Supporting Information for:

Characterizing excited-state intramolecular proton transfer in 3-hydroxyflavone with ultrafast transient infrared spectroscopy

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I. Experimental Methods

a. Transient Infrared (Optical Pump—IR probe)

3HF was obtained commercially from Sigma-Aldrich and used without further purification. Synthesis of 3HTC and its characterization was guided by the procedure published by Gundoz et. al.[1] and is summarized in Section II of this Supporting Information.

Ultrafast UV/Vis and infrared pulses were both sourced from the outputs of a regenerative amplifier (Coherent Astrella, 800 nm, 30 fs, 1 kHz, 3.5 and 3.6 mJ/pulse) which pumped separate optical parametric amplifiers (OPA; Light Conversion, TOPAS Prime). UV/Vis light was generated by one OPA and its associated external crystal stages. The infrared probe pulse was formed by combining the signal and idler via a home-built difference frequency generator (1 mm AgGaS$_2$ crystal, Eksma Optics) and tuned for a center frequency series of 1600 cm^{-1}, 1450 cm^{-1}, and 1350 cm^{-1} to cover the desired range. Frequency bandwidth of the IR pulses were between 200-300 cm^{-1} with ~80 fs pulse width. Generation of IR probe and reference pulses was accomplished by reflections off the front face (probe, ~1% reflection) and back face (reference) of a 1 mm wedged CaF$_2$ window. A translation stage (Aerotech; ANT95L050-MP-PL2-TAS) was utilized to set the delay time τ_2 between pump and probe pulses with a maximum τ_2 of 10 ps. A lens (250 mm focal length, ThorLabs) focused the visible pump beam to a diameter of about 300 μm at the sample; approximate pump fluence was 30 μJ/mm^2 for all experiments. Excitation wavelengths were set to 363 nm and 379 nm for 3HF and 3HTC, respectively (Fig. S2). The probe pulse was then focused into the sample (100 μm diameter) and overlapped with the visible pulse; a pump-probe geometry setup was used and the signal field was self-heterodyned by the probe pulse.

Timing between the visible and IR pulses was found by monitoring the free carrier absorption in a Si wafer, as shown in panel (a) from a difference spectrum calculated as the signal observed in the presence of the pump minus the absorbance signal without the pump. On this graph, absorption corresponds to a signal of negative intensity; due to the direction of the delay stage motion used, negative times correspond to the arrival of the probe after the pump. The derivative of the cumulative function distribution was then fit to a Gaussian profile (b) to extract the full width at half maximum for the instrument response function.

(a)

(b)
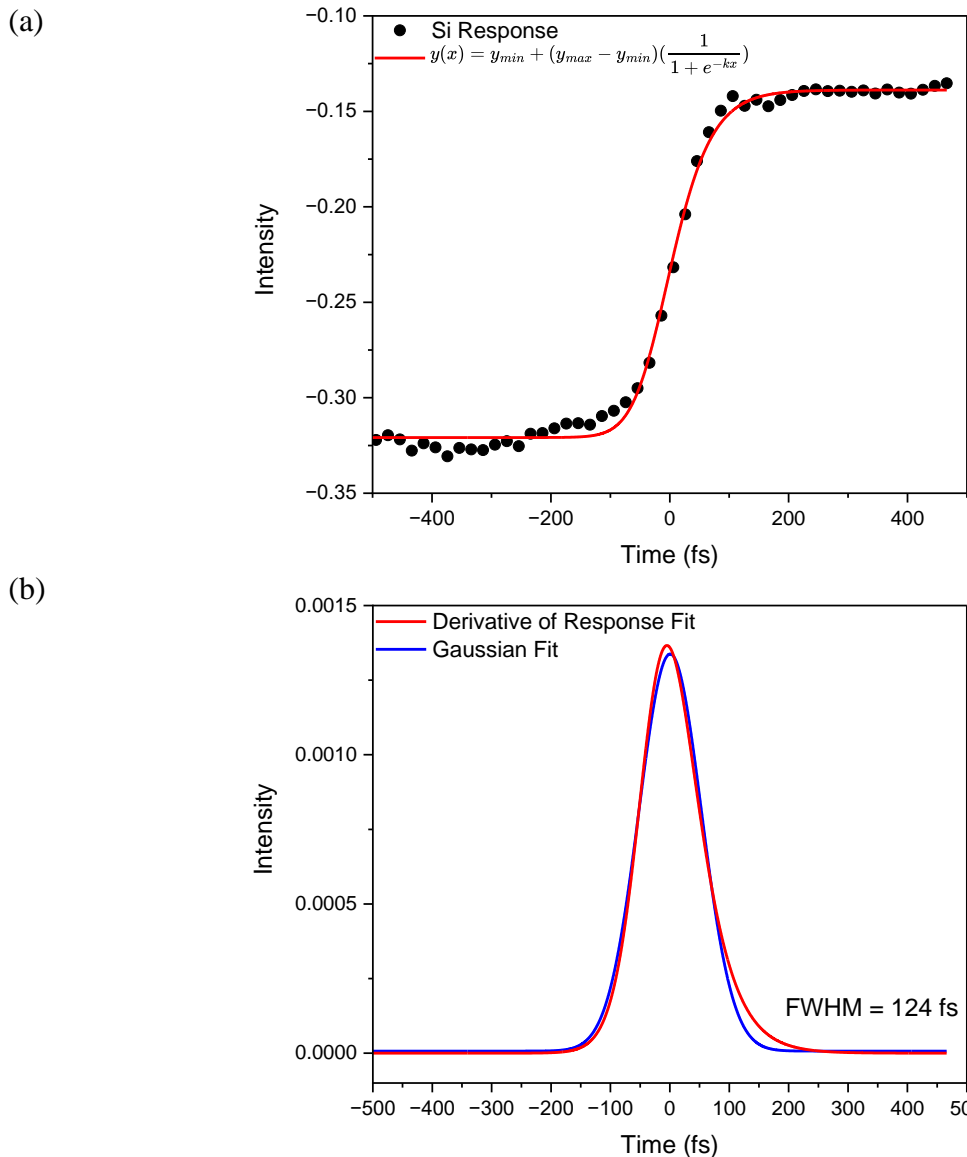
Measurement of the Si pump-probe response yielded the instrument response function (~130 fs FWHM). For detection, a monochromator dispersed the probe and reference lines onto an MCT focal-plane array detector (128×128 pixels, PhaseTech) to visualize the probe frequency axis.

All samples (3HF, 2 mM; 3HTC, 3 mM) were dissolved in $CDCl_3$ and flowed at a rate of about 1 cm/s using a peristaltic pump (APT Instruments, SP10XV1R-509) through a flow cell with 300 μm path length between two 1 mm CaF_2 windows. The sample cell was rastered perpendicular to the probe path to avoid damaging the CaF_2 windows. Multiple batches were used for each measurement to verify reproducibility. TRIR spectra were tracked during collection to ensure that there were no artifacts or contributions due to sample degradation; UV-Vis of the sample solution after collection did not show any new transitions at or lower in energy than the excitation wavelength.

b. Transient Absorption (IR pump—IR probe)

For generation of infrared pulses, a regenerative amplifier (Coherent Astrella, 800 nm, 30 fs, 1 kHz, 3.6 mJ/pulse) was utilized to pump an optical parametric amplifier (OPA; Light Conversion, TOPAS Prime). Infrared pulses were formed by combining the signal and idler via a home-built difference frequency generator (1 mm $AgGaS_2$ crystal, Eksma Optics. IR probe and reference pulses were created from the reflections off the front face (probe, ~1% reflection) and back face (reference) of a wedged CaF_2 window (1 mm). The remaining IR light was transmitted through a pulse shaper (PhaseTech) to generate a pump pulse of the same center frequency and approximate bandwidth. Frequency bandwidth of the IR pulses were 180 cm^{-1} at the FWHM with a center frequency of ~1440 cm^{-1} and ~80 fs pulse width.

Delay time τ_2 between pump and probe pulses was controlled by a translation stage (Aerotech; ANT95L050-MP-PL2-TAS). Both pump and probe pulses focused onto the sample in the pump-probe geometry style (100 μm diameter). The signal field was self-heterodyned by the probe pulse. The probe and reference lines were next dispersed by a monochromator before focusing onto the MCT focal-plane array detector (128 × 128 pixels, PhaseTech).

Samples of 3HF and 3HTC were dissolved in CDCl$_3$ (80 mM) and placed into cells composed of CaF_2 windows (1 mm) and a 300 μm Teflon spacer. Throughout collection, the sample cell was occasionally rastered perpendicular to the probe path in order to probe fresh spots of the sample.

II. Synthesis of 3-hydroxy-2-(thiophen-2-yl)chromen-4-one

The following procedure is modified from reaction #15 listed in Gundoz et. al. for a general reaction path to form 3-hydroxyflavone derivatives.[1]

1. To a round-bottom flask (25 or 50 mL), add 353 µL 2-hydroxyacetophenone, 270 µL 2-thiophenecarboxaldehyde, ~0.5 g NaOH, and about 10 mL of MetOH. Place two stir bars in the flask, attach a Graham condenser, and suspend in an oil bath.

2. Stir and reflux (~400 rpm, 88°C) until the colour changes from pale yellow to orange, about 3 hrs.

3. Remove from oil bath. Cool to room temperature. Add 10 mL 0.5 N NaOH and 8 mmol H_2O_2.

4. Stir 2-3 hrs at room temperature. A solid product should form; the reaction mixture will thicken significantly and stirring rate may need to be decreased.

5. Pour reaction mixture into ~20 mL distilled water surrounded by ice bath.

6. Vacuum filter this diluted reaction mixture using a Büchner funnel. Lyophilize to sublimate any remaining water from the sample; this product will be orange-tinted powder.

7. Since the synthesis is performed in a basic solution, the product will likely be deprotonated. To remedy this, suspend the product in a few mL of water and add small aliquots of dilute HCl until the pH of the slurry is 5-6, mixing after each addition.

8. Vacuum filter the yellow, now-protonated product using a Büchner funnel; rinse with a small amount of cold, distilled water. Sublimate remaining water from the sample via lyophilizer.

Characterization:

Yellow solid, 58.3% yield.

UV-Vis in Fig. S2.

^{1}H-NMR: [300 MHz, line broadening = 0.5 Hz, DMSO-d_6]: δ = 7.30 ppm (t, J = 4.3 Hz, 1H); δ = 7.46 ppm (t, J = 7.3 Hz, 1H); δ = 7.75 ppm (m, 2H); δ = 7.90 ppm (dd, J = 1.2 Hz, J = 5.3 Hz, 1H); δ = 7.96 ppm (d, J = 4.1 Hz, 1H); δ=8.09 ppm (dd, J = 1.5 Hz, J = 7.9, 1H); δ=10.22 ppm (s, 1H).

III. Computational Procedures and Results

Calculations for geometry optimization and vibrational frequencies were performed using ORCA[2] with theory/basis B3LYP-D3BJ/aug-cc-pVDZ.[3-8] TDDFT was employed for excited-state calculations. Frequencies listed in this Supporting Information are scaled by 0.975. Transition states were calculated by NEB with aforementioned theory/basis using the optimized structures as endpoints.

(a)　　　　　　　　　　　(b)　　　　　　　　　　　(c)

(d)　　　　　　　　　　　(e)　　　　　　　　　　　(f)

(g)　　　　　　　　　　　(h)　　　　　　　　　　　(i)
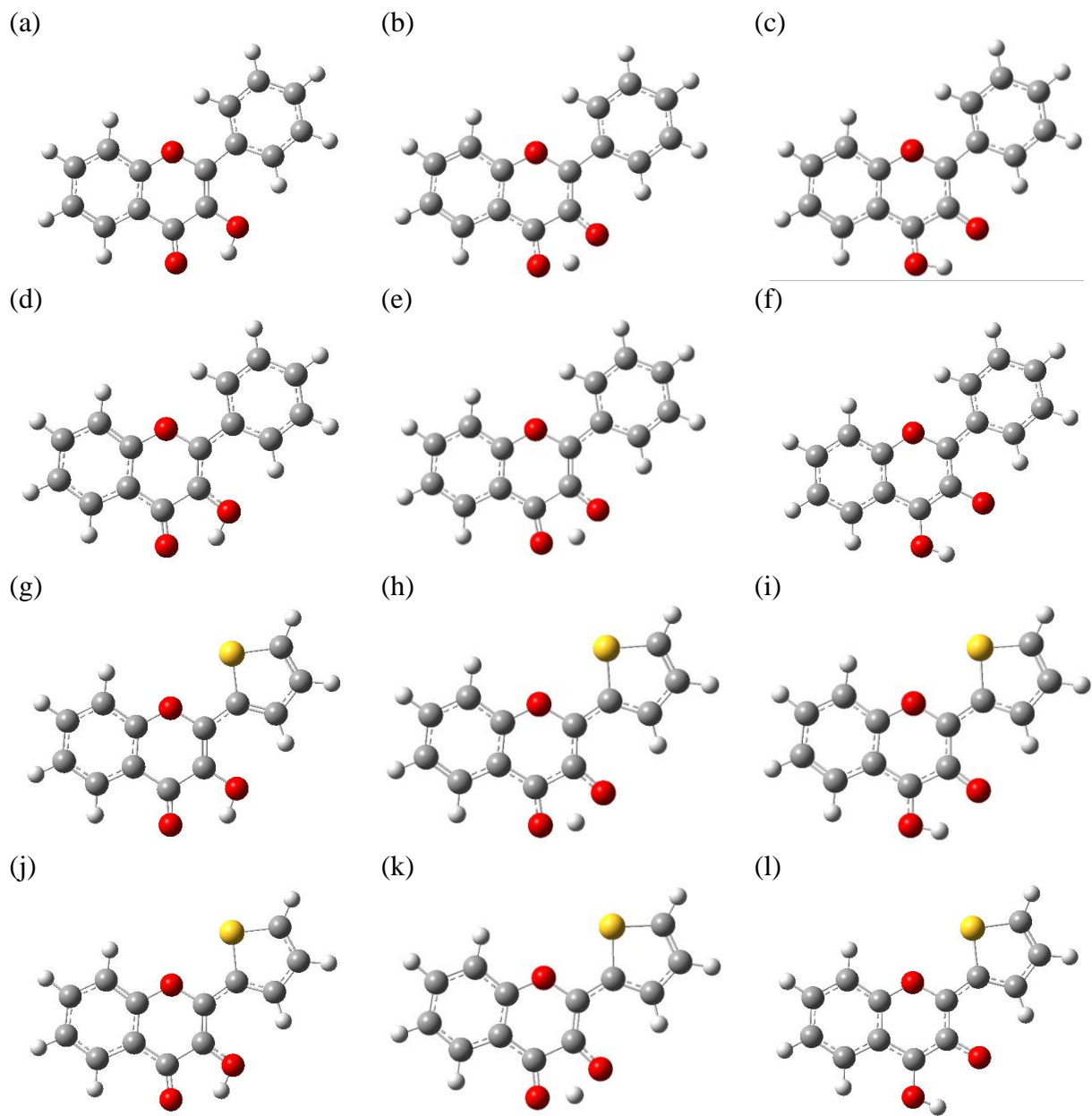
(j)　　　　　　　　　　　(k)　　　　　　　　　　　(l)

Figure S1. Optimized geometries for 3HF (a-f) and 3HTC (g-l). Configurations shown: S_0 (a, g), S_0 transition state (b, h), S_0' (c, i), S_1 (d, j), S_1 transition state (e, k), and S_1' (f, l).

