827000 -0.02758800
C 5.06725800 6.96638800 0.09076000
H 6.14922100 6.99027900 0.18071900
H 4.95482100 9.10189000 -0.02649700
H 2.46495800 9.13658500 -0.24186600
H 1.19892800 6.97377000 -0.24564400
O 2.19793700 4.67787300 -0.04735100
C 6.36901000 4.16185600 0.36100600
C 7.42080100 5.12036000 0.43402900
N 8.32878000 5.83886400 0.50304000
C 6.83519100 2.81475900 0.46302000
N 7.22432000 1.72568200 0.54591100
H 4.48168300 2.28357200 0.25431100
H 2.29411800 1.36596200 0.10350100
H 0.08854800 3.53045900 -0.13439300
C -1.81488000 1.71233000 -0.09432000
C -2.82728900 0.70878500 0.01863900
C -2.39268700 -0.71852800 0.19609100
C -1.06201800 -0.97393200 -0.49951100
H -1.18759800 -0.85078100 -1.58667900
H -0.73150700 -2.00478700 -0.31927000
H -3.18284600 -1.38435600 -0.17516900
H -2.28384100 -0.91678000 1.27660500
C -4.14765300 1.09188100 -0.00361800
C -4.49834000 2.46428400 -0.12987100
C -3.44401900 3.42107300 -0.23638000
O -2.16455000 3.01225700 -0.20980500
C -3.70477700 4.78756500 -0.37803800
C -5.01174500 5.21986800 -0.40318500
C -6.12644300 4.31236800 -0.28223400
C -5.81865400 2.93528200 -0.15900900
O -6.78059700 1.99544500 -0.07580900
C -8.11107400 2.33224900 -0.06250500
C -8.49153000 3.70003800 -0.16936700
C -7.48814100 4.70903900 -0.30481700
C -7.87431600 6.12378700 -0.52404700

C -7.46236400 7.17582800 0.31917700
C -7.81995700 8.48985600 -0.00181600
C -8.60246100 8.77756100 -1.11710500
C -9.01849000 7.73824000 -1.95031300
C -8.64969500 6.42855100 -1.65686200
H -8.95491300 5.61740500 -2.32148600
H -9.62147300 7.94717200 -2.83538400
H -8.88244200 9.80854200 -1.33918500
H -7.47731400 9.29344300 0.65194300
C -6.64180200 6.94471300 1.59079600
O -6.89076200 5.91782800 2.25846900
O -5.79173500 7.82212600 1.86516600
C -9.89331600 3.95489300 -0.09853700
C -10.8126360 2.94439800 0.02473800
C -10.4269610 1.54666200 0.09499000
C -9.00809800 1.29798500 0.05797700
H -8.64354200 0.27238500 0.12909100
O -11.2759950 0.62264100 0.18975000
H -11.8800440 3.16840200 0.07862900
H -10.2361420 4.98960400 -0.13586300
H -5.21091100 6.28402700 -0.52437800
H -2.87054700 5.48297400 -0.46895000
H -4.93389600 0.34070400 0.08190300
H 0.92694800 -0.11713500 -0.57779700
H 0.25766700 -0.22808300 1.05003600

10 Cartesian Coordinates (in Å) of S₁ minimum geometry of DCM-IFC (open)

Neutral (TD-M06-2X/def2-SVP/SMD(water)):

C 0.00000000 0.00000000 0.00000000
C -0.43364800 1.43939300 -0.11356200
C 0.46599700 2.50355800 -0.14966700
C 1.86269300 2.35839600 -0.06788300
C 2.75431900 3.43341000 -0.09059400
C 4.14428800 3.28931600 0.00706700
C 5.03068000 4.37130300 -0.01286400
C 4.41779000 5.70070200 -0.15823300
C 3.01030300 5.77790900 -0.25022400
C 2.34308000 6.99467100 -0.38922300
C 3.07076700 8.17585100 -0.44266700
C 4.46504500 8.13537500 -0.35851700
C 5.12170400 6.91885600 -0.21961400
H 6.20614200 6.92537200 -0.15989700
H 5.04598200 9.05683000 -0.40191300
H 2.55035500 9.12817000 -0.55169900
H 1.25474900 6.98405600 -0.45388500
O 2.21064000 4.67692300 -0.21116800
C 6.43151100 4.12087600 0.10502700
C 7.48081200 5.07086400 0.13389600
N 8.39387500 5.79268200 0.16705400
C 6.89061400 2.78206900 0.22259900
N 7.26446300 1.68456600 0.31782100
H 4.51634000 2.26924300 0.10647800

