Supplementary Materials for

Amphiphilic Adsorption of Human Islet Amyloid Polypeptide Aggregates to Lipid/Aqueous Interfaces

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I. Euler transformation matrix.

$$R=\begin{pmatrix} \cos(\phi)\cos(\theta)\cos(\psi)-\sin(\phi)\sin(\psi) & \cos(\phi)\cos(\theta)\sin(\psi)+\sin(\phi)\cos(\psi) & -\cos(\phi)\sin(\theta) \\ -\sin(\phi)\cos(\theta)\cos(\psi)-\cos(\phi)\sin(\psi) & -\sin(\phi)\cos(\theta)\sin(\psi)+\cos(\phi)\cos(\psi) & \sin(\phi)\sin(\theta) \\ \sin(\theta)\cos(\psi) & \sin(\theta)\sin(\psi) & \cos(\theta) \end{pmatrix} \quad \text{(S1)}$$

II. The chiral and achiral susceptibility elements.

$\chi^{(2)}_{zyx}$ and $\chi^{(2)}_{xyz}$ can be obtained by an integration of the in plane rotation angle ϕ from 0 to 2π as discussed in Simpson *et al*. to yield (1)

$$\chi^{(2)}_{zyx}=-\chi^{(2)}_{zxy}=-\frac{1}{2}N_S\times\left\{\begin{aligned} &\left\langle\cos^2\theta\right\rangle(\beta_{cab}-\beta_{cba}) \\ &+\left\langle\sin^2\theta\sin^2\psi\right\rangle(\beta_{bca}-\beta_{bac}) \\ &+\left\langle\sin^2\theta\cos^2\psi\right\rangle(\beta_{abc}-\beta_{acb}) \\ &+\left\langle\sin^2\theta\sin\psi\cos\psi\right\rangle(\beta_{aac}-\beta_{aca}-\beta_{bbc}+\beta_{bcb}) \\ &+\left\langle\sin\theta\cos\theta\sin\psi\right\rangle(\beta_{bab}-\beta_{bba}-\beta_{cac}+\beta_{cca}) \\ &+\left\langle\sin\theta\cos\theta\cos\psi\right\rangle(-\beta_{aab}+\beta_{aba}-\beta_{cbc}+\beta_{ccb}) \end{aligned}\right\} \quad \text{(S2)}$$

$$\chi^{(2)}_{xyz}=\frac{1}{2}N_S\times\left\{\begin{aligned} &\left\langle\cos^2\theta\right\rangle(\beta_{abc}-\beta_{bac}) \\ &+\left\langle\sin^2\theta\sin^2\psi\right\rangle(\beta_{cab}-\beta_{acb}) \\ &+\left\langle\sin^2\theta\cos^2\psi\right\rangle(\beta_{bca}-\beta_{cba}) \\ &+\left\langle\sin^2\theta\sin\psi\cos\psi\right\rangle(\beta_{aca}-\beta_{bcb}-\beta_{caa}+\beta_{cbb}) \\ &+\left\langle\sin\theta\cos\theta\sin\psi\right\rangle(\beta_{abb}-\beta_{acc}-\beta_{bab}+\beta_{cac}) \\ &+\left\langle\sin\theta\cos\theta\cos\psi\right\rangle(-\beta_{aba}+\beta_{baa}-\beta_{bcc}+\beta_{cbc}) \end{aligned}\right\} \quad \text{(S3)}$$

For the *ssp* SFG spectra, the intensity is proportional to the square of $\chi_{ssp}^{(2)}$,

$$\chi_{ssp}^{(2)} = L_{xxz}\chi_{xxz}^{(2)} \tag{S4}$$

where the L_{xxz} is Fresnel factor, and $\chi_{xxz}^{(2)}$ is shown as reported by Simpson *et al*. (1),

$$\chi_{xxz}^{(2)} = \frac{1}{2}N_S \times \left\{ \begin{array}{l} \left\langle \sin^2\theta\cos\theta \right\rangle \beta_{ccc} + \left\langle \cos\theta \right\rangle (\beta_{aac} - \beta_{bbc}) \\ -\left\langle \sin^2\theta\cos\theta\sin^2\psi \right\rangle (\beta_{bbc} + \beta_{bcb} + \beta_{cbb}) \\ -\left\langle \sin^2\theta\cos\theta\cos^2\psi \right\rangle (\beta_{aac} + \beta_{aca} + \beta_{caa}) \\ +\left\langle \sin^2\theta\cos\theta\sin\psi\cos\psi \right\rangle (\beta_{abc} + \beta_{acb} + \beta_{bac} + \beta_{bca} + \beta_{cab} + \beta_{cba}) \\ +\left\langle \sin\theta\sin\psi \right\rangle (\beta_{bbb} + \beta_{aab} - \beta_{bcc} - \beta_{cbc}) \\ +\left\langle \sin\theta\cos\psi \right\rangle (-\beta_{aaa} - \beta_{bba} + \beta_{acc} + \beta_{cac}) \\ +\left\langle \sin^3\theta\sin\psi \right\rangle (-\beta_{aab} - \beta_{aba} - \beta_{baa} + \beta_{bcc} + \beta_{cbc} + \beta_{ccb}) \\ +\left\langle \sin^3\theta\cos\psi \right\rangle (\beta_{abb} + \beta_{bab} + \beta_{bba} - \beta_{acc} - \beta_{cac} - \beta_{cca}) \\ +\left\langle \sin^3\theta\sin^3\psi \right\rangle (-\beta_{bbb} + \beta_{aab} + \beta_{aba} + \beta_{baa}) \\ +\left\langle \sin^3\theta\cos^3\psi \right\rangle (\beta_{aaa} - \beta_{abb} - \beta_{bab} - \beta_{bba}) \end{array} \right\} \tag{S5}$$

III. Amide I normal modes of a tri-peptide pair.

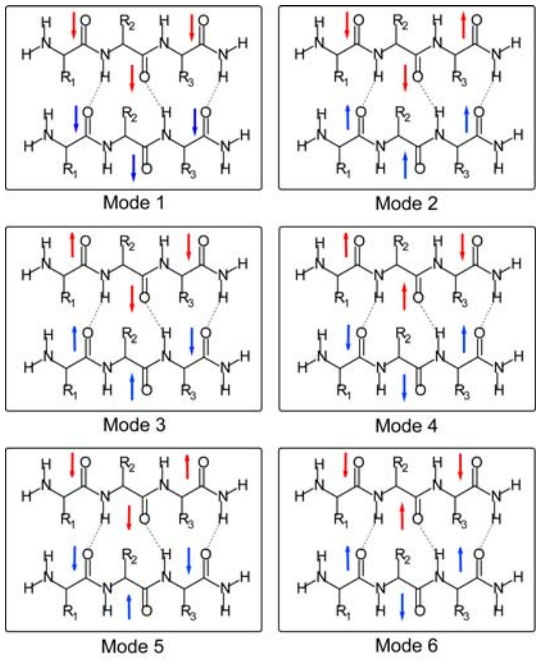

FIGURE S1. Vibrational normal modes of the C=O stretch for a typical tri-peptide pair analog.