Table I. Cartesian coordinates for the S_0, S_1, S_1 transition, and S_1' states of 3HF and 3HTC.

3HF-S$_0$			
C	-0.009134	-0.100205	0.000918
C	-0.005826	-0.075652	1.411103
C	1.223193	-0.104902	2.089034
C	2.437410	-0.157589	1.388613
C	2.409858	-0.179563	0.000842
C	1.185521	-0.151024	-0.698875
H	-0.971677	-0.077162	-0.507636
H	3.373229	-0.178864	1.944513
H	3.348517	-0.219835	-0.552066
H	1.183009	-0.169376	-1.788181
C	-1.057143	0.003810	3.646695
C	0.179712	-0.026939	4.237555
C	-1.230426	-0.020420	2.197416
O	-2.383848	0.006786	1.736394
O	-2.220801	0.056193	4.337667
H	-2.903520	0.062556	3.631227
O	1.301271	-0.082555	3.445513
C	0.511101	-0.008879	5.667219
C	-0.487316	0.089419	6.659268
C	-0.138001	0.108543	8.009751
C	1.201270	0.028900	8.401659
C	2.197811	-0.069911	7.425286
C	1.860288	-0.087511	6.073681
H	-1.531452	0.150778	6.373557
H	-0.923000	0.186462	8.762133
H	1.467125	0.044139	9.458906
H	3.246126	-0.132734	7.718059
H	2.643821	-0.163297	5.324806

3HTC-S$_0$			
C	-2.362142	3.111047	2.001485
C	-1.731492	2.500850	0.898142
C	-1.970356	3.015301	-0.387232
C	-2.817278	4.113689	-0.586846
C	-3.427208	4.697737	0.515870
C	-3.201479	4.198272	1.814640
H	-2.166274	2.700945	2.990970
H	-2.978640	4.484673	-1.597577
H	-4.087850	5.552658	0.370917
H	-3.687908	4.668441	2.668606
C	0.447979	0.779075	-5.131986
C	1.107131	-0.163843	-4.379961
C	0.832097	-0.053652	-2.988846
C	-0.040074	0.981071	-2.692608
H	0.475913	0.921698	-6.208576
H	1.768687	-0.914204	-4.808488
H	1.251351	-0.701443	-2.226097
O	-1.394768	2.478354	-1.500193
O	-0.542349	0.803064	2.118506
O	0.559519	-0.219825	-0.052298
C	-0.839221	1.354278	1.045203
C	-0.267589	0.843252	-0.190525
C	-0.549316	1.402299	-1.409562
H	0.564028	-0.385182	0.914510
S	-0.527229	1.829226	-4.155068

3HF-S$_1$			
C	-1.000513	0.376004	0.000247
C	0.428539	0.393720	-0.000028
C	1.111927	-0.850132	-0.000264
C	0.437297	-2.060154	-0.000426
C	-0.984430	-2.053788	-0.000102
C	-1.681988	-0.842002	0.000303
H	-1.527905	1.327252	0.000464
H	1.002496	-2.989969	-0.000682
H	-1.523753	-2.999981	-0.000142

3HTC-S$_1$			
C	-1.573925	0.638749	0.049843
C	-0.928701	0.005176	-1.059812
C	-1.180560	0.527722	-2.359494
C	-2.025630	1.605197	-2.568068
C	-2.653018	2.213627	-1.452489
C	-2.416558	1.725187	-0.159468
H	-1.385409	0.244747	1.046115
H	-2.190819	1.965333	-3.581802
H	-3.319099	3.061228	-1.608007

H	-2.772233	-0.847372	0.000603
C	2.692762	1.414543	-0.000337
C	3.313509	0.171055	-0.000517
C	1.199350	1.587825	-0.000050
O	0.814093	2.782019	-0.001068
O	3.318719	2.583067	-0.000135
H	2.535864	3.218775	0.000649
O	2.501050	-0.929423	-0.000537
C	4.721743	-0.137971	-0.000369
C	5.719182	0.878729	-0.000341
C	7.065338	0.539939	-0.000058
C	7.466335	-0.806088	0.000213
C	6.493930	-1.818823	0.000156
C	5.143599	-1.498706	-0.000153
H	5.427448	1.923875	-0.000546
H	7.815880	1.330218	-0.000034
H	8.525740	-1.062795	0.000464
H	6.798793	-2.865340	0.000357
H	4.395158	-2.286125	-0.000176

H	-2.903105	2.200624	0.692623
C	1.237118	-1.705974	-7.135750
C	1.907805	-2.657963	-6.379329
C	1.640938	-2.557101	-5.000773
C	0.751163	-1.514182	-4.696509
H	1.272321	-1.568505	-8.213223
H	2.572429	-3.400159	-6.817238
H	2.067689	-3.201513	-4.238373
O	-0.599179	-0.014257	-3.502548
O	0.275393	-1.740036	0.109138
O	1.307167	-2.700013	-2.008463
C	-0.071152	-1.120874	-0.924110
C	0.511404	-1.655011	-2.201458
C	0.243815	-1.094567	-3.434985
H	1.258510	-2.804521	-1.012833
S	0.255684	-0.659213	-6.166752

3HF-S$_1$ Transition State		
C	-3.818802	0.596428	0.008091
C	-2.391244	0.596422	-0.001910
C	-1.708456	-0.654076	-0.012273
C	-2.406714	-1.855752	-0.014437
C	-3.821398	-1.829811	-0.004944
C	-4.512342	-0.610704	0.007103
H	-4.333927	1.554928	0.016611
H	-1.857794	-2.795278	-0.023507
H	-4.373516	-2.768913	-0.006084
H	-5.602263	-0.605393	0.014698
C	-0.109377	1.606611	0.002721
C	0.497246	0.360810	-0.010776
C	-1.590033	1.752948	0.000754
O	-1.918307	2.991810	0.007768
O	0.422130	2.802941	0.016394
H	-0.682835	3.341096	0.012704
O	-0.333991	-0.743638	-0.026032
C	1.900969	0.038745	-0.005977
C	2.889340	1.061590	-0.016618
C	4.237936	0.732113	-0.007932
C	4.647968	-0.611369	0.007940

3HTC-S$_1$ Transition State		
C	-1.303637	1.193804	2.954152
C	-0.683630	0.557649	1.834495
C	-0.948268	1.070761	0.529000
C	-1.800417	2.152966	0.338128
C	-2.402466	2.759746	1.461065
C	-2.145712	2.280468	2.756111
H	-1.096564	0.801991	3.948071
H	-1.987280	2.515681	-0.670798
H	-3.070008	3.608665	1.317385
H	-2.616224	2.760954	3.613885
C	1.504613	-1.120501	-4.258636
C	2.153839	-2.082616	-3.502003
C	1.863968	-1.995467	-2.123140
C	0.980097	-0.953171	-1.823942
H	1.553973	-0.971119	-5.333827
H	2.819894	-2.827127	-3.934514
H	2.267998	-2.650336	-1.355747
O	-0.392944	0.524425	-0.606132
O	0.574308	-1.227577	2.935960
O	1.531438	-2.120292	0.979939
C	0.171719	-0.556160	1.919871

C	3.682845	-1.629064	0.015230
C	2.328512	-1.318017	0.009498
H	2.581289	2.103605	-0.031629
H	4.982582	1.528271	-0.016030
H	5.709296	-0.860686	0.013463
H	3.994535	-2.673775	0.027763
H	1.586351	-2.111841	0.017410

C	0.761906	-1.108849	0.675331
C	0.476805	-0.550885	-0.555410
H	1.269571	-1.986880	2.190124
S	0.517022	-0.076127	-3.289367

3HF-S$_1$'			
C	-1.063329	-0.221095	-0.000811
C	-2.472405	-0.254174	0.012896
C	-3.115233	-1.508056	0.043992
C	-2.392966	-2.697403	0.052877
C	-0.993748	-2.644548	0.040299
C	-0.334508	-1.411002	0.015841
H	-0.561642	0.743553	-0.024125
H	-2.929594	-3.644258	0.075966
H	-0.421524	-3.571747	0.049914
H	0.754607	-1.376610	0.007035
C	-4.684520	0.774799	-0.043929
C	-5.287257	-0.482761	0.003541
C	-3.296705	0.915838	-0.002761
O	-2.675025	2.131330	-0.050537
O	-5.411299	1.901287	-0.144026
O	-4.481386	-1.600641	0.086721
C	-6.702717	-0.759293	0.010185
C	-7.658893	0.277493	0.109649
C	-9.021695	-0.000364	0.088463
C	-9.474731	-1.322696	-0.013288
C	-8.539610	-2.360976	-0.096260
C	-7.173692	-2.092746	-0.082970
H	-7.333662	1.312391	0.224605
H	-9.737326	0.818288	0.165610
H	-10.543008	-1.538791	-0.019485
H	-8.880019	-3.394121	-0.174715
H	-6.457893	-2.907852	-0.153007
H	-3.322477	2.841160	0.033223

3HTC-S$_1$'			
C	-0.927537	0.623477	-0.003480
C	-0.358895	0.008056	-1.135327
C	-0.687868	0.514636	-2.408154
C	-1.549563	1.594325	-2.567608
C	-2.108114	2.190015	-1.429746
C	-1.797793	1.704843	-0.155234
H	-0.680631	0.237510	0.982972
H	-1.776809	1.949014	-3.571369
H	-2.787207	3.034310	-1.544964
H	-2.234898	2.172991	0.726287
C	1.864301	-1.601321	-7.178254
C	2.443964	-2.604406	-6.433969
C	2.102725	-2.550496	-5.059834
C	1.267700	-1.475388	-4.746651
H	1.940643	-1.425656	-8.247156
H	3.086129	-3.370161	-6.865499
H	2.441198	-3.274211	-4.323793
O	-0.188433	-0.065158	-3.549544
O	0.833160	-1.619263	0.160657
O	2.004087	-2.589937	-2.160322
C	0.521540	-1.124009	-1.072864
C	1.100610	-1.603307	-2.240814
C	0.763029	-1.056957	-3.489084
H	1.346483	-2.431672	0.065438
S	0.880764	-0.548225	-6.200806