H 2.31901900 1.37263400 0.03260300
H 0.06613500 3.51504200 -0.22567600
C -1.83906300 1.69190400 -0.14407800
C -2.82778600 0.69913300 -0.03418100
C -2.39580100 -0.73273400 0.12238000
C -1.04515200 -0.97233800 -0.53946500
H -1.14296800 -0.83956100 -1.62848300
H -0.71633500 -2.00437000 -0.36138100
H -3.17438200 -1.38842800 -0.28971700
H -2.32404600 -0.95574300 1.20059600
C -4.16395600 1.07211900 -0.05739500
C -4.50968500 2.44198400 -0.18365900
C -3.47490000 3.39747600 -0.29126500
O -2.19670700 2.99841700 -0.26972400
C -3.72746900 4.77083100 -0.42320200
C -5.03496500 5.20478600 -0.45017100
C -6.11795000 4.29439100 -0.34599100
C -5.83794200 2.93227400 -0.21534400
O -6.81265300 2.00943300 -0.11410700
C -8.12672700 2.35400700 -0.13128000
C -8.48705300 3.75360300 -0.26007700
C -7.50278400 4.70591300 -0.36220000
C -7.83785300 6.14206700 -0.58276300
C -7.82110900 7.11149900 0.43752500
C -8.13629400 8.44147100 0.13657000
C -8.46108900 8.81525100 -1.16397700
C -8.47858000 7.85620800 -2.17485600
C -8.17032300 6.52794300 -1.88459500
H -8.18508200 5.77557200 -2.67513400
H -8.73478500 8.13874400 -3.19682600
H -8.70283700 9.85497500 -1.38623800
H -8.12635900 9.18431900 0.93330400
C -7.48061000 6.72174500 1.83783900
O -7.17555200 5.60153700 2.17855000
O -7.54431900 7.73811900 2.69397000
H -7.31713600 7.41089300 3.58245200
C -9.90188200 4.06033700 -0.25867800
C -10.8319730 3.08649400 -0.15389700
C -10.4663360 1.66465200 -0.03990900
C -9.04805700 1.35948200 -0.02859800
H -8.72958700 0.32100500 0.06147600
O -11.3339810 0.78734200 0.04134100
H -11.8984140 3.31801300 -0.15091600
H -10.2004580 5.10667700 -0.34151200
H -5.24866100 6.26956600 -0.55405200
H -2.88755000 5.45975100 -0.50239200
H -4.94754000 0.31758200 0.02082200
H 0.95379800 -0.13944900 -0.52545700
H 0.19264300 -0.22086900 1.06506400

Anion (TD-M06-2X/def2-SVP/SMD(water)):

C 0.00000000 0.00000000 0.00000000
C -0.43728600 1.43802500 -0.11655700
C 0.45939500 2.50540800 -0.14608100
C 1.85561400 2.36544100 -0.05183200
C 2.74495500 3.44250400 -0.08126400