IV. Categorizing the normal modes via the *ab initio* analysis.

To calculate the overall hyperpolarizability of the β-sheet model from the 89 hyperpolarizability tensors (see Section VI for the details of excluding irrelevant normal modes), we need to classify the corresponding normal modes into A and B modes by considering the ideal and non-ideal A and B modes. In ideal cases (see the transition dipole vectors, Fig. S3a), the transition dipole for the A mode is perpendicular to the backbone of β-strands, while that for the B mode is parallel to the backbone of β-strands. However, from the *ab initio* normal mode analysis and also in reality, the transition dipoles for the A and B modes are not perfectly perpendicular and parallel to the β-strands, and thus non-ideal cases need to be considered. In the non-ideal cases, the deviation can come from inhomogeneous magnitudes of dipole derivatives of single C=O groups, the existence of odd number of strongly coupled C=O stretches, and/or the vibrational coupling of C=O stretch to other functional groups.

In our treatment, the deviation is described by ξ (ξ has a range of 0-90°), which is defined as the angle between the transition dipole and the backbone of β-strands, i.e., ξ = 0º for ideal A mode and ξ = 90º for ideal B mode. ξ is estimated to be 68º for the amide I vibration of a single glycine peptide analog. For the ideal case of a tri-peptide analog (Fig. S3b), i.e., assuming that each amide group possesses identical vibrational magnitude and orientation in a coupled normal mode, the A-type mode of a tri-peptide analog (Fig. S3b) shows ξ = 40º, and the B-type mode of a tri-peptide analog (Fig. S3b) shows ξ = 82º. Giving some reasonable freedom for ξ to vary as the amide I vibrations (i.e. magnitude and orientation) of individual C=O groups may differ in a coupled mode and following the convection of defining A and B modes, here we classify all the normal modes from *ab initio* analysis into A-type and B-type modes. The A-type modes are assigned when $0 \le \xi < 75°$, while the B-type modes are assigned when $75° \le \xi \le 90°$.

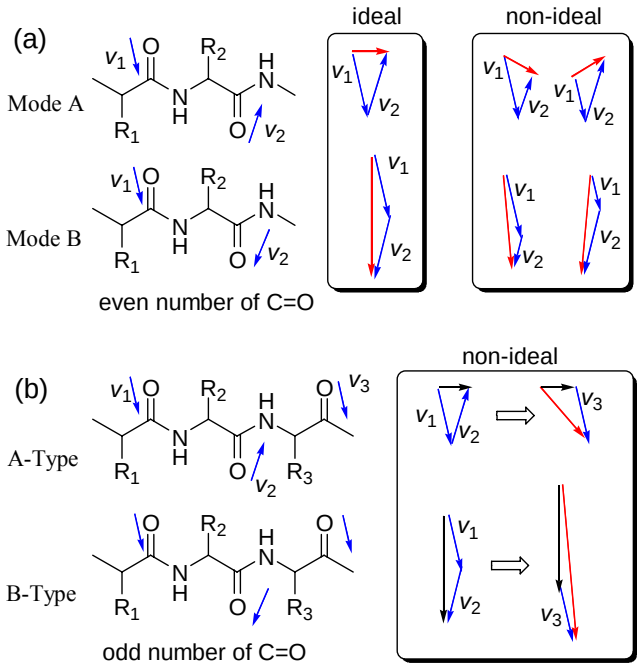

FIGURE S2. The ideal and non-ideal A and B vibrational modes in parallel *β*-sheets.

V. Normal mode analysis for all the possible tri-peptide pairs in the beta-sheet region of hIAPP aggregates.

TABLE S1. The amide I normal modes of the 16 tripeptide pairs (tpps) used for the simulation of the SFG spectra of the hIAPP aggregates. The vibrational frequencies are shown as the result of the *ab initio* normal mode analyses using the B3LYP/6-31g* method without any scaling factors for shifting the frequency. The angle ξ is defined as the angle between the normal mode dipole derivative and the peptide backbone. The percentage of vibration distributed among the peptide backbone atoms is also shown.

tpps	Chemical composition	Modes	Backbone vibration (%)	Freq (cm^{-1})	ξ (degree)	Type
1	Ala8Thr9Gln10	211	94	1721.65	78	B
		212	92	1735.87	89	B
		213	95	1746.54	17	A
		215	97	1769.47	53	A
		216	78	1782.10	58	deleted
		218	96	1794.17	85	B
2	Thr9Gln10Arg11	279	27	1722.56	70	deleted
		280	19	1722.60	87	deleted
		281	65	1745.37	75	B
		283	85	1759.02	82	B
		284	97	1777.91	66	A
		286	98	1794.12	40	A
3	Gln10Arg11Leu12	298	59	1718.08	90	deleted
		301	75	1733.27	88	B
		302	40	1743.44	89	B
		303	50	1750.22	56	A
		304	76	1756.02	62	A
		308	87	1774.93	36	A
4	Arg11Leu12Ala13	263	71	1707.86	84	B
		268	87	1733.76	74	A
		269	90	1750.05	12	A
		270	96	1757.48	82	B
		271	98	1780.96	70	A
		272	99	1804.08	66	A
5	Leu12Ala13Asn14	219	90	1731.62	85	B
		220	70	1733.86	77	B
		221	70	1755.79	72	deleted
		222	80	1762.64	62	A
		224	88	1777.23	64	A
		226	99	1794.15	74	A
6	Ala13Asn14Phe15	228	91	1702.42	70	A
		230	93	1741.56	86	B
		231	96	1753.55	18	A
		232	79	1771.86	63	A
		234	76	1787.40	81	B
		236	97	1808.26	72	A
7	Asn14Phe15Leu16	270	71	1706.49	71	A