IV. Supplemental Data and Data Analysis Descriptions
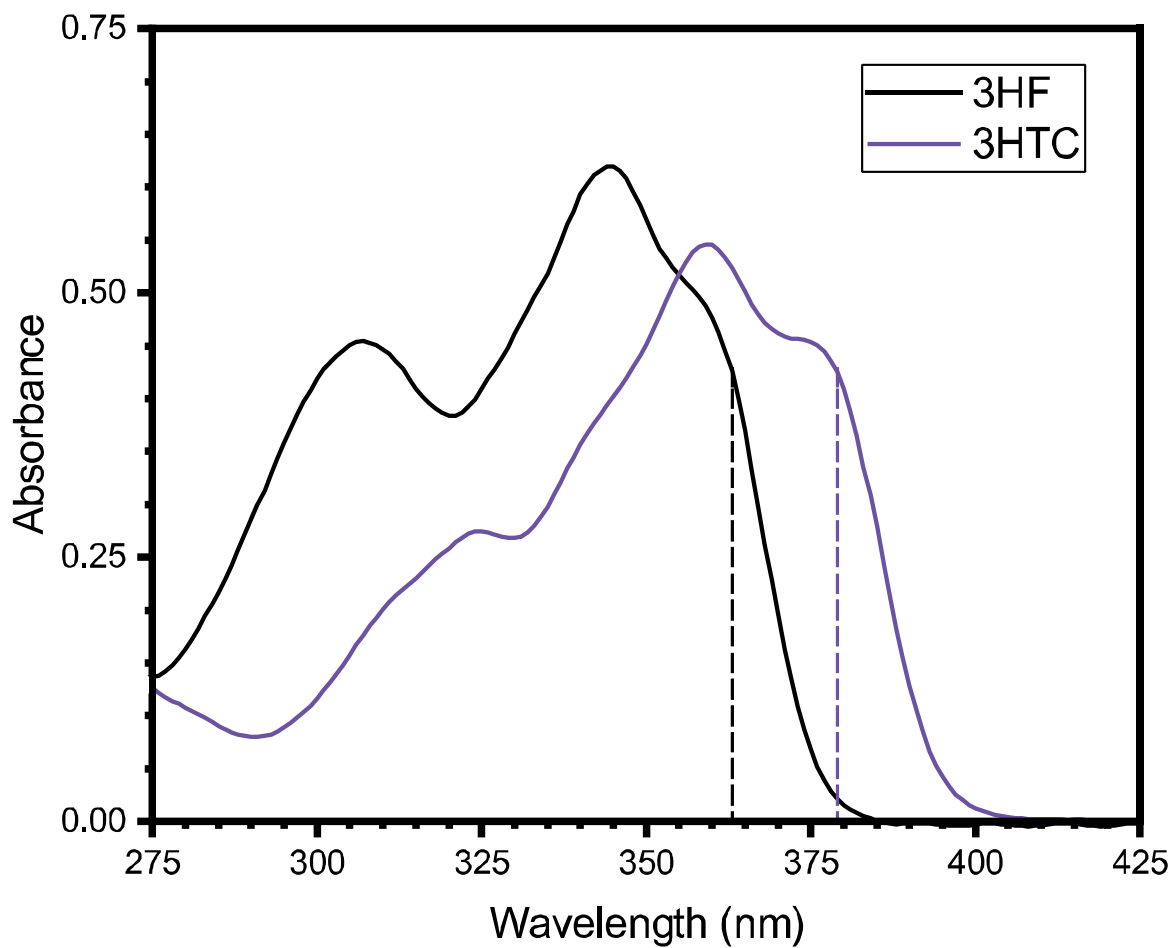
Fig. S2. Steady-state UV-Vis spectra in CDCl$_3$ of 3HF (~45 μM, black) and 3HTC (~60 μM, purple). Excitation wavelengths (3HF, 363 nm; 3HTC, 379 nm) used in this experiment are designated by the dashed lines.
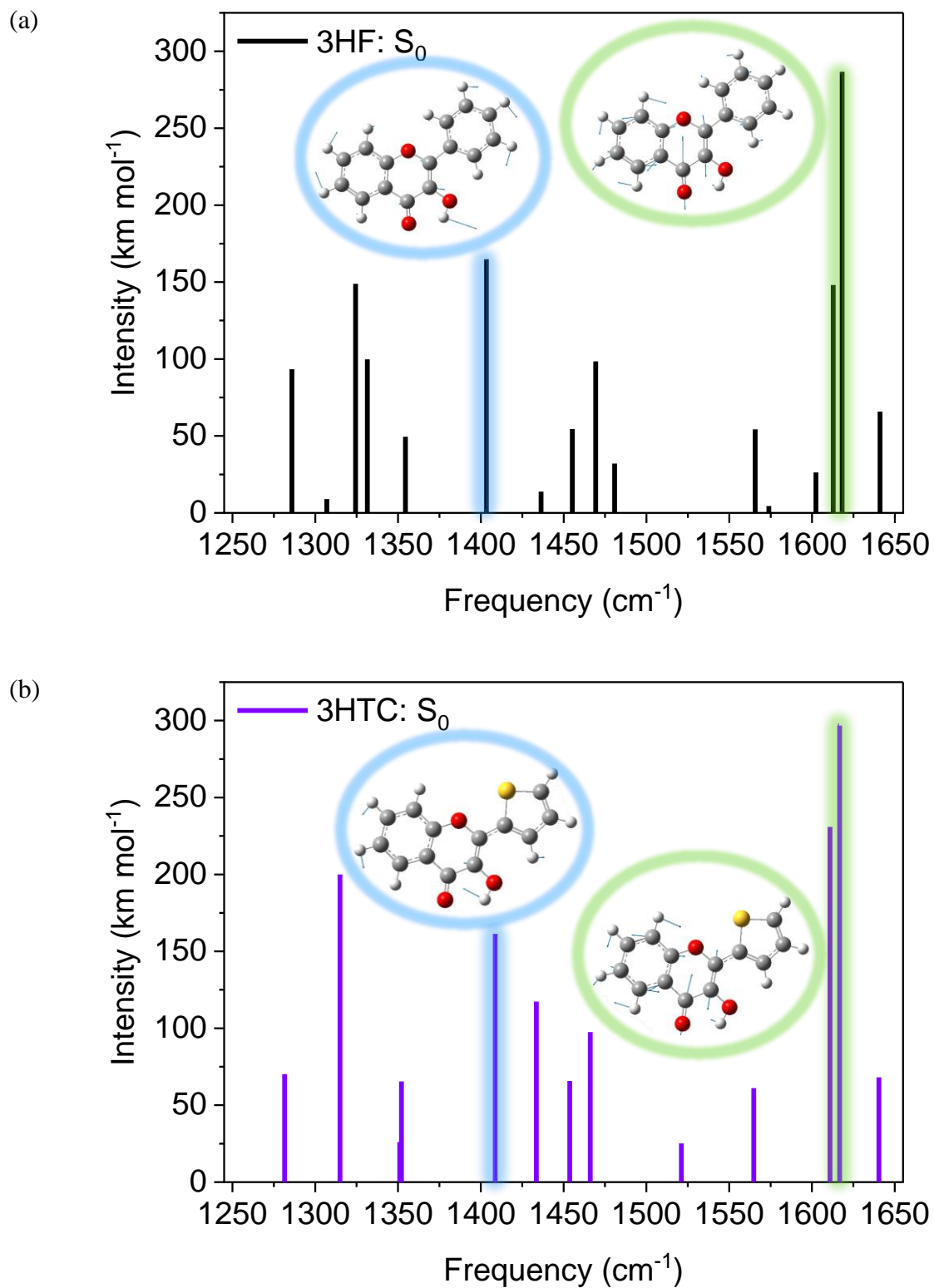
Fig. S3. Computed vibrational spectra for the S_0 state of 3HF (a) and 3HTC (b) with selected vibrational modes visualized, labeled with corresponding colours.
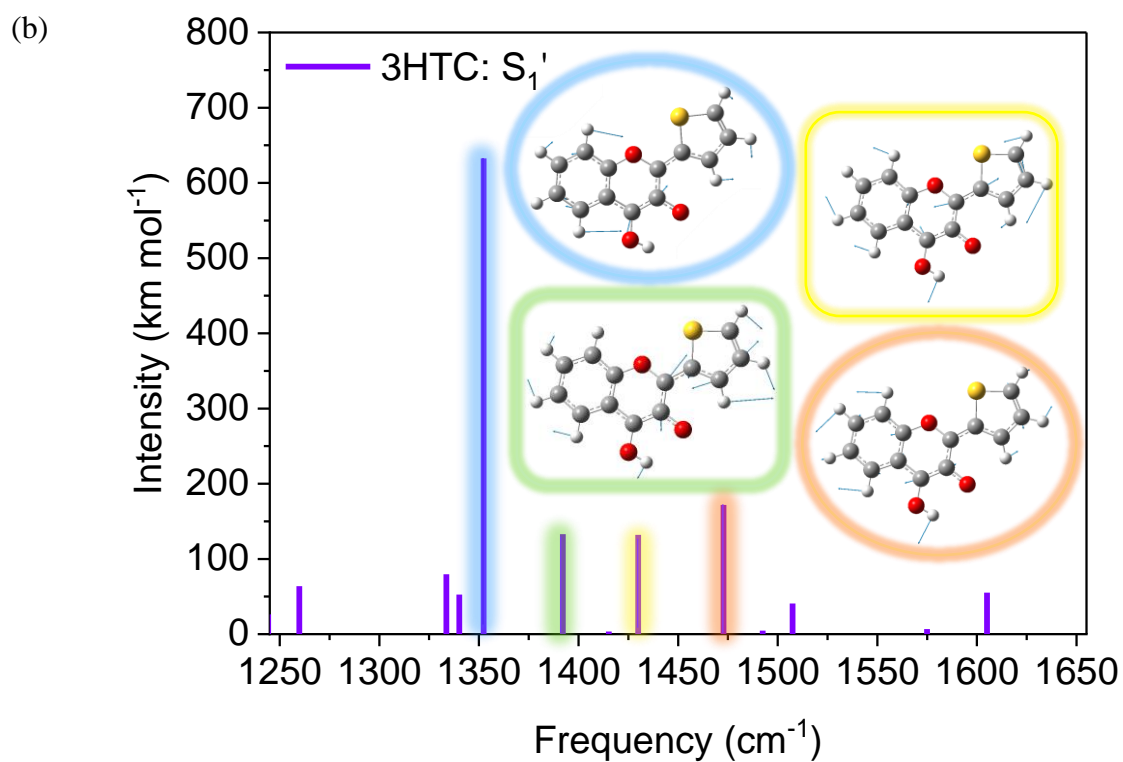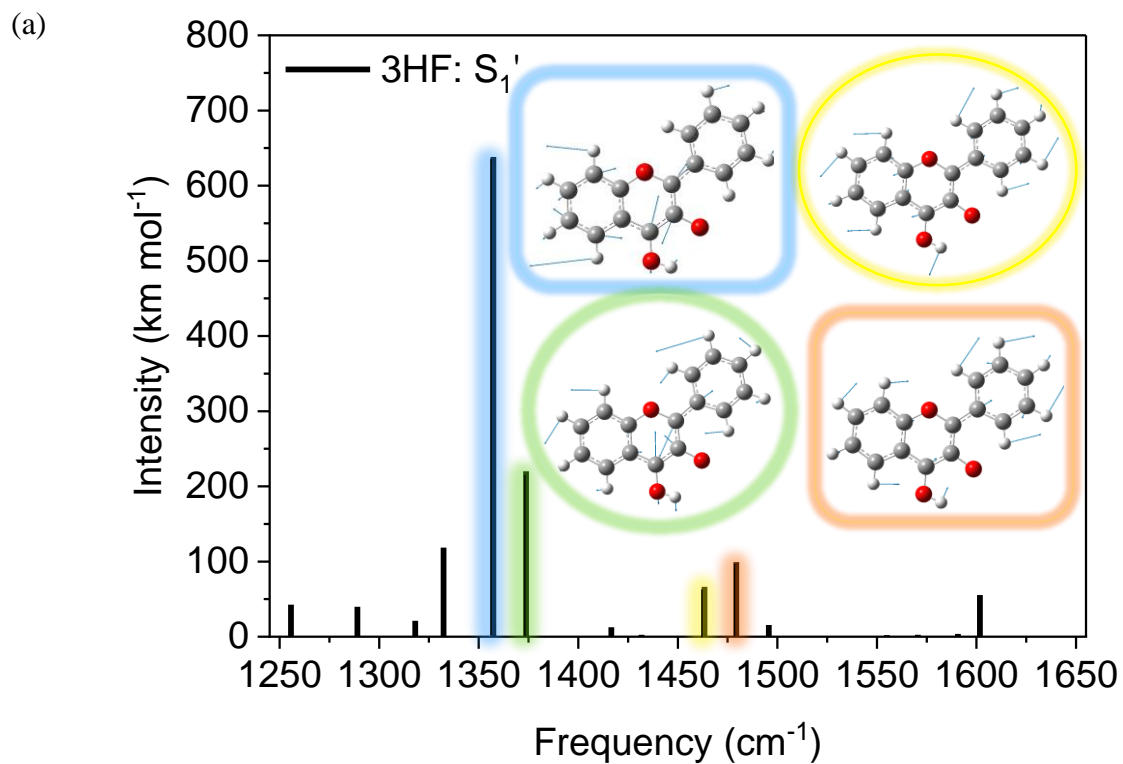
Fig. S4. Computed vibrational spectra for the S$_1$' state of 3HF (a) and 3HTC (b) with selected vibrational modes visualized, labeled with corresponding colours.
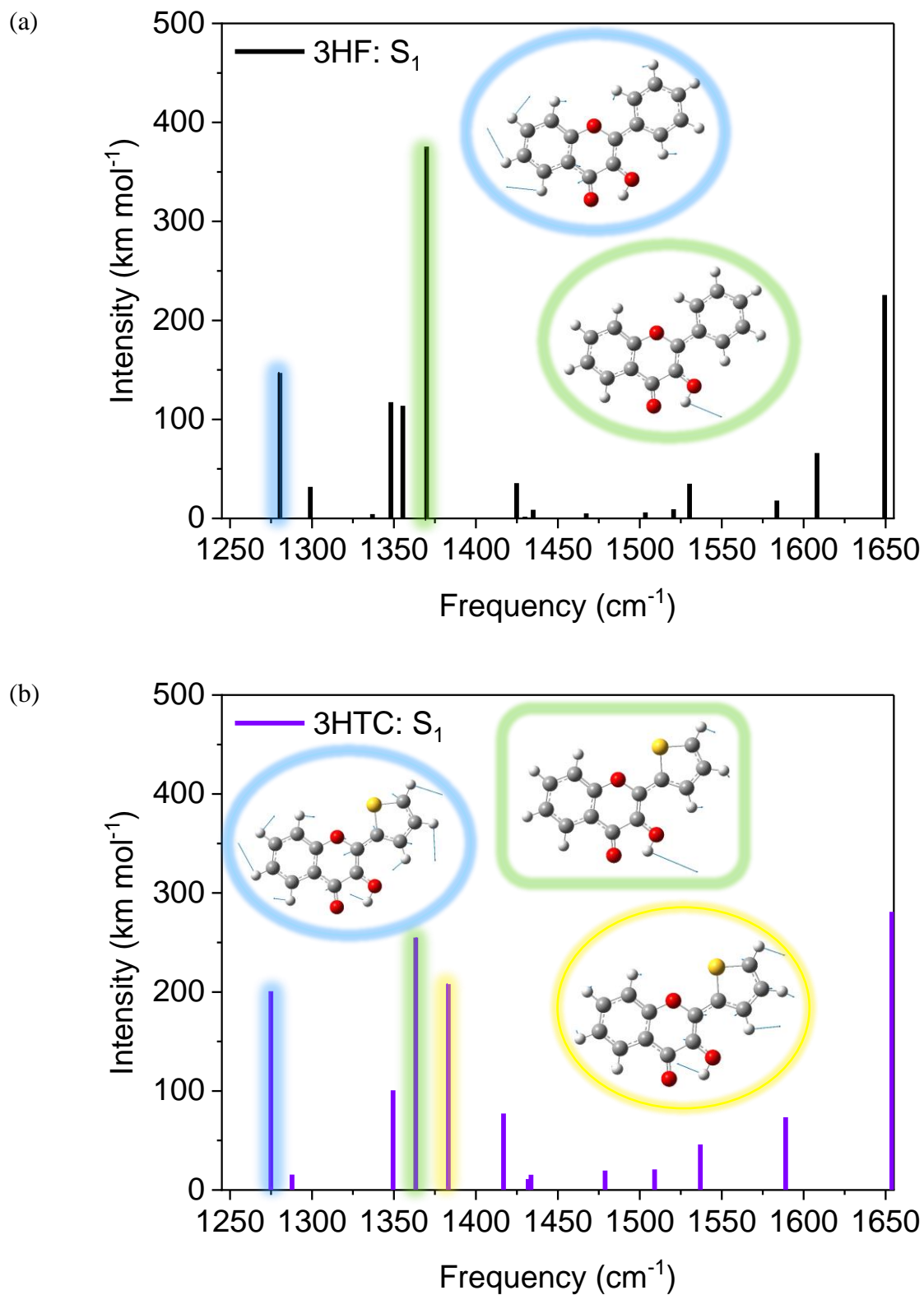
Fig. S5. Computed vibrational spectra for the S$_1$ state of 3HF (a) and 3HTC (b) with selected vibrational modes visualized, labeled with corresponding colours.