C 4.13440000 3.30335400 0.02801100
C 5.01865600 4.38681700 -0.00485200
C 4.40354700 5.71231300 -0.17375900
C 2.99642300 5.78485300 -0.27575700
C 2.32740900 6.99778100 -0.43767400
C 3.05271900 8.17980600 -0.50399300
C 4.44639200 8.14404000 -0.40870900
C 5.10486100 6.93132400 -0.24688600
H 6.18870800 6.94157200 -0.17795700
H 5.02541600 9.06624400 -0.46100400
H 2.53083600 9.12907600 -0.63112700
H 1.23956100 6.98359600 -0.50942100
O 2.19903700 4.68279100 -0.22452600
C 6.41968000 4.14142300 0.12278200
C 7.46838400 5.09245400 0.12350200
N 8.38135400 5.81513800 0.13401100
C 6.88031200 2.80677600 0.27579600
N 7.25545300 1.71272800 0.40132400
H 4.50819500 2.28572200 0.14458700
H 2.31406900 1.38222200 0.06306300
H 0.05673900 3.51516200 -0.22995700
C -1.84307800 1.68541300 -0.16066800
C -2.82913200 0.68757600 -0.07493100
C -2.39418400 -0.74399300 0.07694700
C -1.03134900 -0.97391500 -0.56284800
H -1.11073800 -0.83536000 -1.65264200
H -0.70106500 -2.00552100 -0.38480600
H -3.16303900 -1.39937700 -0.35355900
H -2.34031000 -0.97527100 1.15448900
C -4.16653900 1.05506100 -0.11628600
C -4.51671300 2.42465900 -0.23002900
C -3.48477800 3.38599200 -0.30639900
O -2.20442000 2.99205400 -0.27608500
C -3.74311500 4.76015700 -0.41379400
C -5.05268900 5.18779700 -0.44605000
C -6.13313500 4.27143500 -0.37697400
C -5.84744500 2.90954200 -0.27324900
O -6.81743700 1.97805100 -0.20638500
C -8.13260500 2.31854700 -0.23552800
C -8.49834200 3.71622000 -0.33688300
C -7.51985500 4.68257400 -0.39574100
C -7.85827000 6.11737000 -0.61322400
C -7.78121800 7.09209600 0.39691900
C -8.08957000 8.41777200 0.07695900
C -8.46527800 8.78350900 -1.21329600
C -8.54391300 7.81215200 -2.21073900
C -8.24251400 6.48559500 -1.90982600
H -8.30126600 5.72075600 -2.68701400
H -8.84042400 8.08347300 -3.22500800
H -8.70068000 9.82440500 -1.44026300
H -8.03135400 9.16226700 0.87113500
C -7.39717400 6.73963800 1.83812300
O -7.16120200 5.53467700 2.08035900
O -7.35369500 7.68091400 2.65816100
C -9.91418800 4.01130300 -0.34651900
C -10.8404930 3.02897500 -0.27836700

C -10.4683860 1.60853300 -0.19391800
C -9.04949100 1.31436700 -0.17022000
H -8.72365300 0.27661600 -0.09963900
O -11.3321820 0.72229600 -0.14457700
H -11.9081680 3.25505500 -0.28240700
H -10.2190240 5.05733200 -0.40462400
H -5.27135800 6.25335300 -0.52648600
H -2.90591900 5.45488600 -0.46763400
H -4.94754200 0.29598500 -0.05881300
H 0.96399000 -0.13428900 -0.50771300
H 0.17271600 -0.22440400 1.06778100

11 Cartesian Coordinates (in Å) of S₂/S₁-intersection region (conical intersection not converged) of DCM-IFC (open)

Neutral (TDA-CAM-B3LYP/6-31G(d)/CPCM(water)):

C -0.055444 -0.002764 0.054923
C -0.488129 1.428802 -0.055680
C 0.473628 2.518003 -0.078282
C 1.793389 2.343803 0.015449
C 2.747644 3.466685 -0.005775
C 4.074172 3.291311 0.090931
C 4.993330 4.412306 0.063175
C 4.366347 5.719301 -0.099739
C 2.965026 5.777903 -0.188187
C 2.270210 6.977028 -0.340252
C 2.980026 8.154517 -0.412504
C 4.380149 8.138140 -0.334493
C 5.055766 6.948793 -0.181621
H 6.133445 6.972725 -0.127636
H 4.937383 9.066098 -0.394813
H 2.452538 9.094809 -0.531492
H 1.188329 6.948889 -0.399974
O 2.181508 4.667136 -0.134496
C 6.335490 4.145852 0.191933
C 7.397395 5.099607 0.207950
N 8.307013 5.814961 0.232333
C 6.795185 2.797746 0.338984
N 7.187874 1.715585 0.457386
H 4.451797 2.283037 0.193617
H 2.251640 1.366502 0.111138
H 0.075714 3.521234 -0.166149
C -1.839978 1.734234 -0.108798
C -2.855467 0.739086 -0.033482
C -2.461638 -0.698838 0.141044
C -1.099795 -0.976747 -0.485344
H -1.166312 -0.871576 -1.573727
H -0.787585 -2.001690 -0.272221
H -3.237241 -1.340394 -0.285715
H -2.422174 -0.923670 1.216661
C -4.176971 1.140103 -0.099235
C -4.516958 2.494077 -0.221116
C -3.448407 3.463893 -0.271887
O -2.152243 3.035239 -0.224516