		272	95	1733.30	79	B
		273	93	1763.00	90	B
		274	82	1766.75	59	A
		276	91	1779.10	28	A
		278	98	1799.86	76	B
8	Phe15Leu16Val17	279	94	1727.13	85	B
		280	97	1732.03	69	A
		281	96	1752.63	88	B
		282	84	1767.98	62	A
		283	96	1771.20	76	B
		284	99	1796.22	77	B
9	Ser28Ser29Thr30	189	93	1725.02	65	A
		190	95	1728.08	79	B
		191	97	1753.90	73	A
		192	88	1766.67	73	A
		193	99	1780.89	65	A
		194	99	1795.57	79	B
10	Ser29Thr30Asn31	203	66	1715.90	77	B
		204	91	1722.53	74	A
		205	88	1756.03	82	B
		206	80	1768.61	64	A
		207	93	1769.49	66	A
		208	57	1775.70	64	A
11	Thr30Asn31Val32	225	96	1713.38	84	B
		226	72	1732.90	69	A
		227	97	1761.33	24	A
		228	97	1762.78	74	A
		229	97	1776.27	52	A
		231	87	1800.78	90	B
12	Asn31Val32Gly33	191	95	1716.06	79	B
		192	97	1730.61	71	A
		193	97	1764.02	48	A
		194	97	1769.64	82	B
		195	99	1784.09	76	B
		198	93	1803.40	72	A
13	Val32Gly33Ser34	177	96	1732.28	87	B
		178	98	1736.43	61	A
		179	97	1758.88	78	B
		180	83	1764.60	70	A
		181	99	1785.79	65	A
		182	99	1797.32	49	A
14	Gly33Ser34Asn35	169	94	1737.26	75	B
		170	77	1746.35	83	B
		171	79	1754.69	78	B
		172	87	1759.86	41	A
		173	60	1770.27	60	A
		174	66	1778.17	82	Deleted
15	Ser34Asn35Thr36	202	89	1703.10	80	B
		204	87	1736.63	78	B

		205	95	1749.08	28	A
		206	96	1764.08	47	A
		207	85	1778.40	56	A
		210	97	1817.93	74	A
16	Asn35Thr36Tyr37	255	95	1720.60	73	A
		256	67	1729.26	78	B
		257	74	1760.09	70	A
		259	79	1769.44	28	A
		260	64	1778.55	47	Deleted
		262	100	1805.26	73	A

Among these 96 normal modes in Table S1, 7 of them are eliminated (shown as 'Deleted') for computing the SFG hyperpolarizability of β-sheets (using Eq. 5) because the C=O stretch is coupled strongly with the carbonyl group in the residues with more than 20% of the vibration amplitudes are distributed on the residues. We expect the residues are flexible in the aqueous environment, so that the lack of macroscopic order of these residues at the interface could diminish the SFG signals of the coupled normal modes. We find that eliminating these 7 modes leads to a better matching between the calculated and experimental SFG spectra. Therefore, we conclude that these 7 modes are artifacts that need to be removed in the calculation, due to the lack of dynamic effect of the residues in the simulation here. Subsequently, 89 normal modes from the 16 tpp's are used for calculating the overall hyperpolarizability.

VI. Parallel β-Sheet Hyperpolarizability.

The frequency-dependent vibrational hyperpolarizability of the β-sheet is computed from the hyperpolarizabilities components of N_q=89 normal modes, as follows (Fig. S4):

$$\beta_{lmn}(\omega) = \frac{1}{2}\sum_{q=1}^{N_q} g(\omega, \omega_q)\beta_{lmn,q} \tag{S6}$$

where $g(\omega, \omega_q)$ is a Gaussian function accounting for the broadening of the normal mode ω_q.

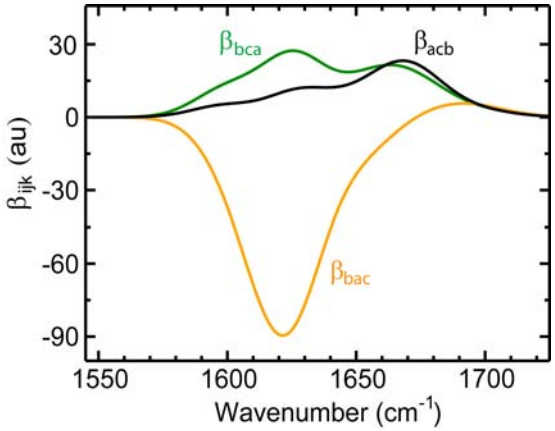

FIGURE S3. The calculated spectra of β_{lmn} components: β_{bca}, β_{bac}, and β_{acb}, where $\beta_{bca,B}$, $\beta_{bac,B}$, and $\beta_{acb,A}$ are taken as the corresponding hyperpolarizability values at the spectral peak positions.

The numerical values of $\beta_{bca,B}$ and $\beta_{bac,B}$ (i.e., the maximum and minimum values of $\beta_{bca,}$ and $\beta_{bac,}$, respectively, at around 1622 cm^{-1} in Fig. S4) and $\beta_{acb,A}$ (the peak value of β_{acb} at around 1660 cm^{-1} in Fig. S4) give the intensity ratios $\beta_{bca,B}/\beta_{acb,A}$ = 1.2 and $\beta_{bac,B}/\beta_{acb,A}$ = -3.8.