(a)

(b)

(c)
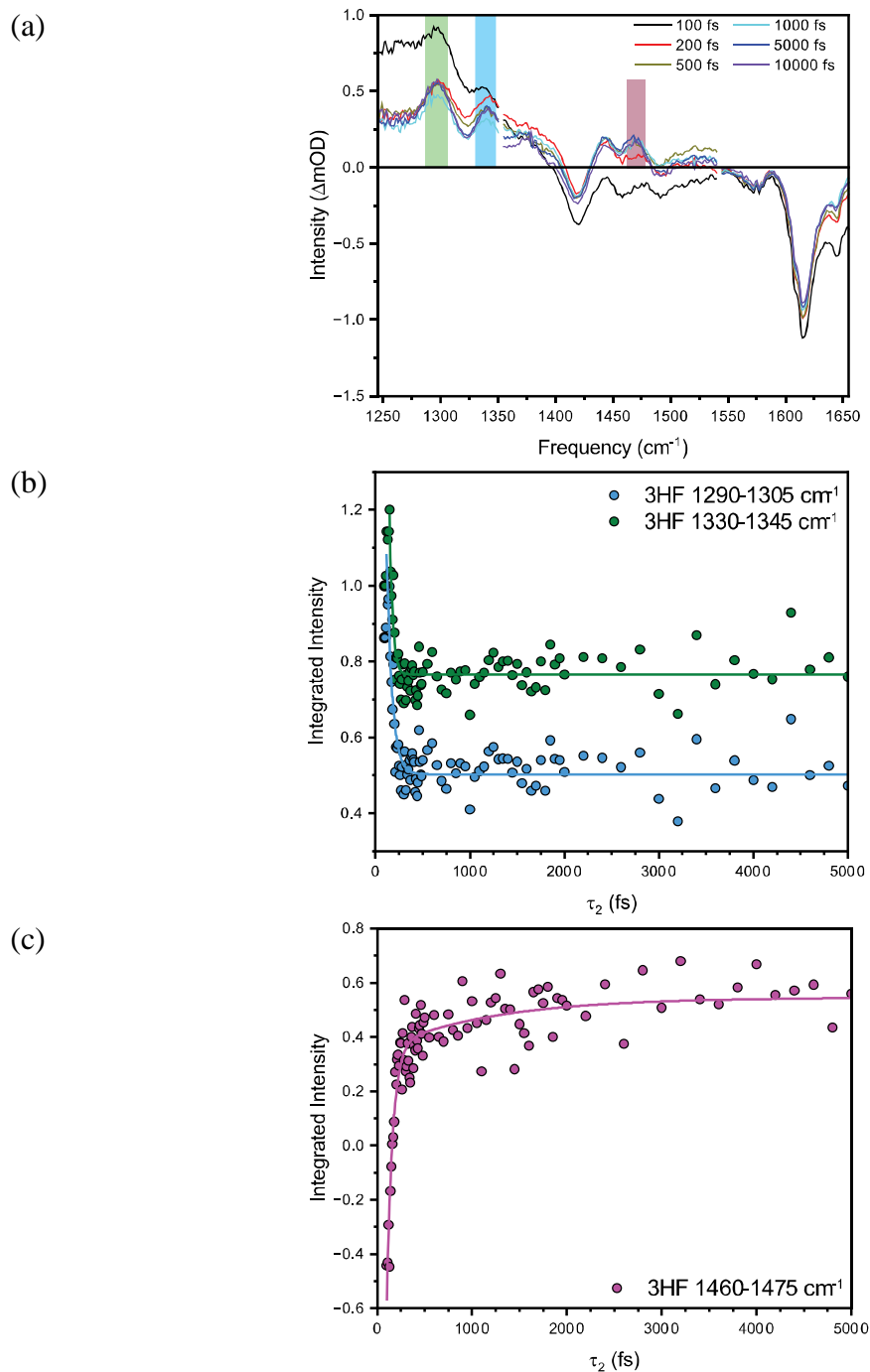
Fig. S6. Integrations of transient infrared data for 3HF (a) over respectively-colored chosen frequency regions. Monoexponential decay fitting was performed for the 1290-1305 cm^{-1} and 1330-1345 cm^{-1} regions (b), giving respective time constants of 57 ± 6 fs and 32 ± 5 fs. The absorbance at 1460-1475 cm^{-1} was fit to a biexponential growth function (c), with time constants of 63 ± 9 fs (amplitude 4.58) and 1.2 ± 0.5 ps (amplitude 0.20).

(a)

(b)

(c)
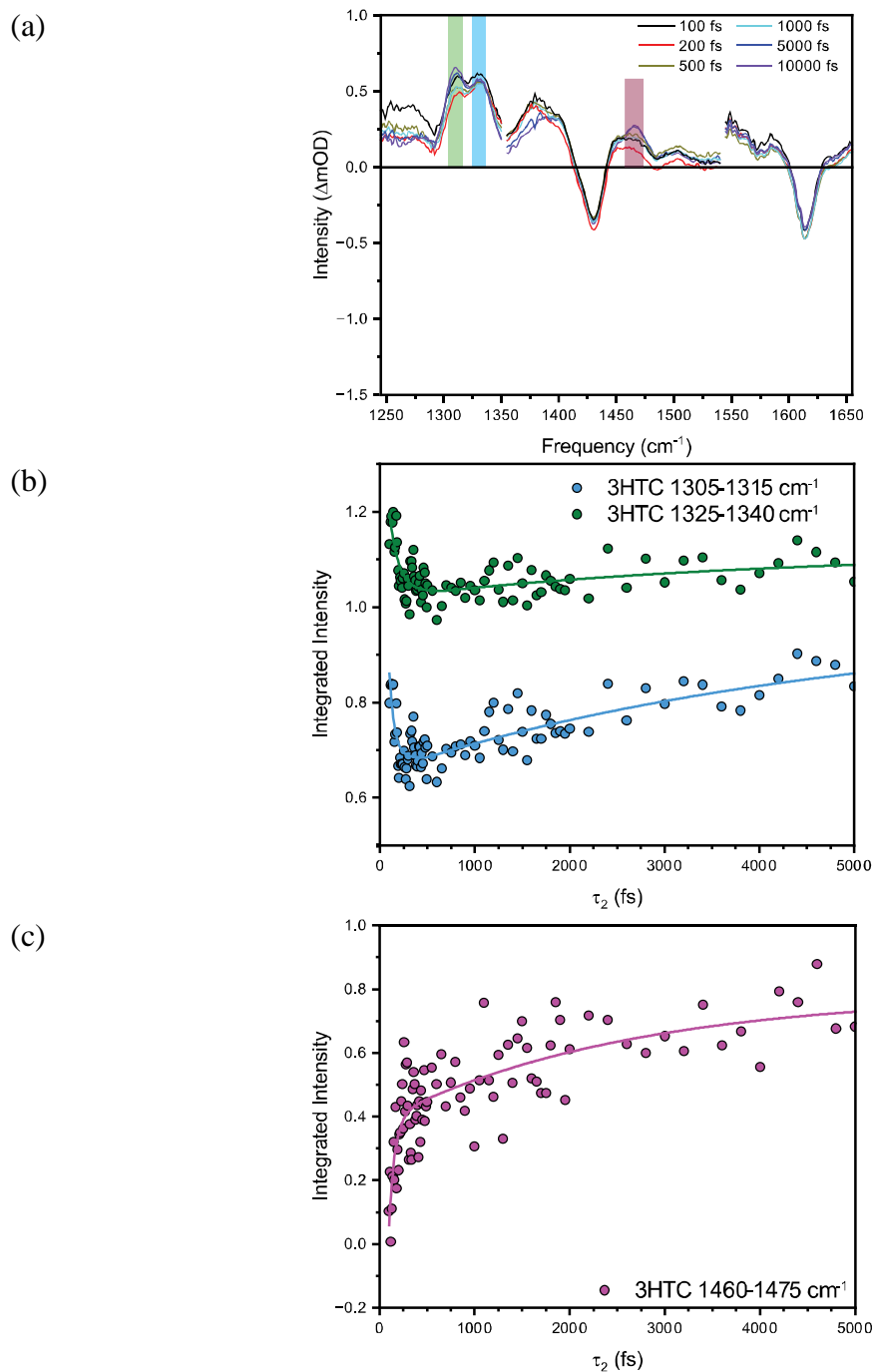
Fig. S7. Integrations of transient infrared data for 3HTC (a) over respectively-colored chosen frequency regions. Fitting was performed for the 1305-1315 cm^{-1} and 1325-1340 cm^{-1} regions using an exponential decay followed by exponential growth (b), giving respective decay time constants of 53 ± 16 fs and 96 ± 28 fs and growth time constants of 4.7 ± 1.3 ps and 4.0 ± 3.0 ps. The 1460-1475 cm^{-1} region was fit to a biexponential growth function (c), with time constants of 64 ± 24 fs (amplitude 1.62) and 2.5 ± 0.7 ps (amplitude 0.40).

(a)

(b)

(c)
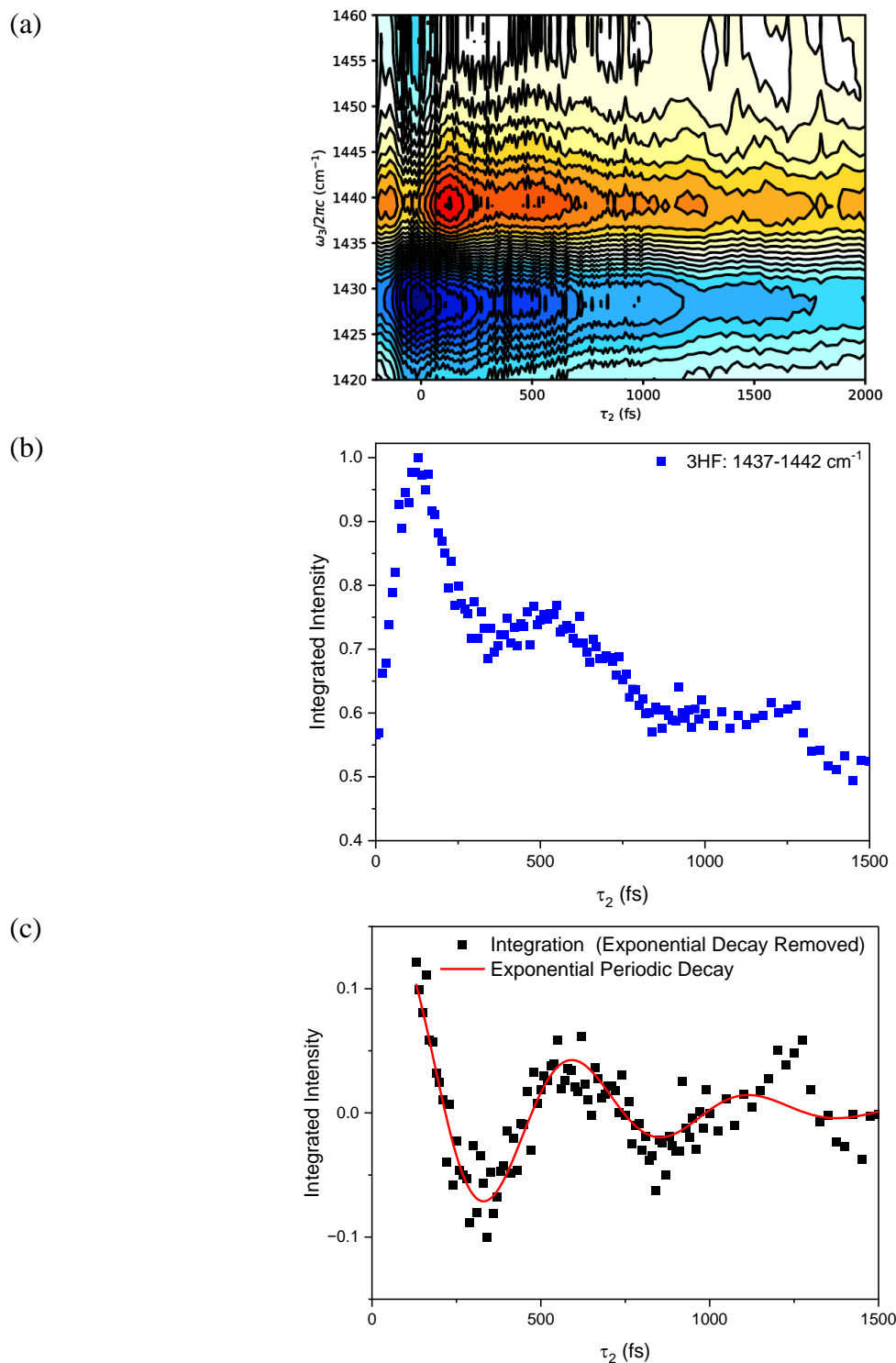
Fig. S8. (a) Ground-state transient absorption contour plot (IR pump-IR probe) of 3HF OH bend transition near 1440 cm^{-1}, where integration over the bleach region (b) displays oscillatory behaviour. After subtraction of the primary exponential decay component, $y = 0.4248 + 0.52278 * e^{\wedge}(-t/913.69603)$, the remaining profile (c) was fit from 100 fs onward with an exponential periodic decay function to extract the oscillation period, 261 ± 6 fs.

(a)

(b)

(c)
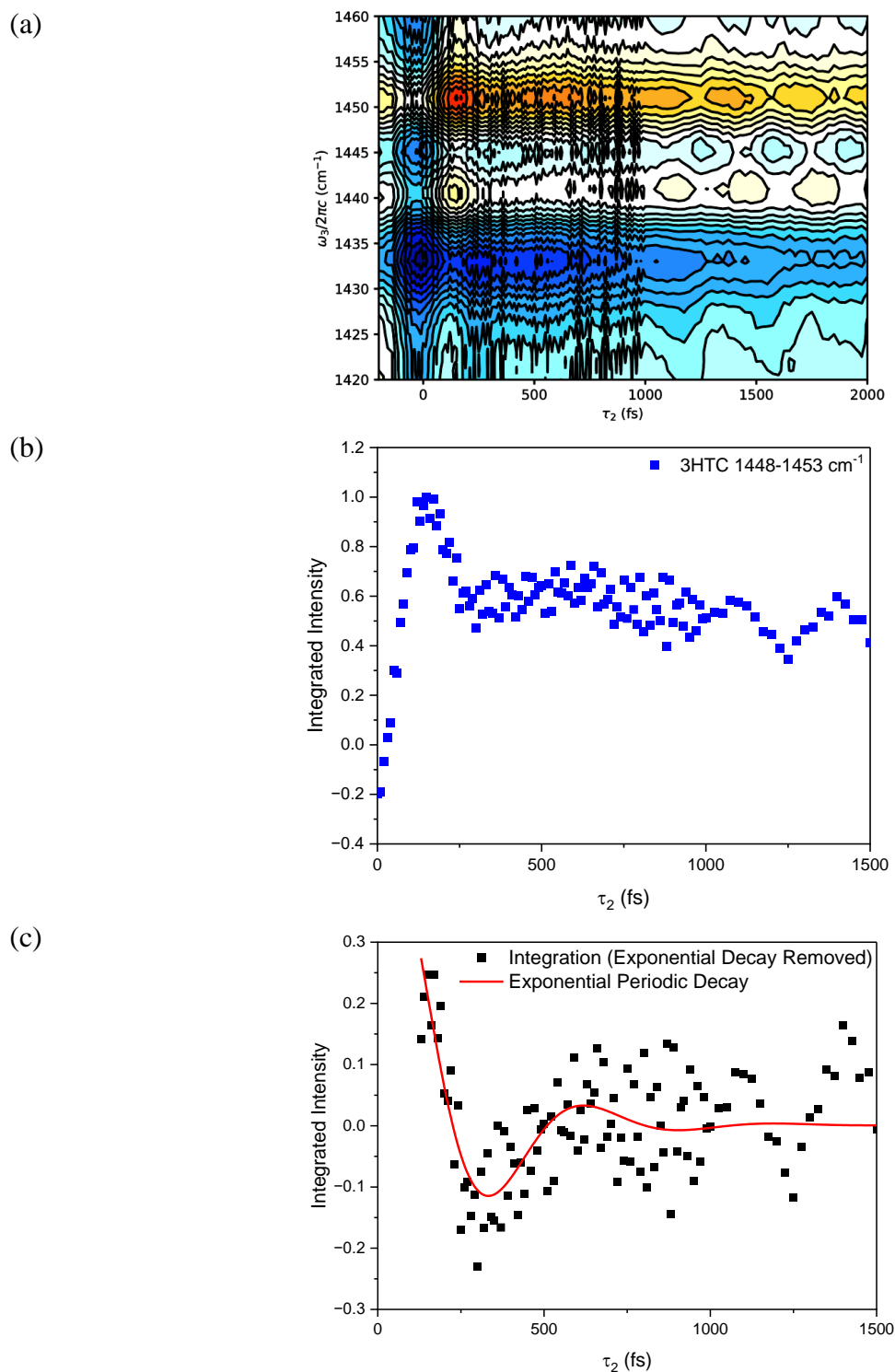
Fig. S9. (a) Ground-state transient absorption contour plot (IR pump-IR probe) of 3HTC OH bend transition near 1450 cm^{-1}. Integration over the bleach region (b) displays oscillatory behaviour. After subtraction of the primary exponential decay component $y = 0.13587 + 0.66472 * e\char`^(-t/1938.01769)$, the remaining profile (c) was fit from 100 fs with an exponential periodic decay function to retrieve the oscillation period, 270 ± 22 fs.