C -3.723815 4.804452 -0.376267
C -5.047620 5.226338 -0.424123
C -6.164036 4.328227 -0.375981
C -5.845048 2.950603 -0.287026
O -6.787626 2.001783 -0.262183
C -8.140763 2.314637 -0.312360
C -8.526703 3.665596 -0.396833
C -7.523597 4.692740 -0.427229
C -7.919396 6.115191 -0.578471
C -7.718179 7.096289 0.413463
C -8.059775 8.430097 0.168327
C -8.625777 8.808744 -1.040559
C -8.841370 7.847742 -2.022734
C -8.484288 6.524815 -1.791315
H -8.635427 5.782467 -2.568446
H -9.279136 8.128556 -2.975744
H -8.896329 9.845214 -1.213166
H -7.893260 9.168779 0.943430
C -7.190662 6.738034 1.760044
O -7.309093 5.661354 2.305431
O -6.565536 7.767948 2.356062
H -6.298823 7.468855 3.246019
C -9.923049 3.876173 -0.413898
C -10.823500 2.835286 -0.373428
C -10.427290 1.451392 -0.306448
C -9.010927 1.250039 -0.270057
H -8.617462 0.240351 -0.206341
O -11.269050 0.500014 -0.273839
H -11.890286 3.043231 -0.389175
H -10.292850 4.895651 -0.459679
H -5.248134 6.287492 -0.511793
H -2.911332 5.521800 -0.420165
H -4.961265 0.392946 -0.051804
H 0.895485 -0.142358 -0.463654
H 0.136797 -0.210876 1.117792

Anion (TDA-CAM-B3LYP/6-31G(d)/CPCM(water)):

C -0.076086 -0.323959 -0.238855
C -0.437532 1.082289 -0.587214
C 0.512945 2.184598 -0.576699
C 1.604526 2.237947 0.186544
C 2.440115 3.461559 0.204195
C 3.453402 3.678622 1.051503
C 4.187172 4.931818 1.042552
C 3.869249 5.827334 -0.069865
C 2.787058 5.491801 -0.898552
C 2.366046 6.295178 -1.958496
C 3.067950 7.447439 -2.236195
C 4.177148 7.801619 -1.452936
C 4.560874 7.017600 -0.386961
H 5.421280 7.319290 0.194047
H 4.734823 8.703126 -1.681607
H 2.764955 8.077560 -3.065971
H 1.506164 5.978456 -2.541334
O 2.064244 4.353869 -0.721597
C 5.063798 5.175615 2.073699