VII. Solving for the orientation angle ψ directly by the numerical simulation.

The intensity ratio of B mode to A mode $I_{B/A}$ is calculated numerically by

$$I_{\mathrm{B/A}}(\psi) = \left| \frac{\chi^{(2)}_{psp,B}(\psi)}{\chi^{(2)}_{psp,A}(\psi)} \right|^2 \approx \left| \frac{R(\chi^{(2)}_{psp,B}(\psi))}{R(\chi^{(2)}_{psp,A}(\psi))} \right|^2 \quad \text{(S7)}$$

Here, $R\left(\chi^{(2)}_{psp,A}(\psi)\right)$ is taken as the peak value around 1622 cm^{-1} of the real $\chi^{(2)}_{psp}(\psi)$ function, and $R\left(\chi^{(2)}_{psp,B}(\psi)\right)$ is taken as the peak value around 1660 cm^{-1} of the real $\chi^{(2)}_{psp}(\psi)$ function. The approximation in Eq. S5 is made because the imaginary part of $\chi^{(2)}_{psp}(\psi)$ is negligibly (~10^3 times) smaller than the real part. For examples, a few $R\left(\chi^{(2)}_{psp}\right)$ functions with ψ-angles labeled are shown in Fig. S4, all the $R\left(\chi^{(2)}_{psp}\right)$ functions used ($0 \le \psi \le 360^\circ$, with an interval of 5°) are shown in Fig. S5. In Figure S4 or S5, the ratios of $R(\chi^{(2)}_{psp,B}) / R(\chi^{(2)}_{psp,A})$ are shown to vary with the change of ψ.

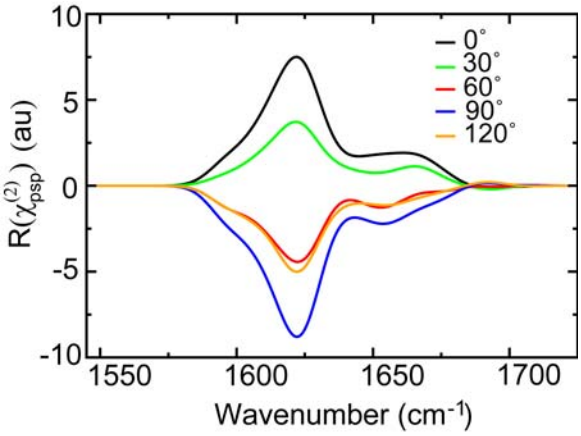

FIGURE S4. The real parts of a few $\chi^{(2)}_{psp}(\psi)$ functions with the ψ-angles labeled.

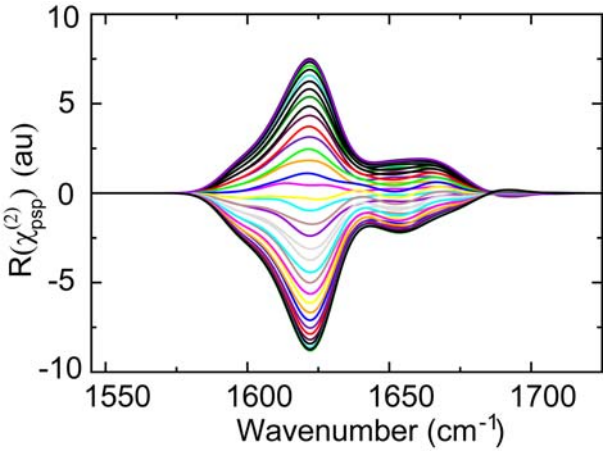

FIGURE S5. The real parts of the $\chi^{(2)}_{psp}(\psi)$ functions for ψ = 0-360°, with an interval of 5°.

VIII. Calculated SFG spectra for the 1st and 2nd β-strand

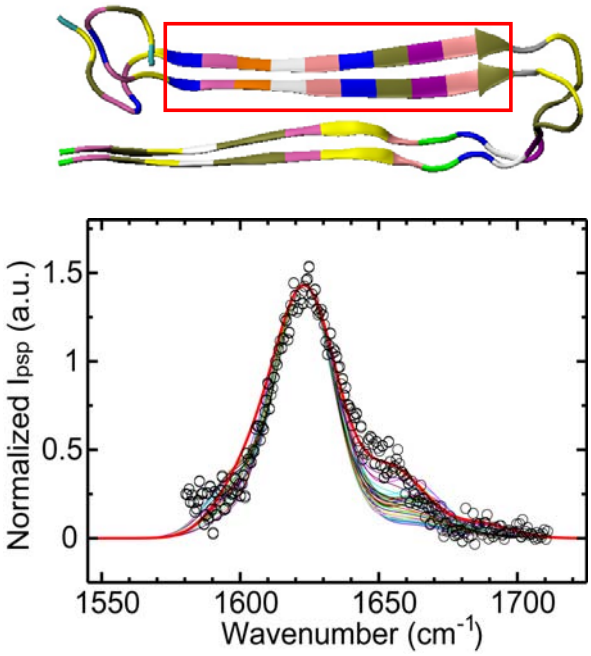

FIGURE S6. Calculated psp SFG spectra with different ψ-angles (every 5° from 0 to 180°) contributed by the first β-sheet region (i.e. the region inside the box of two parallel hIAPP molecules, top panel). The circles are experimentally measured data, and the thick red curve is the calculated SFG spectrum for the 2-strand β-sheet regions with ψ=48°.

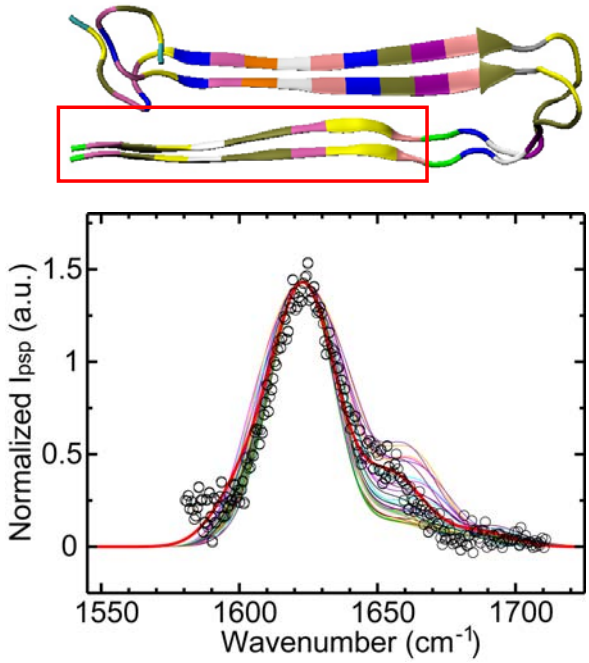

FIGURE S7. Calculated psp spectra with different ψ-angles (every 5° from 0 to 180°) contributed by the 2nd β-sheet region (i.e. the region inside the box of two parallel hIAPP molecules, top panel). The circles are experimentally measured data, and the thick red curve is the calculated SFG spectrum for the 2-strand β-sheet regions with ψ=48°.