Fig. S10. Low-frequency motions involving the proton transfer coordinate in S_0 of 3HF: (a) 102 cm^{-1} out-of-plane motion. (b) 118 cm^{-1} in-plane mode. Analogous low-frequency motions in S_0 of 3HTC: (c) 102 cm^{-1} and (d) 107 cm^{-1} out-of-plane motions, (e) 250 cm^{-1} in-plane motion.

Table II. Transient infrared spectral data for 3HF and 3HTC at pump-probe delay times listed in the main text.

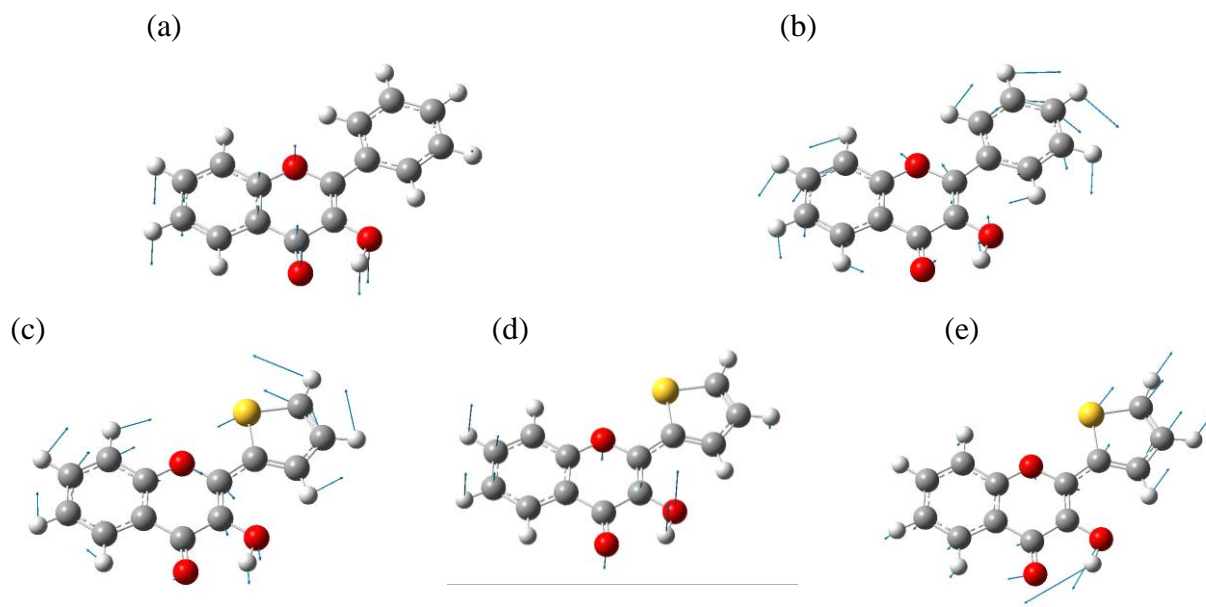| TRIR Data	3HF							3HTC					
Frequency	100 fs	200 fs	500 fs	1000 fs	5000 fs	10000 fs		100 fs	200 fs	500 fs	1000 fs	5000 fs	10000 fs
(cm⁻¹)	ΔmOD	ΔmOD	ΔmOD	ΔmOD	ΔmOD	ΔmOD		ΔmOD	ΔmOD	ΔmOD	ΔmOD	ΔmOD	ΔmOD
1245	0.73149	0.36241	0.35037	0.29591	0.33369	0.37506		0.37401	0.17944	0.25708	0.21260	0.23834	0.18249
1246	0.74058	0.35765	0.31287	0.32819	0.31946	0.36138		0.38144	0.16978	0.26167	0.24137	0.22255	0.18168
1247	0.75730	0.32750	0.33278	0.31208	0.30448	0.36341		0.37693	0.17762	0.28577	0.23901	0.21244	0.19309
1248	0.75585	0.30284	0.38334	0.30460	0.29240	0.37648		0.34978	0.19779	0.28905	0.23084	0.22088	0.20400
1249	0.74445	0.30702	0.41775	0.32062	0.28794	0.38195		0.32117	0.21426	0.26576	0.23228	0.23497	0.20394
1250	0.77553	0.34427	0.37786	0.31060	0.29321	0.35063		0.34895	0.20244	0.26257	0.24194	0.21190	0.18918
1251	0.82255	0.38192	0.32924	0.27495	0.29109	0.32455		0.39519	0.19039	0.28389	0.25553	0.18454	0.17360
1252	0.82779	0.38196	0.35708	0.25236	0.27447	0.35192		0.39984	0.21094	0.30274	0.26398	0.20195	0.17433
1253	0.80022	0.35302	0.38417	0.27542	0.29047	0.37250		0.41535	0.21863	0.29779	0.24907	0.21975	0.18655
1254	0.76600	0.32214	0.38036	0.30495	0.31785	0.34867		0.43287	0.20496	0.28211	0.22910	0.22910	0.18315
1255	0.75181	0.31413	0.36850	0.28582	0.30461	0.29385		0.40904	0.19487	0.27661	0.23197	0.24417	0.15127
1256	0.76944	0.32176	0.36190	0.27441	0.28266	0.28023		0.37940	0.19924	0.25204	0.22883	0.23386	0.16054
1257	0.78213	0.32713	0.35534	0.27664	0.27369	0.30701		0.37382	0.20705	0.23236	0.21877	0.20485	0.20076
1258	0.75120	0.31805	0.33984	0.25679	0.27389	0.32137		0.39434	0.20082	0.26390	0.22396	0.19302	0.20170
1259	0.76780	0.31606	0.34232	0.25176	0.27166	0.34258		0.40957	0.19769	0.28044	0.22886	0.19433	0.17471
1260	0.82617	0.32921	0.36183	0.26641	0.27963	0.36192		0.40054	0.19999	0.26374	0.22541	0.19213	0.14687
1261	0.82978	0.34480	0.36924	0.26879	0.31637	0.34581		0.37519	0.19368	0.25690	0.22022	0.17565	0.13592
1262	0.82331	0.35054	0.36614	0.27366	0.32073	0.34023		0.37104	0.18999	0.25554	0.21450	0.17151	0.13457
1263	0.82990	0.33929	0.35878	0.27348	0.29388	0.35009		0.38961	0.19415	0.24842	0.21315	0.18408	0.14118
1264	0.81787	0.31683	0.35070	0.23948	0.30707	0.32755		0.39277	0.19668	0.23691	0.22240	0.18814	0.16104
1265	0.81849	0.32488	0.35312	0.23252	0.31392	0.31137		0.38908	0.18834	0.24722	0.22602	0.19056	0.16653
1266	0.83248	0.36308	0.36323	0.27318	0.28917	0.32268		0.38982	0.17808	0.27024	0.21521	0.19624	0.15196
1267	0.81061	0.37386	0.36275	0.29990	0.27849	0.33066		0.39160	0.18991	0.25709	0.20199	0.19629	0.14807
1268	0.79400	0.36367	0.36554	0.28715	0.29739	0.34329		0.39881	0.20211	0.24673	0.20966	0.19510	0.15592
1269	0.80919	0.35579	0.37520	0.25971	0.32455	0.36074		0.40734	0.19808	0.26030	0.23421	0.19409	0.16427
1270	0.81702	0.35691	0.36868	0.27886	0.31382	0.35523		0.40062	0.19306	0.25419	0.23440	0.18548	0.16396
1271	0.81943	0.33998	0.36528	0.30162	0.29198	0.33993		0.39464	0.19697	0.25258	0.22630	0.18012	0.16625
1272	0.82075	0.30571	0.37984	0.28959	0.29334	0.33819		0.40287	0.20595	0.27103	0.22906	0.18764	0.17703
1273	0.80229	0.31523	0.38874	0.28381	0.31057	0.35491		0.41039	0.20206	0.26596	0.22603	0.20092	0.18142
1274	0.79448	0.35168	0.37531	0.28582	0.32823	0.35694		0.40138	0.19562	0.25505	0.21704	0.20674	0.18661
1275	0.81744	0.37141	0.35036	0.28524	0.33403	0.32941		0.37769	0.19681	0.26394	0.21170	0.20265	0.19796
1276	0.82584	0.36179	0.36009	0.29140	0.32711	0.32267		0.37027	0.18951	0.27052	0.21690	0.20769	0.19685
1277	0.80696	0.34428	0.37717	0.29510	0.32080	0.34166		0.37599	0.17959	0.25555	0.21464	0.20594	0.18826
1278	0.78109	0.34352	0.36827	0.29484	0.32777	0.36351		0.37456	0.17799	0.22167	0.19439	0.18779	0.18630
1279	0.78759	0.35329	0.37938	0.32625	0.34289	0.37201		0.35675	0.17591	0.20725	0.19026	0.19947	0.19156
1280	0.81574	0.37061	0.39828	0.34968	0.35857	0.37773		0.33932	0.16929	0.21845	0.20094	0.22266	0.19492
1281	0.82785	0.39242	0.39248	0.32094	0.37070	0.39511		0.33874	0.16125	0.23509	0.20402	0.21577	0.19085

1282	0.80858	0.40412	0.39159	0.31439	0.38373	0.40715	0.33157	0.15976	0.23246	0.19337	0.19824	0.19466
1283	0.80160	0.40859	0.40605	0.34207	0.39735	0.42040	0.31717	0.15716	0.21046	0.18102	0.19374	0.19694
1284	0.84833	0.41696	0.42430	0.36377	0.40602	0.44556	0.31029	0.14266	0.18673	0.17938	0.20632	0.18322
1285	0.86468	0.42253	0.43492	0.36565	0.40396	0.44484	0.30647	0.13194	0.17529	0.16904	0.19649	0.18428
1286	0.84524	0.43016	0.44323	0.36862	0.41518	0.43254	0.29824	0.12779	0.17649	0.15886	0.17361	0.19259
1287	0.85043	0.45073	0.46107	0.39754	0.46401	0.45680	0.28222	0.11947	0.17902	0.16831	0.17600	0.17876
1288	0.86643	0.47195	0.47479	0.40638	0.48955	0.50098	0.26684	0.10321	0.16992	0.15436	0.17493	0.17501
1289	0.87604	0.48385	0.49183	0.41697	0.48317	0.52503	0.25401	0.09801	0.15640	0.12963	0.16584	0.17727
1290	0.87476	0.48418	0.52780	0.48561	0.49129	0.50240	0.23768	0.12316	0.15514	0.14690	0.17151	0.15009
1291	0.85673	0.47330	0.52739	0.48129	0.50299	0.49502	0.21617	0.11721	0.14161	0.14868	0.17122	0.12873
1292	0.84993	0.47644	0.49845	0.41136	0.51103	0.52616	0.20879	0.08314	0.12895	0.12738	0.16153	0.13527
1293	0.89610	0.52492	0.51555	0.43837	0.52554	0.55485	0.24219	0.09547	0.16324	0.14360	0.16582	0.15727
1294	0.92205	0.55115	0.53882	0.47281	0.53798	0.56041	0.27352	0.11742	0.19138	0.16407	0.18166	0.18676
1295	0.90200	0.53515	0.53942	0.45677	0.54379	0.55322	0.27719	0.12043	0.19061	0.16648	0.20383	0.21646
1296	0.90216	0.54250	0.54296	0.45962	0.54938	0.56510	0.27647	0.12932	0.20617	0.17673	0.23328	0.24040
1297	0.91620	0.56435	0.54539	0.47381	0.55215	0.57863	0.29333	0.15895	0.22906	0.20163	0.26569	0.26895
1298	0.91823	0.57417	0.54326	0.47448	0.55165	0.57237	0.32525	0.20237	0.24936	0.23544	0.29548	0.30678
1299	0.89941	0.56499	0.54706	0.45964	0.55257	0.54882	0.34351	0.23183	0.28093	0.26719	0.32037	0.34317
1300	0.88312	0.55452	0.54027	0.45266	0.53925	0.53491	0.36568	0.24623	0.30279	0.29618	0.35217	0.37614
1301	0.88207	0.55504	0.52191	0.46108	0.51164	0.54077	0.40707	0.26222	0.31308	0.32710	0.39832	0.41328
1302	0.87289	0.55452	0.52814	0.45422	0.50368	0.53636	0.44669	0.30119	0.35713	0.36418	0.44800	0.46688
1303	0.85462	0.54562	0.53192	0.43575	0.50029	0.51715	0.46995	0.34315	0.40302	0.39544	0.47946	0.51467
1304	0.83533	0.52951	0.50616	0.42028	0.48144	0.49235	0.48090	0.36658	0.41681	0.41545	0.49029	0.54078
1305	0.81719	0.51679	0.48232	0.40802	0.46379	0.47052	0.50589	0.38463	0.43321	0.44325	0.51837	0.57048
1306	0.80609	0.51404	0.46781	0.39490	0.44885	0.45983	0.53127	0.40399	0.46432	0.47202	0.55490	0.60005
1307	0.79952	0.51415	0.45536	0.38085	0.42976	0.45207	0.53969	0.42629	0.49792	0.48793	0.57754	0.61831
1308	0.77463	0.48989	0.44301	0.37605	0.40555	0.40955	0.55494	0.45324	0.50880	0.49680	0.59567	0.63728
1309	0.74608	0.45864	0.43231	0.36985	0.38397	0.36407	0.57511	0.47140	0.51063	0.50764	0.60910	0.65395
1310	0.73272	0.44860	0.42322	0.34545	0.37090	0.36023	0.58679	0.47095	0.52481	0.52334	0.61398	0.65854
1311	0.70207	0.43991	0.40779	0.30772	0.35509	0.35819	0.59704	0.47460	0.52841	0.53106	0.61864	0.65335
1312	0.66528	0.42733	0.38476	0.28216	0.33362	0.34266	0.60095	0.48619	0.52172	0.52776	0.62014	0.64277
1313	0.65227	0.41621	0.36077	0.28525	0.31124	0.32335	0.59253	0.49422	0.52093	0.52158	0.60997	0.63187
1314	0.63799	0.39652	0.34775	0.27241	0.29158	0.30185	0.59375	0.49392	0.52377	0.52571	0.59213	0.62672
1315	0.61538	0.38042	0.34232	0.24262	0.27500	0.27895	0.59488	0.48767	0.52309	0.52918	0.57712	0.61819
1316	0.59692	0.38515	0.33203	0.22922	0.26074	0.25752	0.57277	0.48036	0.51517	0.51147	0.57179	0.59373
1317	0.58115	0.37504	0.31974	0.22613	0.25242	0.24455	0.56262	0.46955	0.51117	0.49103	0.55932	0.57255
1318	0.56683	0.34951	0.30786	0.21972	0.24434	0.23653	0.56915	0.46219	0.51135	0.48329	0.53948	0.55986
1319	0.55456	0.34072	0.29610	0.20370	0.22737	0.22301	0.56433	0.46932	0.50569	0.48842	0.52840	0.54552
1320	0.53950	0.33380	0.28816	0.19569	0.21780	0.20925	0.55487	0.47630	0.49726	0.49004	0.52431	0.53778
1321	0.52664	0.32485	0.28494	0.19931	0.21875	0.19951	0.55178	0.47845	0.49462	0.48620	0.52207	0.53591
1322	0.52671	0.32944	0.28268	0.19880	0.21544	0.19325	0.55909	0.48593	0.50444	0.49149	0.52022	0.52876
1323	0.52026	0.33490	0.27615	0.19035	0.20970	0.19375	0.57315	0.49363	0.51438	0.50311	0.52701	0.52711
1324	0.50134	0.33353	0.26937	0.18412	0.20852	0.19935	0.58709	0.49892	0.52110	0.51466	0.53910	0.53519