C 5.812896 6.372370 2.287334
N 6.435843 7.319872 2.516115
C 5.266058 4.192051 3.092685
N 5.447712 3.424192 3.939321
H 3.676586 2.924451 1.795547
H 1.896726 1.450218 0.873087
H 0.210886 3.076399 -1.112324
C -1.758090 1.420135 -0.840589
C -2.824576 0.482110 -0.694381
C -2.495453 -0.942065 -0.371813
C -1.086698 -1.329128 -0.812715
H -1.017004 -1.343901 -1.905791
H -0.847317 -2.331523 -0.454213
H -3.264417 -1.591549 -0.799441
H -2.551460 -1.065055 0.719558
C -4.124461 0.958087 -0.752465
C -4.385475 2.329721 -0.843906
C -3.243274 3.227558 -0.985918
O -1.997632 2.706793 -1.095402
C -3.419460 4.585636 -1.001637
C -4.694323 5.099302 -0.787793
C -5.860518 4.286104 -0.561030
C -5.661281 2.885817 -0.679497
O -6.670401 2.015681 -0.579272
C -7.965461 2.428016 -0.239842
C -8.198453 3.797879 -0.017434
C -7.137503 4.754744 -0.214083
C -7.405409 6.213135 -0.092868
C -6.762109 7.037322 0.848761
C -7.011183 8.412946 0.830216
C -7.911590 8.982725 -0.061310
C -8.561647 8.167959 -0.984354
C -8.294169 6.803872 -1.000802
H -8.781182 6.169988 -1.736538
H -9.262664 8.592032 -1.697714
H -8.099443 10.052612 -0.040460
H -6.479510 9.031896 1.545442
C -5.815093 6.506256 1.929665
O -6.077560 5.374616 2.398501
O -4.759387 7.167398 2.109057
C -9.497226 4.094962 0.429278
C -10.462945 3.115987 0.592408
C -10.238269 1.722932 0.311141
C -8.907643 1.432087 -0.109995
H -8.623212 0.402596 -0.305977
O -11.150808 0.834430 0.431654
H -11.454691 3.393177 0.943528
H -9.742267 5.129803 0.654536
H -4.816806 6.175000 -0.747715
H -2.563232 5.240420 -1.143244
H -4.949888 0.262928 -0.635833
H 0.936126 -0.531449 -0.592754
H -0.046205 -0.408082 0.856798