IX. The dipole derivative vector and polarizability tensors for the used normal modes of tpps 1-16 (see Table S1).

In the following, the dipole derivative vectors are in the unit of $[KM/mol]^{1/2}$, the polarizability tensors are in the unit of $Å^2/amu^{1/2}$.

****

tpps: 1

---

mode 211, freq = 1721.6492

Dipole derivatives

-3.223380

6.022440

27.774568

Polarizability derivatives:

0.142082	-0.285204	0.005726
-0.285204	0.270548	0.326493
0.005726	0.326493	0.669965

---

mode 212, freq = 1735.8680

Dipole derivatives

-2.761790

-0.368535

16.616677

Polarizability derivatives:

0.007291	-0.261709	0.186637
-0.261709	-0.294594	0.325812
0.186637	0.325812	-0.693755

---

mode 213, freq = 1746.5389

Dipole derivatives

-0.450787
1.686200
-0.269101

Polarizability derivatives:

0.154188	-0.049748	0.048961
-0.049748	0.466609	-0.140310
0.048961	-0.140310	0.731476

---

mode 215, freq = 1769.4651

Dipole derivatives

2.371718
-6.787641
8.630794

Polarizability derivatives:

-0.016608	-0.042673	0.031214
-0.042673	-0.154465	0.182825
0.031214	0.182825	-0.617527

---

mode 216, freq = 1782.1003

Dipole derivatives

3.533190
10.767677
-17.080579

Polarizability derivatives:

-0.057928	-0.042252	-0.069147
-0.042252	-0.106922	-0.193261
-0.069147	-0.193261	1.116565

---

mode 218, freq = 1794.1693

Dipole derivatives

-0.452547
0.630985
-8.230743

Polarizability derivatives:

-0.026320	0.065460	-0.029431
0.065460	-0.039001	0.022707
-0.029431	0.022707	0.108837

```
**************************************************
tpps: 2
--------------------------------------------------
mode 281, freq = 1745.3705

 Dipole derivatives
    -1.342925
    -6.947429
    25.086643

 Polarizability derivatives:
      0.109254     -0.061417     -0.183646
     -0.061417     -0.308480      0.222782
     -0.183646      0.222782     -1.223822
--------------------------------------------------
mode 283, freq = 1759.0164

 Dipole derivatives
    -0.611593
     0.878604
     6.080262

 Polarizability derivatives:
     -0.047017     -0.006844      0.171045
     -0.006844      0.042362      0.215345
      0.171045      0.215345      0.274255
--------------------------------------------------
mode 284, freq = 1777.9148

 Dipole derivatives
     6.463507
     9.587161
    20.410091

 Polarizability derivatives:
      0.005490     -0.032526      0.176115
     -0.032526      0.107484      0.393030
      0.176115      0.393030      1.240054
--------------------------------------------------
mode 286, freq = 1794.1245

 Dipole derivatives
     4.021669
     6.658073
     3.769520

 Polarizability derivatives:
      0.072060      0.175271      0.114716
      0.175271      0.137859      0.237736
      0.114716      0.237736      0.214295
**************************************************
tpps: 3
--------------------------------------------------
```

mode 301, freq = 1733.2744

Dipole derivatives
-3.967853
-0.769177
-26.845367

Polarizability derivatives:

0.154438	0.375367	0.091256
0.375367	0.376855	-0.073054
0.091256	-0.073054	1.035345

---

mode 302, freq = 1743.4389

Dipole derivatives
5.161583
0.437951
-22.239016

Polarizability derivatives:

0.053353	0.107801	0.197835
0.107801	0.013658	-0.371740
0.197835	-0.371740	0.819319

---

mode 303, freq = 1750.2200

Dipole derivatives
4.222425
-7.676803
-10.626396

Polarizability derivatives:

0.185370	0.085255	0.237851
0.085255	-0.124583	-0.189143
0.237851	-0.189143	-0.616847

---

mode 304, freq = 1756.0226

Dipole derivatives
-3.178628
-6.316144
-11.240339

Polarizability derivatives:

-0.165346	0.228702	-0.221718
0.228702	-0.116183	-0.263616
-0.221718	-0.263616	-1.019920

---

mode 308, freq = 1774.9256

Dipole derivatives
-1.520174
-6.525922

4.552914

Polarizability derivatives:

0.144368	0.045007	-0.165107
0.045007	0.151745	-0.277694
-0.165107	-0.277694	0.015127

****

tpps: 4

---

mode 263, freq = 1707.8594

Dipole derivatives

3.826037
-2.267386
21.025994

Polarizability derivatives:

0.059055	-0.119310	-0.015307
-0.119310	-0.166684	0.280114
-0.015307	0.280114	-0.781009

---

mode 268, freq = 1733.7631

Dipole derivatives

2.549127
5.480807
19.160818

Polarizability derivatives:

0.151762	-0.092633	0.219921
-0.092633	0.498644	0.397757
0.219921	0.397757	0.897391

---

mode 269, freq = 1750.0497

Dipole derivatives

0.438472
5.961702
1.261867

Polarizability derivatives:

0.210263	0.054215	0.154551
0.054215	0.254832	0.055381
0.154551	0.055381	0.518749

---

mode 270, freq = 1757.4826

Dipole derivatives

3.693383
-2.050698
13.898124

Polarizability derivatives:

```
      0.055252      -0.036569       0.036037
     -0.036569      -0.030103       0.234833
      0.036037       0.234833      -0.151147
-------------------------------------------------
mode 271, freq = 1780.9556

 Dipole derivatives
      7.288150
      7.287083
     18.512160

 Polarizability derivatives:
      0.071588       0.074906       0.292343
      0.074906       0.106265       0.214724
      0.292343       0.214724       1.194345
-------------------------------------------------
mode 272, freq = 1804.0779

 Dipole derivatives
      4.205550
      4.548626
      9.487931

 Polarizability derivatives:
      0.140705       0.063717       0.154186
      0.063717       0.017269       0.157681
      0.154186       0.157681       0.378958
*************************************************
tpps: 5
-------------------------------------------------
mode 219, freq = 1731.6213

 Dipole derivatives
     -9.681366
     -5.429154
    -17.987795

 Polarizability derivatives:
     -0.113365       0.010954      -0.186078
      0.010954      -0.223173      -0.443187
     -0.186078      -0.443187      -0.434374
-------------------------------------------------
mode 220, freq = 1733.8624

 Dipole derivatives
     -6.297865
      3.804177
    -14.795884

 Polarizability derivatives:
      0.128468       0.126616       0.194343
      0.126616       0.329971      -0.464125
      0.194343      -0.464125       0.937963
```