1325	0.49024	0.33382	0.27501	0.19666	0.21647	0.20357	0.59380	0.50706	0.53469	0.52238	0.54011	0.54249
1326	0.49637	0.33888	0.28698	0.21045	0.22544	0.21471	0.59202	0.51677	0.53893	0.52427	0.54084	0.54799
1327	0.50907	0.34977	0.29572	0.21426	0.23421	0.23077	0.59161	0.52948	0.53470	0.52556	0.55171	0.55731
1328	0.50242	0.36634	0.29847	0.22096	0.25331	0.23355	0.60903	0.55030	0.55218	0.53751	0.56724	0.57606
1329	0.49667	0.37898	0.30572	0.22950	0.26522	0.24427	0.61920	0.56026	0.56494	0.54840	0.57320	0.58336
1330	0.50864	0.38305	0.32305	0.24018	0.26756	0.27225	0.60915	0.55182	0.55615	0.54879	0.56709	0.57377
1331	0.51925	0.38769	0.33973	0.26234	0.29446	0.28522	0.60903	0.54929	0.55812	0.54774	0.56720	0.57866
1332	0.51860	0.39748	0.34569	0.27735	0.32316	0.28747	0.61363	0.55367	0.56091	0.54821	0.56518	0.58162
1333	0.51119	0.41005	0.34479	0.27526	0.32875	0.29638	0.60886	0.55804	0.55162	0.54956	0.55578	0.56674
1334	0.51502	0.41632	0.36066	0.28422	0.33402	0.31676	0.59883	0.56236	0.54976	0.55086	0.56002	0.56073
1335	0.52513	0.41912	0.37650	0.29851	0.34789	0.33986	0.58923	0.55306	0.54351	0.54617	0.55477	0.55782
1336	0.52868	0.42457	0.37117	0.30182	0.36352	0.35388	0.58163	0.52638	0.51976	0.53076	0.52025	0.54083
1337	0.52509	0.43145	0.36419	0.30012	0.36551	0.35576	0.56933	0.51287	0.50179	0.50830	0.49548	0.51244
1338	0.52102	0.44216	0.37397	0.30509	0.37137	0.35566	0.54803	0.50387	0.49253	0.48275	0.48013	0.48419
1339	0.52126	0.45615	0.39745	0.31939	0.39698	0.36422	0.52015	0.47887	0.47967	0.45690	0.45505	0.46341
1340	0.51786	0.45985	0.39249	0.32077	0.40425	0.37461	0.49867	0.45514	0.45359	0.43182	0.42735	0.43793
1341	0.50781	0.45846	0.37888	0.31340	0.39536	0.38237	0.48312	0.43709	0.42410	0.40846	0.40118	0.40538
1342	0.49422	0.46528	0.39133	0.31100	0.39430	0.38395	0.46145	0.41954	0.40275	0.38953	0.37358	0.37135
1343	0.48284	0.47316	0.37124	0.29435	0.38776	0.36929	0.42162	0.40750	0.36829	0.38115	0.33705	0.33801
1344	0.47032	0.46609	0.33424	0.28025	0.37192	0.35460	0.38841	0.39257	0.32990	0.36577	0.30237	0.30714
1345	0.45281	0.43785	0.34209	0.29692	0.35702	0.36217	0.39163	0.36244	0.31411	0.32317	0.28589	0.28099
1346	0.44964	0.42765	0.35933	0.29625	0.35438	0.36001	0.37853	0.33391	0.30577	0.29014	0.27054	0.26205
1347	0.44761	0.43596	0.35257	0.27182	0.35454	0.33900	0.34669	0.31998	0.29483	0.27731	0.24931	0.24371
1348	0.41655	0.42853	0.32169	0.25927	0.33723	0.32017	0.33822	0.31922	0.28402	0.26463	0.22913	0.21664
1349	0.39700	0.41282	0.30988	0.24570	0.31691	0.31481	0.32039	0.31094	0.27352	0.25301	0.20779	0.19441
1350 <grating change>	0.39415	0.39775	0.31726	0.22721	0.30054	0.31362	0.29074	0.29142	0.26043	0.23847	0.18839	0.18204
1355	0.30852	0.34534	0.28143	0.26111	0.20148	0.13528	0.21163	0.17493	0.20625	0.17600	0.13358	0.09329
1356	0.31028	0.34302	0.27628	0.25057	0.18875	0.13541	0.22027	0.18008	0.21710	0.18891	0.13994	0.08994
1357	0.30417	0.33999	0.26414	0.24226	0.19238	0.13200	0.22348	0.19108	0.22675	0.20178	0.14191	0.09947
1358	0.28895	0.33493	0.25309	0.23976	0.20134	0.13055	0.22338	0.20342	0.23410	0.21004	0.14344	0.12005
1359	0.27209	0.32524	0.25322	0.24322	0.19561	0.13953	0.22623	0.21383	0.23980	0.21516	0.15420	0.13641
1360	0.26060	0.31889	0.25434	0.24704	0.18992	0.14457	0.23441	0.22147	0.24354	0.22167	0.16679	0.14294
1361	0.25578	0.32014	0.24756	0.24560	0.19684	0.13676	0.24705	0.22653	0.24654	0.23197	0.17335	0.13973
1362	0.24651	0.31760	0.24089	0.23734	0.20001	0.13531	0.25868	0.22994	0.25421	0.24152	0.17695	0.13317
1363	0.23091	0.30921	0.23849	0.22191	0.19629	0.14332	0.26834	0.23590	0.26743	0.24770	0.18167	0.13132
1364	0.21917	0.30500	0.23718	0.20118	0.20111	0.14252	0.28073	0.25152	0.28137	0.25136	0.19071	0.14222
1365	0.21212	0.29938	0.23467	0.19199	0.20949	0.13866	0.29580	0.27489	0.29487	0.25504	0.20492	0.16309
1366	0.20509	0.28233	0.23084	0.21206	0.20837	0.14703	0.31085	0.29795	0.30933	0.26250	0.22214	0.18472
1367	0.19642	0.27082	0.23239	0.23946	0.20913	0.15418	0.32568	0.31033	0.32683	0.27920	0.23272	0.19868
1368	0.18890	0.27651	0.24081	0.24967	0.22058	0.15135	0.33957	0.31056	0.34371	0.30489	0.23289	0.20236
1369	0.19293	0.28045	0.24139	0.24007	0.22875	0.15978	0.34913	0.31882	0.34350	0.32539	0.23721	0.20579

1370	0.20411	0.27601	0.22987	0.22141	0.22744	0.18108	0.35670	0.33961	0.33398	0.33724	0.24960	0.21278
1371	0.20170	0.27521	0.21707	0.21469	0.22313	0.19091	0.37075	0.35642	0.34979	0.35078	0.25957	0.21829
1372	0.18966	0.28048	0.21431	0.22191	0.21999	0.18720	0.38812	0.36251	0.38568	0.36464	0.26843	0.22164
1373	0.18398	0.28768	0.22609	0.23296	0.21902	0.18183	0.40119	0.36145	0.41322	0.37196	0.28282	0.22541
1374	0.18334	0.29206	0.22524	0.23687	0.21482	0.18432	0.41621	0.37414	0.41412	0.37623	0.29796	0.23340
1375	0.18523	0.28842	0.19980	0.22991	0.20846	0.19357	0.43377	0.40584	0.39152	0.38100	0.30865	0.24622
1376	0.19583	0.27130	0.19306	0.22506	0.21914	0.18709	0.43294	0.41524	0.38943	0.38292	0.31623	0.25645
1377	0.20368	0.25058	0.20566	0.22615	0.23160	0.17534	0.42442	0.39590	0.41521	0.38862	0.31251	0.26226
1378	0.17977	0.25090	0.18584	0.22405	0.19492	0.20290	0.45228	0.38682	0.42980	0.41368	0.28163	0.26908
1379	0.14454	0.26286	0.15217	0.21460	0.13979	0.22968	0.48348	0.39442	0.42783	0.43251	0.25763	0.27661
1380	0.13782	0.26217	0.15302	0.19985	0.13137	0.18861	0.45994	0.40366	0.42353	0.41003	0.28688	0.28255
1381	0.14555	0.25479	0.16575	0.19486	0.15613	0.13580	0.43404	0.39910	0.41929	0.38677	0.32834	0.29300
1382	0.14693	0.25175	0.16372	0.20502	0.17960	0.12721	0.44972	0.37843	0.41464	0.39530	0.34241	0.30902
1383	0.14301	0.25447	0.15981	0.20532	0.17480	0.13389	0.45689	0.36868	0.41081	0.39891	0.35207	0.31489
1384	0.13622	0.25459	0.15909	0.19152	0.14505	0.13066	0.43991	0.37353	0.40678	0.38561	0.36092	0.31133
1385	0.12697	0.23660	0.15262	0.18633	0.12491	0.11224	0.43512	0.36746	0.39938	0.38110	0.34371	0.31854
1386	0.11518	0.21484	0.14872	0.18840	0.11817	0.09078	0.44048	0.35487	0.39327	0.38348	0.31825	0.33077
1387	0.10091	0.21353	0.15777	0.18382	0.11167	0.08248	0.43339	0.35291	0.39402	0.37795	0.31916	0.33107
1388	0.08644	0.21700	0.14810	0.17271	0.10565	0.07551	0.41297	0.34821	0.38872	0.37379	0.33184	0.32711
1389	0.07439	0.21011	0.10733	0.15986	0.10298	0.06093	0.38988	0.32980	0.37092	0.37593	0.33537	0.32803
1390	0.06640	0.20597	0.09425	0.15088	0.10321	0.05497	0.38527	0.31274	0.36112	0.36368	0.32856	0.32937
1391	0.05850	0.20537	0.11858	0.14799	0.10243	0.05672	0.39729	0.30405	0.36342	0.33866	0.31902	0.32475
1392	0.04175	0.19262	0.12628	0.14888	0.09452	0.04418	0.39801	0.29768	0.36039	0.32968	0.31985	0.30983
1393	0.02311	0.17744	0.11475	0.14649	0.08687	0.02599	0.38560	0.29374	0.35448	0.33399	0.32666	0.30197
1394	0.01506	0.17838	0.10916	0.13446	0.08991	0.02353	0.37264	0.29428	0.35624	0.33311	0.32691	0.32116
1395	0.00986	0.18020	0.10869	0.12256	0.08929	0.02722	0.36073	0.29089	0.35420	0.32906	0.32040	0.33771
1396	0.00060	0.17004	0.10669	0.12023	0.07626	0.02622	0.35000	0.27922	0.34108	0.32673	0.31177	0.32822
1397	-0.00446	0.16302	0.10116	0.12498	0.07118	0.02768	0.34461	0.27104	0.33376	0.32347	0.30810	0.31688
1398	-0.00698	0.16171	0.09080	0.12776	0.07599	0.03014	0.34547	0.27014	0.33682	0.31903	0.31187	0.31559
1399	-0.02084	0.15129	0.07491	0.11577	0.06914	0.02086	0.34871	0.26870	0.33768	0.31651	0.31957	0.31503
1400	-0.04035	0.13500	0.05871	0.09648	0.05565	0.00374	0.34686	0.26190	0.33354	0.31230	0.32441	0.31285
1401	-0.05243	0.12422	0.04888	0.08521	0.05115	-0.00958	0.33372	0.24853	0.32698	0.30072	0.31961	0.31038
1402	-0.06676	0.11473	0.04205	0.07633	0.04220	-0.02046	0.31868	0.23397	0.31528	0.28601	0.30660	0.30316
1403	-0.09037	0.10131	0.03331	0.06193	0.01901	-0.03279	0.30801	0.22127	0.29797	0.27251	0.28854	0.28903
1404	-0.10932	0.08699	0.02113	0.04321	-0.00058	-0.04736	0.29066	0.20407	0.28304	0.25810	0.26702	0.27482
1405	-0.12097	0.07181	0.00516	0.02253	-0.01180	-0.06319	0.26484	0.18256	0.26926	0.24114	0.24565	0.26054
1406	-0.13781	0.05183	-0.01382	0.00197	-0.02795	-0.07793	0.24119	0.16515	0.24507	0.22166	0.22956	0.23775
1407	-0.15811	0.03085	-0.03176	-0.01674	-0.04726	-0.09159	0.21962	0.15061	0.21649	0.20023	0.21272	0.20807
1408	-0.17421	0.01469	-0.04468	-0.03293	-0.06150	-0.10548	0.19443	0.13184	0.19567	0.17712	0.18597	0.17786
1409	-0.19285	-0.00396	-0.05790	-0.04970	-0.07767	-0.12018	0.16574	0.10260	0.17198	0.14978	0.15703	0.14612
1410	-0.21908	-0.03003	-0.07669	-0.06946	-0.10062	-0.13631	0.13632	0.06390	0.13794	0.11822	0.13246	0.11225
1411	-0.24466	-0.05441	-0.09986	-0.09053	-0.12027	-0.15482	0.11075	0.03196	0.10802	0.08983	0.10496	0.08132
1412	-0.26584	-0.07316	-0.12266	-0.11170	-0.13341	-0.17342	0.08811	0.01087	0.08504	0.06466	0.07308	0.05332