12 Frequencies (cm^{-1}) and IR intensities (km/mol) of normal modes of DCM-IFC (open) at M06-2X/def2-SVP/SMD(water)

| Frequency (cm^{-1}) | IR intensity (km/mol) | Frequency (cm^{-1}) | IR intensity (km/mol) | Frequency (cm^{-1}) | IR intensity (km/mol) |
|--------------------------------|-----------------------|--------------------------------|-----------------------|--------------------------------|-----------------------|
| 12.78 | 5.12 | 14.53 | 0.55 | 16.95 | 1.91 |
| 19.42 | 2.25 | 29.76 | 0.88 | 34.03 | 0.12 |
| 42.28 | 6.50 | 42.46 | 2.95 | 55.65 | 1.93 |
| 62.82 | 2.00 | 66.17 | 1.79 | 78.59 | 0.63 |
| 79.83 | 4.36 | 90.24 | 3.39 | 96.47 | 3.97 |
| 105.04 | 0.12 | 125.43 | 0.27 | 139.96 | 7.73 |
| 144.36 | 5.51 | 156.70 | 12.12 | 165.05 | 1.69 |
| 171.10 | 3.60 | 173.37 | 0.84 | 179.91 | 0.75 |
| 187.82 | 1.16 | 210.28 | 8.16 | 225.08 | 3.44 |
| 247.64 | 3.02 | 254.79 | 0.68 | 257.78 | 1.42 |
| 262.82 | 4.91 | 268.39 | 0.03 | 285.51 | 5.72 |
| 296.64 | 0.14 | 300.98 | 2.51 | 312.05 | 0.29 |
| 327.51 | 2.09 | 356.87 | 1.25 | 369.55 | 4.76 |
| 377.00 | 3.38 | 387.38 | 61.86 | 405.29 | 10.67 |
| 410.01 | 5.96 | 418.29 | 43.23 | 428.14 | 8.39 |
| 441.56 | 6.87 | 455.54 | 2.24 | 464.77 | 23.69 |
| 475.77 | 10.51 | 478.51 | 58.10 | 486.65 | 3.83 |
| 500.12 | 2.69 | 513.84 | 24.70 | 516.33 | 22.38 |
| 519.83 | 20.32 | 523.29 | 14.09 | 534.68 | 1.69 |
| 540.41 | 7.89 | 556.57 | 18.17 | 571.73 | 40.78 |
| 575.03 | 136.50 | 584.52 | 59.18 | 596.95 | 45.29 |
| 602.29 | 28.92 | 607.66 | 5.01 | 622.33 | 43.35 |
| 640.91 | 39.44 | 643.57 | 139.91 | 650.50 | 33.82 |
| 654.06 | 33.93 | 660.67 | 23.29 | 664.50 | 16.59 |
| 680.69 | 17.39 | 690.58 | 13.66 | 700.00 | 15.99 |
| 712.27 | 18.81 | 721.48 | 14.64 | 729.97 | 226.23 |
| 733.32 | 1.15 | 745.94 | 27.35 | 760.12 | 3.18 |
| 769.30 | 43.33 | 779.63 | 0.23 | 782.64 | 74.40 |
| 786.33 | 80.49 | 795.68 | 5.71 | 801.36 | 25.61 |
| 810.18 | 42.29 | 811.28 | 27.91 | 831.94 | 0.44 |
| 841.25 | 12.47 | 843.74 | 97.29 | 848.15 | 34.29 |
| 854.46 | 27.02 | 868.66 | 7.61 | 875.16 | 128.56 |
| 880.43 | 7.02 | 905.85 | 1.63 | 907.93 | 31.19 |