---
mode 222, freq = 1762.6423

Dipole derivatives
-3.788146
3.825708
-5.974742

Polarizability derivatives:
0.079353 -0.011963 0.158773
-0.011963 0.217616 -0.295335
0.158773 -0.295335 0.788832
---
mode 224, freq = 1777.2253

Dipole derivatives
-8.819697
9.330798
-16.888728

Polarizability derivatives:
0.261318 -0.026711 0.390200
-0.026711 0.121625 -0.052267
0.390200 -0.052267 0.653111
---
mode 226, freq = 1794.1483

Dipole derivatives
-4.632624
2.610293
-7.546519

Polarizability derivatives:
0.085586 -0.034478 0.162354
-0.034478 -0.025849 -0.129504
0.162354 -0.129504 0.364481
****
tpps: 6
---
mode 228, freq = 1702.4219

Dipole derivatives
-11.664925
7.847741
-17.540108

Polarizability derivatives:
0.321481 0.131007 0.321808
0.131007 0.208007 -0.408520
0.321808 -0.408520 0.758951
---
mode 230, freq = 1741.5623

Dipole derivatives
-6.375957
-1.284883
-18.933144

Polarizability derivatives:
-0.058606 0.103305 -0.208181
0.103305 -0.262453 -0.385988
-0.208181 -0.385988 -0.376072

---

mode 231, freq = 1753.5503

Dipole derivatives
1.607893
7.074316
-1.552035

Polarizability derivatives:
0.104629 -0.008890 0.124753
-0.008890 0.423963 0.029836
0.124753 0.029836 0.772148

---

mode 232, freq = 1771.8553

Dipole derivatives
-4.859917
-2.954821
-3.273494

Polarizability derivatives:
-0.116244 -0.000822 -0.173854
-0.000822 -0.185317 -0.352672
-0.173854 -0.352672 -0.455193

---

mode 234, freq = 1787.4012

Dipole derivatives
-10.835349
-4.391900
-25.384218

Polarizability derivatives:
-0.347016 0.006113 -0.437000
0.006113 -0.082502 -0.160590
-0.437000 -0.160590 -1.271700

---

mode 236, freq = 1808.2554

Dipole derivatives
-6.385531
-3.426758
-8.306175

Polarizability derivatives:

-0.272324	-0.112424	-0.123455
-0.112424	0.025062	-0.143605
-0.123455	-0.143605	-0.329442

****

tpps: 7

---

mode 270, freq = 1706.4888

Dipole derivatives

-7.018350
5.110254
-12.967378

Polarizability derivatives:

0.436892	0.024864	0.302638
0.024864	0.350383	-0.357728
0.302638	-0.357728	0.596067

---

mode 272, freq = 1733.3020

Dipole derivatives

-8.050115
-4.222331
-21.098791

Polarizability derivatives:

-0.039166	0.146344	-0.284358
0.146344	-0.174072	-0.391889
-0.284358	-0.391889	-0.694664

---

mode 273, freq = 1762.9969

Dipole derivatives

-5.936307
0.071886
-13.768114

Polarizability derivatives:

-0.002749	-0.029128	0.194837
-0.029128	0.003029	-0.243900
0.194837	-0.243900	0.557495

---

mode 274, freq = 1766.7541

Dipole derivatives

-2.846871
6.461099
-10.258568

Polarizability derivatives:

0.097955	0.010636	0.121355
0.010636	0.264618	-0.369660

```
     0.121355      -0.369660       0.907226
-------------------------------------------------
mode 276, freq = 1779.0977

 Dipole derivatives
    -2.762973
    -7.317160
     2.723438

 Polarizability derivatives:
     -0.330509       0.038245      -0.414024
      0.038245      -0.150941      -0.197009
     -0.414024      -0.197009      -1.095909
-------------------------------------------------
mode 278, freq = 1799.8601

 Dipole derivatives
    -2.665911
     2.612899
    -9.912952

 Polarizability derivatives:
     -0.048016      -0.014690       0.141566
     -0.014690      -0.001067      -0.137165
      0.141566      -0.137165       0.364571
*************************************************
tpps: 8
-------------------------------------------------
mode 279, freq = 1727.1336

 Dipole derivatives
   -10.488647
     2.413828
   -26.716659

 Polarizability derivatives:
      0.166344       0.085986       0.182422
      0.085986      -0.002753      -0.445744
      0.182422      -0.445744       0.453638
-------------------------------------------------
mode 280, freq = 1732.0327

 Dipole derivatives
    -6.220005
    -5.504337
   -12.974683

 Polarizability derivatives:
     -0.176970       0.065881      -0.350067
      0.065881      -0.445800      -0.248704
     -0.350067      -0.248704      -0.953719
-------------------------------------------------
mode 281, freq = 1752.6326
```

Dipole derivatives
-2.218693
0.573372
-14.538174

Polarizability derivatives:
0.045212 0.024379 -0.003600
0.024379 0.052313 -0.176493
-0.003600 -0.176493 -0.026766
---
mode 282, freq = 1767.9829

Dipole derivatives
-5.959116
-6.420077
-10.614852

Polarizability derivatives:
-0.286902 -0.018943 -0.148940
-0.018943 -0.156399 -0.401703
-0.148940 -0.401703 -1.204557
---
mode 283, freq = 1771.2044

Dipole derivatives
-2.642517
-3.472519
-14.120341

Polarizability derivatives:
-0.099682 0.026419 -0.284522
0.026419 -0.110119 -0.028152
-0.284522 -0.028152 -0.860646
---
mode 284, freq = 1796.2230

Dipole derivatives
-7.452277
-2.704909
-9.018305

Polarizability derivatives:
-0.140649 -0.056369 -0.271016
-0.056369 -0.018477 -0.124147
-0.271016 -0.124147 -0.282841
****
tpps: 9
---
mode 189, freq = 1725.0247