1413	-0.28611	-0.09034	-0.13826	-0.13279	-0.14693	-0.18680	0.06161	-0.01087	0.05636	0.03420	0.04355	0.02226
1414	-0.30834	-0.10803	-0.15146	-0.15157	-0.16522	-0.19850	0.03269	-0.03589	0.02392	0.00112	0.01510	-0.00946
1415	-0.33285	-0.12686	-0.17085	-0.16549	-0.18814	-0.21431	0.00639	-0.06170	-0.00313	-0.02647	-0.01646	-0.03590
1416	-0.35099	-0.14767	-0.18962	-0.17644	-0.20249	-0.22555	-0.01947	-0.08926	-0.02539	-0.04763	-0.04517	-0.05941
1417	-0.35795	-0.16738	-0.20005	-0.18567	-0.20028	-0.22694	-0.04625	-0.11718	-0.04522	-0.06460	-0.06633	-0.08204
1418	-0.36338	-0.17445	-0.20264	-0.19018	-0.19371	-0.23013	-0.06884	-0.13681	-0.06249	-0.08191	-0.08487	-0.09982
1419	-0.37069	-0.16922	-0.19940	-0.18875	-0.19091	-0.23630	-0.08795	-0.15093	-0.08135	-0.10260	-0.10536	-0.11614
1420	-0.37398	-0.16569	-0.19268	-0.18280	-0.19170	-0.23309	-0.11128	-0.17487	-0.10969	-0.12747	-0.13009	-0.14226
1421	-0.36935	-0.16383	-0.18388	-0.17267	-0.19087	-0.22123	-0.13853	-0.20654	-0.13966	-0.15515	-0.15807	-0.17411
1422	-0.35595	-0.15610	-0.17337	-0.15834	-0.18183	-0.20807	-0.16522	-0.23507	-0.15916	-0.18330	-0.18682	-0.20083
1423	-0.34058	-0.14115	-0.15945	-0.14148	-0.16432	-0.19347	-0.19043	-0.25942	-0.18110	-0.21073	-0.21575	-0.22411
1424	-0.32766	-0.12059	-0.14063	-0.12483	-0.14294	-0.17754	-0.21618	-0.28347	-0.21581	-0.23834	-0.24514	-0.24896
1425	-0.31140	-0.09845	-0.11717	-0.11208	-0.12858	-0.16565	-0.24824	-0.31521	-0.25149	-0.27075	-0.27586	-0.27934
1426	-0.29005	-0.07581	-0.09158	-0.09653	-0.11581	-0.15414	-0.28275	-0.35209	-0.28127	-0.30527	-0.30536	-0.31188
1427	-0.26823	-0.05057	-0.06824	-0.06240	-0.08296	-0.12982	-0.30577	-0.37998	-0.30691	-0.33124	-0.32759	-0.33597
1428	-0.25246	-0.02656	-0.04751	-0.02486	-0.04361	-0.09700	-0.31956	-0.39691	-0.32474	-0.34773	-0.34170	-0.35223
1429	-0.24597	-0.00937	-0.02724	-0.00865	-0.02437	-0.06873	-0.33344	-0.40757	-0.33013	-0.35862	-0.34999	-0.36616
1430	-0.23245	0.00425	-0.00501	0.00448	-0.01236	-0.04854	-0.34312	-0.41226	-0.33022	-0.36200	-0.35435	-0.37359
1431	-0.20298	0.01848	0.01959	0.03173	0.00818	-0.03401	-0.34204	-0.41019	-0.32940	-0.35696	-0.35466	-0.37007
1432	-0.17755	0.03395	0.04235	0.05980	0.03325	-0.01589	-0.32775	-0.40106	-0.31838	-0.34857	-0.34671	-0.35694
1433	-0.16540	0.05314	0.06323	0.08034	0.05700	0.00724	-0.30428	-0.38489	-0.29658	-0.33695	-0.32891	-0.33706
1434	-0.15909	0.07990	0.08675	0.09571	0.07531	0.02759	-0.28118	-0.36187	-0.27429	-0.31602	-0.30327	-0.31366
1435	-0.15352	0.10420	0.10717	0.11152	0.09171	0.04629	-0.25494	-0.33050	-0.24889	-0.28372	-0.27188	-0.28472
1436	-0.14571	0.11353	0.11676	0.13248	0.11155	0.06785	-0.21729	-0.28999	-0.21249	-0.24249	-0.23603	-0.24755
1437	-0.13351	0.12242	0.12737	0.15177	0.12759	0.08658	-0.17463	-0.24731	-0.17010	-0.20346	-0.19376	-0.21065
1438	-0.11648	0.14061	0.14697	0.16227	0.13848	0.09865	-0.13376	-0.20870	-0.12658	-0.16978	-0.14672	-0.17857
1439	-0.09752	0.14996	0.16235	0.16394	0.16335	0.11101	-0.09267	-0.17356	-0.07824	-0.12193	-0.10638	-0.14012
1440	-0.08166	0.14782	0.16943	0.16361	0.19585	0.12609	-0.05053	-0.13664	-0.03008	-0.06345	-0.07413	-0.09464
1441	-0.07502	0.15166	0.17702	0.17322	0.20167	0.13945	-0.00917	-0.08987	0.00391	-0.02425	-0.03918	-0.05479
1442	-0.07450	0.16001	0.18579	0.18825	0.19123	0.14644	0.02891	-0.03925	0.03301	0.00132	-0.00075	-0.02184
1443	-0.07278	0.16306	0.19158	0.19683	0.19321	0.14442	0.06182	0.00263	0.07371	0.03515	0.03621	0.00908
1444	-0.06861	0.16744	0.19241	0.19903	0.19383	0.13969	0.09170	0.03184	0.11051	0.07262	0.06914	0.03804
1445	-0.06486	0.17532	0.18976	0.19574	0.18161	0.13722	0.12054	0.05118	0.13090	0.10365	0.09680	0.06410
1446	-0.06945	0.16883	0.19098	0.18208	0.17719	0.13322	0.14734	0.07235	0.14935	0.12366	0.11925	0.08732
1447	-0.08344	0.14685	0.19123	0.16149	0.18273	0.12677	0.16712	0.09471	0.16914	0.13534	0.13723	0.10600
1448	-0.09940	0.12903	0.17343	0.14673	0.17674	0.12124	0.17246	0.10429	0.17842	0.14780	0.15218	0.11728
1449	-0.11101	0.12122	0.14673	0.13971	0.16126	0.11622	0.17202	0.10811	0.18322	0.16048	0.16618	0.12792
1450	-0.11588	0.11851	0.13180	0.13531	0.14958	0.10970	0.17966	0.12036	0.19594	0.16838	0.18029	0.14619
1451	-0.12555	0.10704	0.12881	0.12675	0.13934	0.10330	0.18920	0.12923	0.20702	0.17332	0.18920	0.16072
1452	-0.14708	0.08216	0.12915	0.11253	0.12794	0.09791	0.19227	0.12534	0.20697	0.17714	0.19038	0.16303
1453	-0.16877	0.06476	0.11867	0.10355	0.12219	0.09055	0.18889	0.12126	0.20053	0.17752	0.19139	0.16362
1454	-0.18011	0.06306	0.10213	0.10138	0.12143	0.08187	0.18478	0.12180	0.19475	0.17547	0.19612	0.16952
1455	-0.17668	0.06660	0.10333	0.09650	0.11633	0.07687	0.18914	0.12057	0.19621	0.17606	0.20263	0.18037

1456	-0.17342	0.06098	0.11227	0.09320	0.11075	0.07724	0.19392	0.12045	0.20331	0.18018	0.20771	0.18972
1457	-0.18776	0.03754	0.10594	0.09984	0.11444	0.08250	0.18628	0.12690	0.20997	0.18590	0.20942	0.19164
1458	-0.19688	0.02222	0.09586	0.10446	0.12743	0.09153	0.17873	0.13044	0.21169	0.19023	0.21445	0.19812
1459	-0.18480	0.03497	0.09705	0.09864	0.14467	0.10342	0.18227	0.12595	0.20937	0.19176	0.22670	0.21661
1460	-0.17581	0.06046	0.10978	0.09473	0.15657	0.11796	0.18838	0.12698	0.21427	0.19313	0.23857	0.23326
1461	-0.17711	0.07890	0.12717	0.10345	0.16219	0.13140	0.19098	0.13295	0.22374	0.19430	0.24627	0.24222
1462	-0.17239	0.07376	0.13726	0.12810	0.17004	0.13703	0.18980	0.12687	0.22013	0.19228	0.25208	0.24973
1463	-0.16538	0.05810	0.13572	0.14630	0.17773	0.14010	0.18542	0.11752	0.20926	0.19074	0.25812	0.25928
1464	-0.16794	0.05539	0.12560	0.13318	0.17901	0.14852	0.17949	0.12216	0.20726	0.19470	0.26498	0.27093
1465	-0.17184	0.05778	0.12246	0.12048	0.18094	0.15002	0.17720	0.12506	0.21196	0.19702	0.26752	0.27795
1466	-0.16606	0.05590	0.13728	0.13544	0.19056	0.14025	0.18009	0.11388	0.21689	0.19291	0.26348	0.27645
1467	-0.14689	0.05691	0.16273	0.15962	0.20583	0.14444	0.17965	0.10453	0.21795	0.19034	0.26038	0.27301
1468	-0.12452	0.06132	0.18121	0.17706	0.21252	0.16589	0.17593	0.10286	0.21310	0.18979	0.25984	0.27016
1469	-0.12102	0.06112	0.17024	0.18257	0.18899	0.18040	0.17832	0.09996	0.20281	0.18253	0.25581	0.26460
1470	-0.13099	0.06272	0.14738	0.18121	0.16365	0.18059	0.17738	0.09504	0.19283	0.17086	0.24668	0.25537
1471	-0.13617	0.07580	0.14395	0.18105	0.17736	0.17050	0.15927	0.09094	0.18924	0.16149	0.23391	0.24307
1472	-0.13501	0.08507	0.14634	0.17814	0.19240	0.15751	0.14167	0.08326	0.18562	0.15023	0.21958	0.22862
1473	-0.12903	0.07896	0.13976	0.17091	0.17573	0.14830	0.13951	0.06996	0.17679	0.13696	0.20595	0.21345
1474	-0.11610	0.06968	0.13513	0.17016	0.15394	0.14555	0.14183	0.05860	0.16800	0.13660	0.19505	0.19990
1475	-0.10467	0.06761	0.13569	0.17136	0.14107	0.13996	0.14010	0.05153	0.16053	0.14353	0.18501	0.18828
1476	-0.11237	0.07579	0.13252	0.15407	0.12856	0.11274	0.13265	0.04423	0.15021	0.13036	0.17048	0.17629
1477	-0.12422	0.07941	0.11985	0.12979	0.11243	0.07989	0.12024	0.03661	0.13818	0.10644	0.15529	0.16056
1478	-0.11506	0.06160	0.09793	0.12122	0.09306	0.06834	0.10525	0.03023	0.12795	0.09612	0.14602	0.13886
1479	-0.10135	0.04249	0.08446	0.11491	0.07533	0.06070	0.09197	0.02159	0.11865	0.09120	0.13682	0.11701
1480	-0.10278	0.03977	0.08782	0.09853	0.06345	0.04213	0.08301	0.00888	0.10855	0.08137	0.12198	0.10056
1481	-0.11944	0.04257	0.08573	0.08484	0.05726	0.03060	0.07604	-0.00270	0.09693	0.07216	0.10397	0.08958
1482	-0.14068	0.03825	0.07104	0.07754	0.04830	0.02632	0.06919	-0.00984	0.08453	0.06464	0.08758	0.08249
1483	-0.14900	0.01881	0.05693	0.06763	0.02247	0.00725	0.06199	-0.01258	0.07383	0.05357	0.07830	0.07674
1484	-0.15004	-0.00077	0.04486	0.05774	-0.00463	-0.02205	0.05586	-0.01373	0.06934	0.04348	0.07495	0.07036
1485	-0.15869	-0.00111	0.03125	0.05381	-0.00906	-0.04335	0.05301	-0.01612	0.07481	0.04252	0.07309	0.06286
1486	-0.16960	-0.00290	0.02357	0.04434	-0.00844	-0.04968	0.05434	-0.01587	0.08526	0.04858	0.07116	0.05871
1487	-0.17455	-0.02071	0.02480	0.02440	-0.01810	-0.04329	0.05910	-0.01122	0.09402	0.05641	0.07017	0.06045
1488	-0.17211	-0.03144	0.02168	0.01364	-0.02288	-0.03920	0.06365	-0.00898	0.09643	0.06054	0.07462	0.06340
1489	-0.17063	-0.03099	0.01276	0.01511	-0.01993	-0.04356	0.06571	-0.00817	0.09385	0.06100	0.08131	0.06544
1490	-0.18534	-0.03965	0.01077	0.01170	-0.02304	-0.05074	0.06556	0.00082	0.09358	0.06339	0.07985	0.06825
1491	-0.20105	-0.05241	0.01429	0.00775	-0.02962	-0.05567	0.06946	0.01368	0.09822	0.06778	0.07893	0.07134
1492	-0.19372	-0.05314	0.01509	0.01525	-0.02956	-0.05528	0.08270	0.02023	0.10634	0.07133	0.09189	0.07314
1493	-0.18057	-0.04525	0.01345	0.02187	-0.02411	-0.05256	0.09068	0.02165	0.11165	0.07369	0.10184	0.07322
1494	-0.17908	-0.03861	0.01537	0.01903	-0.01950	-0.05062	0.08483	0.02212	0.11150	0.07680	0.09619	0.07404
1495	-0.18179	-0.04409	0.03316	0.02107	-0.02527	-0.04913	0.08161	0.02524	0.11400	0.08570	0.09030	0.08314
1496	-0.17993	-0.05187	0.05593	0.03037	-0.03425	-0.04605	0.08672	0.03096	0.12080	0.09571	0.09166	0.09504
1497	-0.16820	-0.03324	0.05098	0.03385	-0.02354	-0.03894	0.09108	0.03552	0.12523	0.09303	0.09501	0.09166
1498	-0.15325	-0.00304	0.03673	0.03082	-0.00421	-0.03494	0.09428	0.03772	0.12565	0.08620	0.09625	0.08129