| 915.91 | 74.64 | 918.74 | 24.50 | 934.73 | 65.57 |
| 936.64 | 28.96 | 938.82 | 32.64 | 941.95 | 1.51 |
| 946.29 | 41.09 | 985.58 | 76.77 | 1001.85 | 0.10 |
| 1007.34 | 1.20 | 1011.35 | 45.12 | 1013.51 | 22.15 |
| 1023.73 | 423.65 | 1027.05 | 0.64 | 1045.83 | 5.09 |
| 1048.49 | 0.24 | 1055.22 | 0.03 | 1073.25 | 73.40 |
| 1074.13 | 14.46 | 1078.80 | 9.22 | 1085.06 | 109.94 |
| 1097.75 | 229.28 | 1111.57 | 60.36 | 1128.25 | 214.21 |
| 1134.17 | 7.75 | 1151.21 | 2480.15 | 1156.74 | 274.76 |
| 1157.42 | 8.01 | 1160.22 | 27.70 | 1161.76 | 185.84 |
| 1180.75 | 637.45 | 1185.33 | 15.86 | 1200.40 | 1055.06 |
| 1206.81 | 627.10 | 1213.79 | 440.56 | 1227.32 | 200.95 |
| 1228.24 | 512.14 | 1238.93 | 117.04 | 1244.60 | 227.41 |
| 1260.95 | 33.50 | 1262.49 | 533.75 | 1263.28 | 47.96 |
| 1269.84 | 937.55 | 1283.83 | 233.47 | 1291.58 | 165.47 |
| 1299.63 | 66.00 | 1315.05 | 91.51 | 1319.62 | 1353.14 |
| 1335.98 | 876.67 | 1343.13 | 29.16 | 1351.07 | 34.49 |
| 1359.70 | 13.64 | 1367.58 | 233.71 | 1371.41 | 16.77 |
| 1385.07 | 40.16 | 1387.98 | 117.27 | 1400.60 | 327.04 |
| 1404.51 | 499.27 | 1416.08 | 118.44 | 1422.97 | 21.40 |
| 1425.88 | 37.53 | 1430.13 | 50.02 | 1448.57 | 802.10 |
| 1448.94 | 1325.91 | 1452.97 | 63.99 | 1469.71 | 407.32 |
| 1484.62 | 108.67 | 1495.23 | 2130.09 | 1520.43 | 1242.23 |
| 1526.03 | 2715.91 | 1533.00 | 236.91 | 1545.35 | 2608.43 |
| 1549.77 | 57.63 | 1587.92 | 6738.37 | 1613.31 | 166.17 |
| 1636.58 | 401.79 | 1648.78 | 400.28 | 1662.86 | 213.07 |
| 1666.41 | 95.13 | 1671.15 | 282.86 | 1677.01 | 1334.56 |
| 1689.72 | 48.56 | 1691.64 | 488.28 | 1704.22 | 256.12 |
| 1711.83 | 858.95 | 1729.54 | 111.41 | 1731.35 | 354.70 |
| 1824.56 | 834.98 | 2347.09 | 311.80 | 2363.32 | 931.99 |
| 3051.27 | 39.49 | 3057.68 | 16.96 | 3075.89 | 42.80 |
| 3115.88 | 32.70 | 3142.70 | 45.72 | 3144.22 | 19.23 |
| 3223.89 | 0.07 | 3224.45 | 0.03 | 3227.76 | 5.36 |
| 3234.40 | 1.81 | 3234.93 | 0.64 | 3235.63 | 28.30 |
| 3237.96 | 7.54 | 3238.44 | 2.55 | 3240.86 | 29.68 |
| 3244.00 | 1.17 | 3244.70 | 2.63 | 3244.74 | 1.43 |
| 3250.86 | 1.24 | 3255.68 | 3.00 | 3258.85 | 1.43 |
| 3259.82 | 7.89 | 3296.40 | 7.13 | 3762.87 | 328.20 |