Dipole derivatives
-3.136585

-7.212267
-15.026292

Polarizability derivatives:

0.221857	0.232617	0.070367
0.232617	0.626549	0.160100
0.070367	0.160100	0.935434

---

mode 190, freq = 1728.0779

Dipole derivatives
-4.061495
5.478081
-28.612543

Polarizability derivatives:

-0.074893	0.346328	-0.092482
0.346328	-0.185930	0.366903
-0.092482	0.366903	-0.766344

---

mode 191, freq = 1753.9034

Dipole derivatives
-1.205536
2.913700
-9.170361

Polarizability derivatives:

-0.018058	0.043732	-0.040754
0.043732	-0.250573	0.175354
-0.040754	0.175354	-0.199968

---

mode 192, freq = 1766.6679

Dipole derivatives
-4.472257
-3.036573
-8.985957

Polarizability derivatives:

0.112315	0.165833	0.239622
0.165833	0.274587	0.244855
0.239622	0.244855	0.584872

---

mode 193, freq = 1780.8912

Dipole derivatives
-2.579729
-9.470803
-20.618347

Polarizability derivatives:

0.195667	0.101178	0.165461

```
     0.101178       0.117949       0.247329
     0.165461       0.247329       1.252744
-------------------------------------------------
mode 194, freq = 1795.5717

 Dipole derivatives
    -1.625072
    -1.522485
    -7.633568

 Polarizability derivatives:
     -0.013873       0.035111       0.025174
     0.035111      -0.001897       0.087350
     0.025174       0.087350       0.267739
*************************************************
tpps: 10
-------------------------------------------------
mode 203, freq = 1715.9019

 Dipole derivatives
     0.564232
     3.726988
   -16.163959

 Polarizability derivatives:
     -0.358276       0.322612      -0.171150
     0.322612      -0.322188       0.398419
    -0.171150       0.398419      -0.644241
-------------------------------------------------
mode 204, freq = 1722.5251

 Dipole derivatives
    -6.236260
    -6.679524
   -21.948492

 Polarizability derivatives:
      0.203694       0.340635       0.127856
     0.340635       0.239285       0.239091
     0.127856       0.239091       0.685415
-------------------------------------------------
mode 205, freq = 1756.0329

 Dipole derivatives
     1.458152
    -2.458283
   -16.998258

 Polarizability derivatives:
     -0.044561       0.167411       0.110458
     0.167411       0.017520       0.214777
     0.110458       0.214777      -0.288660
-------------------------------------------------
```

mode 206, freq = 1768.6126

Dipole derivatives
4.074127
5.128606
-9.557227

Polarizability derivatives:
-0.377753 0.114616 -0.147326
0.114616 -0.144001 0.061811
-0.147326 0.061811 -1.230777
---
mode 207, freq = 1769.4931

Dipole derivatives
0.965845
3.843676
-8.711611

Polarizability derivatives:
-0.068364 0.132651 -0.188336
0.132651 -0.374100 0.193004
-0.188336 0.193004 -0.691743
---
mode 208, freq = 1775.6965

Dipole derivatives
-12.383351
9.044044
-13.762336

Polarizability derivatives:
0.005785 -0.055896 -0.029829
-0.055896 0.135778 -0.013463
-0.029829 -0.013463 -0.309996
****
tpps: 11
---
mode 225, freq = 1713.3767

Dipole derivatives
5.324220
2.605341
-22.665230

Polarizability derivatives:
-0.094667 0.233797 0.100359
0.233797 -0.246723 0.215442
0.100359 0.215442 -0.834893
---
mode 226, freq = 1732.9042

Dipole derivatives

-1.109512
-6.967979
-18.576703

Polarizability derivatives:

0.260177	0.345953	0.121905
0.345953	0.323266	0.446189
0.121905	0.446189	0.805055

---

mode 227, freq = 1761.3301

Dipole derivatives
-1.202636
-4.800514
1.789030

Polarizability derivatives:

0.070317	0.027423	-0.033558
0.027423	0.322133	0.051984
-0.033558	0.051984	0.421898

---

mode 228, freq = 1762.7797

Dipole derivatives
2.833102
-6.757346
-22.001375

Polarizability derivatives:

0.057024	0.143125	-0.065934
0.143125	0.243277	0.428688
-0.065934	0.428688	0.450665

---

mode 229, freq = 1776.2702

Dipole derivatives
3.426547
-7.617416
-9.273353

Polarizability derivatives:

0.072322	-0.068870	-0.131964
-0.068870	-0.006676	0.224505
-0.131964	0.224505	1.139325

---

mode 231, freq = 1800.7791

Dipole derivatives
-3.780510
-0.126840
-15.388804

Polarizability derivatives:

```
      0.109330      -0.132650       0.128980
     -0.132650      -0.040986       0.155034
      0.128980       0.155034       0.541241
*****************************************************
tpps: 12
-------------------------------------------------
mode 191, freq = 1716.0596

 Dipole derivatives
     -4.295337
     -3.631233
     18.976904

 Polarizability derivatives:
      0.147733      -0.195127       0.024851
     -0.195127       0.468095      -0.178678
      0.024851      -0.178678       0.863126
-------------------------------------------------
mode 192, freq = 1730.6055

 Dipole derivatives
     -0.522517
      8.345588
     23.828412

 Polarizability derivatives:
     -0.125119      -0.254758       0.072530
     -0.254758      -0.218346      -0.366959
      0.072530      -0.366959      -0.814514
-------------------------------------------------
mode 193, freq = 1764.0227

 Dipole derivatives
      0.399903
     -5.274796
      5.889872

 Polarizability derivatives:
      0.134324      -0.048236       0.034276
     -0.048236       0.189828      -0.072655
      0.034276      -0.072655       0.745486
-------------------------------------------------
mode 194, freq = 1769.6421

 Dipole derivatives
     -1.720960
      2.714228
     18.875052

 Polarizability derivatives:
     -0.102599      -0.100636      -0.145995
     -0.100636       0.037646      -0.301281
     -0.145995      -0.301281       0.242348
```

---
mode 195, freq = 1784.0886

Dipole derivatives
-3.757132
-4.982090
19.627597

Polarizability derivatives:
0.051479 0.049293 -0.196410
0.049293 -0.045202 -0.063672
-0.196410 -0.063672 1.357887
---
mode 198, freq = 1803.4044