Table S3: Vibrational frequencies and IR intensities for ground state neutral DCM-IFC (open).

| Frequency (cm ⁻¹) | IR intensity (km/mol) | Frequency (cm ⁻¹) | IR intensity (km/mol) | Frequency (cm ⁻¹) | IR intensity (km/mol) |
|-------------------------------|-----------------------|-------------------------------|-----------------------|-------------------------------|-----------------------|
| 13.70 | 7.23 | 15.25 | 2.82 | 18.31 | 3.54 |
| 25.47 | 17.13 | 30.64 | 1.25 | 35.33 | 2.79 |
| 42.26 | 2.19 | 47.81 | 5.05 | 62.02 | 4.38 |
| 63.04 | 1.19 | 76.21 | 0.38 | 79.19 | 0.09 |
| 86.65 | 4.55 | 90.13 | 3.11 | 97.13 | 6.70 |
| 106.36 | 1.39 | 129.54 | 9.66 | 143.23 | 2.59 |
| 145.84 | 27.81 | 156.98 | 13.33 | 164.39 | 1.52 |
| 170.92 | 3.83 | 173.77 | 0.88 | 179.85 | 4.51 |
| 187.72 | 1.43 | 210.27 | 12.82 | 225.64 | 10.40 |
| 246.37 | 19.08 | 256.06 | 0.54 | 259.57 | 5.08 |
| 262.99 | 5.86 | 269.01 | 0.40 | 286.50 | 2.30 |
| 296.69 | 2.93 | 302.50 | 2.64 | 311.83 | 0.43 |
| 330.40 | 2.81 | 356.66 | 0.99 | 369.54 | 5.78 |
| 377.28 | 5.33 | 387.23 | 63.74 | 402.16 | 16.50 |
| 408.50 | 4.89 | 418.31 | 43.84 | 441.15 | 3.90 |
| 441.82 | 6.30 | 456.34 | 3.59 | 464.52 | 18.89 |
| 476.70 | 8.60 | 479.81 | 48.52 | 486.76 | 5.07 |
| 500.28 | 2.48 | 516.28 | 29.34 | 517.92 | 30.99 |
| 523.32 | 17.22 | 524.90 | 10.23 | 534.41 | 1.78 |
| 540.49 | 9.43 | 558.62 | 8.00 | 572.17 | 48.05 |
| 585.24 | 39.06 | 597.64 | 73.84 | 602.29 | 28.23 |
| 607.63 | 5.24 | 622.87 | 50.01 | 641.90 | 21.90 |
| 644.00 | 150.03 | 652.05 | 24.35 | 657.85 | 7.63 |
| 664.60 | 2.85 | 676.20 | 34.83 | 688.66 | 3.63 |
| 694.35 | 25.39 | 698.76 | 16.15 | 712.05 | 18.84 |
| 723.22 | 17.29 | 728.42 | 154.14 | 734.33 | 40.38 |
| 745.77 | 17.66 | 758.97 | 0.37 | 776.60 | 37.40 |
| 782.52 | 72.94 | 784.05 | 4.20 | 788.51 | 70.01 |
| 799.71 | 24.11 | 801.07 | 20.87 | 811.37 | 24.54 |
| 839.87 | 2.73 | 840.56 | 3.87 | 843.58 | 88.62 |
| 848.24 | 73.73 | 849.03 | 108.79 | 855.13 | 10.31 |
| 869.48 | 7.82 | 873.58 | 121.63 | 880.11 | 6.12 |
| 905.79 | 2.07 | 908.13 | 30.93 | 915.72 | 80.76 |
| 919.70 | 18.90 | 934.82 | 70.79 | 936.47 | 29.12 |
| 938.56 | 17.63 | 942.00 | 4.30 | 946.28 | 47.44 |
| 985.48 | 71.66 | 1004.16 | 0.34 | 1007.30 | 1.16 |
| 1010.98 | 49.77 | 1011.50 | 20.16 | 1023.68 | 437.06 |
| 1025.70 | 2.46 | 1045.56 | 9.37 | 1048.47 | 0.21 |
| 1051.68 | 0.38 | 1067.44 | 18.24 | 1073.25 | 73.94 |
| 1074.10 | 14.23 | 1085.78 | 159.31 | 1099.34 | 119.93 |
| 1109.50 | 12.71 | 1123.20 | 235.13 | 1134.25 | 6.85 |
| 1147.50 | 14.83 | 1151.10 | 2659.52 | 1156.66 | 282.79 |
| 1160.06 | 24.18 | 1177.04 | 14.12 | 1180.52 | 706.20 |
| 1186.89 | 8.94 | 1200.12 | 1197.70 | 1210.59 | 595.08 |
| 1226.90 | 266.04 | 1227.50 | 526.13 | 1238.67 | 109.34 |
| 1244.64 | 238.77 | 1255.73 | 9.45 | 1261.75 | 9.57 |
| 1262.37 | 738.75 | 1264.60 | 167.54 | 1273.50 | 887.99 |
| 1291.14 | 209.52 | 1298.47 | 72.46 | 1314.65 | 122.64 |
| 1318.22 | 1245.68 | 1336.30 | 857.92 | 1341.57 | 10.56 |
| 1346.03 | 24.66 | 1359.70 | 11.67 | 1367.73 | 222.09 |
| 1371.27 | 19.92 | 1385.87 | 13.97 | 1388.03 | 123.27 |
| 1404.13 | 515.58 | 1416.01 | 110.67 | 1422.61 | 16.17 |
| 1425.43 | 25.60 | 1430.43 | 38.68 | 1445.49 | 586.30 |
| 1447.80 | 2098.87 | 1448.70 | 235.23 | 1452.88 | 71.07 |
| 1470.75 | 428.26 | 1481.29 | 80.57 | 1494.24 | 2513.03 |
| 1519.27 | 1637.39 | 1521.86 | 744.93 | 1527.08 | 2030.63 |
| 1544.57 | 2158.53 | 1547.23 | 192.13 | 1582.23 | 6760.83 |
| 1606.95 | 289.81 | 1629.01 | 366.15 | 1646.97 | 407.71 |
| 1657.99 | 203.41 | 1662.20 | 213.57 | 1670.91 | 279.27 |
| 1676.30 | 1606.96 | 1682.75 | 295.73 | 1690.23 | 536.74 |
| 1704.01 | 345.18 | 1706.03 | 510.59 | 1712.48 | 1079.29 |
| 1726.51 | 242.95 | 1730.05 | 24.25 | 2346.52 | 316.26 |
| 2362.90 | 939.78 | 3050.97 | 39.92 | 3057.42 | 17.41 |
| 3075.65 | 43.22 | 3115.89 | 33.08 | 3142.28 | 46.51 |
| 3143.84 | 19.50 | 3214.58 | 0.27 | 3224.19 | 0.16 |
| 3225.13 | 3.00 | 3227.31 | 5.73 | 3234.44 | 1.80 |
| 3235.95 | 27.90 | 3236.71 | 4.21 | 3237.84 | 7.45 |
| 3240.01 | 32.03 | 3240.17 | 1.25 | 3242.78 | 0.63 |
| 3244.67 | 1.44 | 3244.74 | 5.34 | 3250.89 | 1.28 |
| 3255.12 | 2.66 | 3259.40 | 7.79 | 3296.36 | 7.14 |

Table S4: Vibrational frequencies and IR intensities for ground state anionic DCM-IFC (open).

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