Dipole derivatives
2.174395
-4.026322
12.051699

Polarizability derivatives:
-0.033756 0.037183 0.009293
0.037183 0.041142 -0.159801
0.009293 -0.159801 0.462115
****
tpps: 13
---
mode 177, freq = 1732.2806

Dipole derivatives
-6.791804
-1.674796
27.611125

Polarizability derivatives:
-0.047038 -0.123030 -0.294123
-0.123030 0.149156 -0.358703
-0.294123 -0.358703 0.778671
---
mode 178, freq = 1736.4341

Dipole derivatives
-1.322573
8.956164
15.781953

Polarizability derivatives:
-0.205027 -0.162885 0.148405
-0.162885 -0.416726 -0.313350
0.148405 -0.313350 -0.975930
---
mode 179, freq = 1758.8810

Dipole derivatives
-0.522381
-1.934589
8.775225

Polarizability derivatives:
0.008013 0.058967 0.035310
0.058967 -0.050751 -0.069267
0.035310 -0.069267 0.551214
---
mode 180, freq = 1764.6010

Dipole derivatives
0.357177
3.174392
8.638068

Polarizability derivatives:
-0.179479 -0.111958 -0.090759
-0.111958 -0.055708 -0.275755
-0.090759 -0.275755 -0.535821
---
mode 181, freq = 1785.7855

Dipole derivatives
-10.183732
10.611093
20.928756

Polarizability derivatives:
-0.244601 0.056682 0.379637
0.056682 -0.201717 -0.424323
0.379637 -0.424323 -1.131804
---
mode 182, freq = 1797.3155

Dipole derivatives
-0.752738
2.177311
-2.411740

Polarizability derivatives:
0.016033 0.086347 -0.035985
0.086347 0.044960 0.008599
-0.035985 0.008599 0.294698
****
tpps: 14
---
mode 169, freq = 1737.2624

Dipole derivatives
8.786592
-7.089788

-24.563800

Polarizability derivatives:

0.172097	0.118056	-0.134633
0.118056	0.386269	0.481676
-0.134633	0.481676	0.232428

---

mode 170, freq = 1746.3538

Dipole derivatives

6.121279
2.095419
-16.066421

Polarizability derivatives:

-0.039286	0.054272	0.239762
0.054272	-0.464151	0.316929
0.239762	0.316929	-1.286360

---

mode 171, freq = 1754.6940

Dipole derivatives

5.165506
-1.181315
-1.424833

Polarizability derivatives:

-0.063822	-0.004630	-0.006624
-0.004630	0.116068	0.080100
-0.006624	0.080100	-0.495992

---

mode 172, freq = 1759.8559

Dipole derivatives

1.875308
3.831166
-2.726046

Polarizability derivatives:

-0.143605	-0.086601	0.188487
-0.086601	-0.091090	-0.007543
0.188487	-0.007543	-0.899592

---

mode 173, freq = 1770.2677

Dipole derivatives

4.404028
-8.714015
-14.368228

Polarizability derivatives:

0.212885	-0.088363	-0.224722
-0.088363	0.188951	0.254377

```
    -0.224722       0.254377       1.190801
**************************************************
tpps: 15
--------------------------------------------------
mode 202, freq = 1703.1002

 Dipole derivatives
    -8.039868
    -3.912058
    20.844316

 Polarizability derivatives:
      0.137692      -0.178810      -0.164587
     -0.178810       0.085339      -0.203818
     -0.164587      -0.203818       0.818971
--------------------------------------------------
mode 204, freq = 1736.6326

 Dipole derivatives
    -2.212152
     4.100336
    19.004875

 Polarizability derivatives:
     -0.154369      -0.131883       0.170951
     -0.131883      -0.404974      -0.308564
      0.170951      -0.308564      -0.186808
--------------------------------------------------
mode 205, freq = 1749.0795

 Dipole derivatives
    -4.285234
     8.053679
     0.044859

 Polarizability derivatives:
     -0.288396      -0.013873       0.105793
     -0.013873      -0.497724      -0.104790
      0.105793      -0.104790      -0.807100
--------------------------------------------------
mode 206, freq = 1764.0832

 Dipole derivatives
    -4.910749
     7.286319
     6.085605

 Polarizability derivatives:
     -0.146893       0.100253       0.193198
      0.100253      -0.234936      -0.306254
      0.193198      -0.306254      -0.404702
--------------------------------------------------
mode 207, freq = 1778.4005
```

Dipole derivatives
-1.041311
5.072931
7.508160

Polarizability derivatives:
-0.072685 -0.081807 0.200998
-0.081807 -0.176873 -0.208214
0.200998 -0.208214 -0.638492
---
mode 210, freq = 1817.9292

Dipole derivatives
-6.861310
4.001284
12.276700

Polarizability derivatives:
-0.164981 0.108936 0.278178
0.108936 0.038773 -0.161051
0.278178 -0.161051 -0.462648
****
tpps: 16
---
mode 255, freq = 1720.5980

Dipole derivatives
4.380911
-6.270008
-20.407248

Polarizability derivatives:
0.136420 0.205532 -0.232334
0.205532 0.495151 0.461826
-0.232334 0.461826 0.547951
---
mode 256, freq = 1729.2552

Dipole derivatives
5.561231
2.765731
-11.432390

Polarizability derivatives:
-0.114251 0.091087 0.113264
0.091087 -0.156145 0.370603
0.113264 0.370603 -1.042101
---
mode 257, freq = 1760.0892

Dipole derivatives
3.899353

3.030053
-7.548042

Polarizability derivatives:
-0.232450 -0.007680 0.221000
-0.007680 -0.144846 0.064180
0.221000 0.064180 -1.065311
---
mode 259, freq = 1769.4399

Dipole derivatives
0.224604
6.148051
-3.329265

Polarizability derivatives:
-0.146080 -0.017684 0.159117
-0.017684 -0.220196 0.119141
0.159117 0.119141 -0.992832
---
mode 262, freq = 1805.2552

Dipole derivatives
3.137904
3.676814
-11.969332

Polarizability derivatives:
-0.094268 -0.011871 0.111627
-0.011871 0.016353 0.144723
0.111627 0.144723 -0.461097

SUPPORTING REFERENCES

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