1499	-0.14573	0.00693	0.04914	0.02802	0.00073	-0.04116	0.09970	0.03852	0.12440	0.09142	0.09388	0.08221
1500	-0.14339	0.00477	0.06690	0.03149	0.00518	-0.03964	0.10301	0.04152	0.12758	0.09973	0.09363	0.08708
1501	-0.14084	0.00463	0.06967	0.04229	0.02000	-0.02067	0.10222	0.04825	0.13619	0.10168	0.09923	0.08767
1502	-0.13414	0.00893	0.07426	0.05140	0.02705	-0.00732	0.10487	0.05405	0.13821	0.10223	0.10583	0.08953
1503	-0.12466	0.01522	0.08648	0.05373	0.02444	-0.00735	0.11054	0.05598	0.13322	0.10444	0.10955	0.09346
1504	-0.11902	0.01809	0.09508	0.05061	0.03040	-0.00769	0.10967	0.05412	0.13408	0.10703	0.10908	0.09347
1505	-0.11901	0.01957	0.09418	0.04862	0.04120	-0.00530	0.10347	0.05126	0.13830	0.10745	0.10506	0.08883
1506	-0.12302	0.02356	0.08454	0.05361	0.04332	-0.00306	0.09791	0.05007	0.13646	0.10339	0.09913	0.08208
1507	-0.12732	0.02257	0.08046	0.05536	0.03883	-0.00147	0.09108	0.04639	0.12956	0.09667	0.09258	0.07614
1508	-0.12768	0.01327	0.08829	0.04776	0.03319	0.00079	0.08231	0.03688	0.12179	0.08990	0.08735	0.07236
1509	-0.12036	0.00791	0.08952	0.04310	0.02934	0.00742	0.07821	0.02436	0.11773	0.08491	0.08660	0.06852
1510	-0.11206	0.00963	0.08263	0.04455	0.02997	0.01779	0.07891	0.01478	0.11595	0.08205	0.08640	0.06423
1511	-0.11843	0.01012	0.08649	0.04374	0.03703	0.02618	0.07694	0.01532	0.10941	0.08001	0.07650	0.06133
1512	-0.13007	0.01052	0.09827	0.04452	0.04534	0.02744	0.07208	0.01989	0.10167	0.07551	0.06435	0.05866
1513	-0.12855	0.01483	0.10498	0.05410	0.04803	0.02049	0.06743	0.01800	0.10010	0.06651	0.06294	0.05396
1514	-0.12092	0.01393	0.10643	0.06157	0.04908	0.02049	0.06129	0.01401	0.10112	0.06144	0.06378	0.04814
1515	-0.11486	0.00610	0.10638	0.05908	0.05313	0.03317	0.05399	0.01255	0.10053	0.06389	0.05993	0.04248
1516	-0.10409	0.01281	0.10908	0.05649	0.05968	0.03482	0.05278	0.01004	0.09942	0.06125	0.06062	0.03728
1517	-0.08990	0.03208	0.11515	0.06166	0.06662	0.02477	0.05640	0.00599	0.09760	0.05330	0.06505	0.03467
1518	-0.08313	0.03649	0.12145	0.07508	0.07123	0.02790	0.05447	0.00470	0.09281	0.05414	0.06077	0.03829
1519	-0.08650	0.03704	0.12796	0.07085	0.07443	0.02787	0.04976	0.01080	0.08420	0.05998	0.05265	0.04535
1520	-0.09562	0.05592	0.13552	0.02722	0.07800	-0.00058	0.04949	0.02428	0.07353	0.05940	0.05178	0.04961
1521	-0.09643	0.06354	0.14048	0.00790	0.07800	-0.01363	0.04563	0.02367	0.07050	0.05460	0.05103	0.04630
1522	-0.08402	0.04009	0.13889	0.04781	0.07137	0.01630	0.03445	0.00120	0.07815	0.05061	0.04466	0.03547
1523	-0.07846	0.01752	0.12915	0.07041	0.06052	0.04096	0.03018	-0.00970	0.08087	0.05010	0.04064	0.02630
1524	-0.08711	0.00874	0.11629	0.05619	0.05279	0.04108	0.03516	-0.00313	0.07502	0.05210	0.04151	0.02336
1525	-0.09969	-0.00001	0.11099	0.05852	0.05826	0.03823	0.03682	-0.00653	0.07157	0.05235	0.04198	0.02451
1526	-0.10571	-0.00552	0.11092	0.07155	0.06844	0.03459	0.03061	-0.01764	0.06983	0.05033	0.03800	0.02478
1527	-0.09894	0.00155	0.10913	0.06481	0.06918	0.02493	0.02008	-0.01975	0.06594	0.04821	0.02972	0.02077
1528	-0.09033	0.01075	0.11180	0.05861	0.06908	0.02596	0.02262	-0.01223	0.07338	0.05030	0.03166	0.02248
1529	-0.08734	0.01193	0.12171	0.06885	0.07397	0.04360	0.04226	-0.00189	0.09410	0.05677	0.04750	0.03327
1530	-0.08007	0.00757	0.12672	0.07187	0.07046	0.04836	0.04720	-0.00135	0.09593	0.05804	0.05000	0.03481
1531	-0.07068	0.00157	0.12408	0.06185	0.05756	0.03526	0.03235	-0.00947	0.07710	0.05260	0.03727	0.02492
1532	-0.07426	-0.00246	0.12269	0.05692	0.04942	0.02920	0.02485	-0.01089	0.07101	0.04873	0.03681	0.02073
1533	-0.07844	-0.00129	0.12455	0.06265	0.04759	0.03451	0.02906	-0.00738	0.07950	0.05024	0.04884	0.02376
1534	-0.06340	0.00528	0.12651	0.07333	0.04734	0.04288	0.03605	-0.00761	0.08820	0.05654	0.05909	0.02731
1535	-0.04747	0.00464	0.12158	0.06850	0.04990	0.04606	0.03943	-0.00565	0.09496	0.05996	0.06223	0.03009
1536	-0.04844	-0.00847	0.10990	0.04326	0.05605	0.03967	0.03737	0.00174	0.09920	0.05618	0.06051	0.03226
1537	-0.06005	-0.01659	0.10844	0.03367	0.06183	0.02767	0.03593	0.00364	0.09655	0.05195	0.06640	0.03380
1538	-0.07238	-0.01695	0.11717	0.04615	0.06111	0.01623	0.03564	-0.00157	0.08981	0.05067	0.07535	0.03352
1539	-0.07614	-0.02423	0.11663	0.05110	0.04751	0.01235	0.03089	-0.00429	0.08899	0.05054	0.06607	0.02962
1540	-0.07495	-0.03453	0.10348	0.04198	0.02964	0.01876	0.02561	-0.00494	0.09264	0.05000	0.05067	0.02739

<grating change>												
1545	-0.03766	-0.01562	-0.02561	-0.03052	-0.04048	-0.01033		0.29757	0.25846	0.19874	0.23468	0.25232	0.23478
1546	-0.03428	-0.02112	-0.02472	-0.02894	-0.04362	-0.01189		0.28305	0.24125	0.19394	0.22665	0.24511	0.22268
1547	-0.01795	-0.01734	-0.01371	-0.01600	-0.03997	-0.00113		0.30434	0.26019	0.21732	0.24592	0.27209	0.23793
1548	-0.01999	-0.01752	-0.01677	-0.01576	-0.03518	-0.00321		0.34457	0.29568	0.24495	0.26949	0.30232	0.26626
1549	-0.02653	-0.01695	-0.02497	-0.02234	-0.03277	-0.00854		0.36155	0.31226	0.25287	0.27671	0.30962	0.27830
1550	-0.01801	-0.00965	-0.02390	-0.02391	-0.03443	-0.00276		0.32592	0.28618	0.22932	0.25750	0.28268	0.25456
1551	-0.01440	-0.00878	-0.02287	-0.02675	-0.03813	-0.00032		0.28936	0.25790	0.20768	0.23777	0.25859	0.23170
1552	-0.03011	-0.02204	-0.03003	-0.03497	-0.04138	-0.01124		0.29287	0.26028	0.21198	0.23747	0.26374	0.23703
1553	-0.04403	-0.03316	-0.03735	-0.03741	-0.04286	-0.01867		0.30592	0.27148	0.21819	0.24179	0.27139	0.24353
1554	-0.04550	-0.03474	-0.04086	-0.03129	-0.04270	-0.01534		0.30229	0.26856	0.20901	0.23664	0.26274	0.23313
1555	-0.04900	-0.03917	-0.04683	-0.03080	-0.04321	-0.01571		0.28055	0.24106	0.18981	0.21790	0.24492	0.21541
1556	-0.05818	-0.04723	-0.05407	-0.03875	-0.04609	-0.02331		0.25236	0.20550	0.16955	0.19334	0.22689	0.19996
1557	-0.06303	-0.04619	-0.05315	-0.04429	-0.05196	-0.02793		0.23980	0.20345	0.15822	0.18170	0.21655	0.19320
1558	-0.06665	-0.04298	-0.04965	-0.04598	-0.05798	-0.02898		0.24296	0.22333	0.15641	0.18403	0.21423	0.19557
1559	-0.08032	-0.05624	-0.05792	-0.04912	-0.05941	-0.03242		0.24619	0.21867	0.15766	0.18829	0.21499	0.20277
1560	-0.09512	-0.07167	-0.06659	-0.05121	-0.05732	-0.03379		0.24590	0.19883	0.15693	0.18972	0.21720	0.20772
1561	-0.09695	-0.06624	-0.05850	-0.04849	-0.05606	-0.02744		0.24462	0.19521	0.15158	0.18796	0.22053	0.20437
1562	-0.10089	-0.06285	-0.05784	-0.05312	-0.06161	-0.03100		0.24326	0.20005	0.14765	0.18553	0.22182	0.20005
1563	-0.12075	-0.08435	-0.08655	-0.07399	-0.07649	-0.05718		0.24102	0.19733	0.15023	0.18415	0.21832	0.20202
1564	-0.13112	-0.09836	-0.10898	-0.08953	-0.08912	-0.07338		0.23319	0.18896	0.15061	0.17944	0.21220	0.20138
1565	-0.11750	-0.08471	-0.10027	-0.08607	-0.09205	-0.06070		0.21589	0.17752	0.14069	0.16659	0.20333	0.18909
1566	-0.11044	-0.07917	-0.08963	-0.08349	-0.09441	-0.05459		0.18936	0.15820	0.12082	0.14316	0.18386	0.16418
1567	-0.12415	-0.09709	-0.09535	-0.09301	-0.10115	-0.07093		0.16411	0.13391	0.09824	0.11734	0.15762	0.13642
1568	-0.13803	-0.11049	-0.10698	-0.10509	-0.10726	-0.08394		0.16428	0.12060	0.08828	0.11214	0.14720	0.12937
1569	-0.14382	-0.11118	-0.11808	-0.11417	-0.11322	-0.08678		0.17963	0.11906	0.08964	0.12127	0.14952	0.13776
1570	-0.14921	-0.11484	-0.12897	-0.12086	-0.12551	-0.09524		0.16591	0.11366	0.08381	0.10904	0.13503	0.12729
1571	-0.15782	-0.12377	-0.13931	-0.12723	-0.14039	-0.10939		0.13057	0.10097	0.06854	0.08147	0.10787	0.10087
1572	-0.16796	-0.12968	-0.14703	-0.13442	-0.14713	-0.11754		0.11508	0.08740	0.05381	0.07160	0.09455	0.08651
1573	-0.16329	-0.12457	-0.14166	-0.12946	-0.14034	-0.11188		0.12300	0.08261	0.04867	0.07752	0.09741	0.08824
1574	-0.13103	-0.10581	-0.11631	-0.10182	-0.12168	-0.09209		0.13988	0.09383	0.05830	0.08283	0.10694	0.09799
1575	-0.11399	-0.09748	-0.10419	-0.08931	-0.11526	-0.08640		0.15616	0.10797	0.07095	0.08645	0.11493	0.10758
1576	-0.14572	-0.11662	-0.13009	-0.12074	-0.13722	-0.11425		0.16468	0.11052	0.07389	0.08983	0.11577	0.11042
1577	-0.16861	-0.12787	-0.14725	-0.14224	-0.15263	-0.13480		0.16089	0.10424	0.06935	0.08621	0.11098	0.10540
1578	-0.14547	-0.11001	-0.12683	-0.11950	-0.13914	-0.12198		0.14809	0.09597	0.06392	0.07536	0.10476	0.09628
1579	-0.12567	-0.09669	-0.11196	-0.09894	-0.12522	-0.10981		0.14535	0.09355	0.06659	0.07499	0.10369	0.09496
1580	-0.13079	-0.09992	-0.11823	-0.10105	-0.12265	-0.11131		0.15780	0.09881	0.07712	0.08911	0.10930	0.10429
1581	-0.12525	-0.08986	-0.10759	-0.09294	-0.10919	-0.09775		0.16757	0.10476	0.08180	0.09852	0.11547	0.11258
1582	-0.10094	-0.06277	-0.07743	-0.06778	-0.08423	-0.06859		0.17464	0.11227	0.08371	0.10117	0.12303	0.11825
1583	-0.08114	-0.04320	-0.06271	-0.04828	-0.07018	-0.05299		0.19662	0.12953	0.10171	0.11273	0.13917	0.13022
1584	-0.07327	-0.03465	-0.06255	-0.03994	-0.06729	-0.04961		0.21978	0.14672	0.12536	0.12812	0.15434	0.14443
1585	-0.07249	-0.02679	-0.05372	-0.03573	-0.06158	-0.03851		0.21378	0.14498	0.12766	0.13008	0.15067	0.14904

1586	-0.07146	-0.02245	-0.04127	-0.03101	-0.05319	-0.02715	0.19207	0.13364	0.11482	0.12273	0.13697	0.14348
1587	-0.06435	-0.02768	-0.03911	-0.02386	-0.04768	-0.03028	0.18244	0.13074	0.10556	0.11793	0.13097	0.13289
1588	-0.05772	-0.03355	-0.03876	-0.01956	-0.04431	-0.03489	0.18132	0.13185	0.10295	0.11572	0.13238	0.12425
1589	-0.06046	-0.03294	-0.03215	-0.02339	-0.04224	-0.02843	0.17838	0.12833	0.10417	0.11286	0.13505	0.12210
1590	-0.07669	-0.03901	-0.03467	-0.03356	-0.04654	-0.02714	0.17251	0.12021	0.10312	0.10724	0.13202	0.12142
1591	-0.10194	-0.05710	-0.05371	-0.04579	-0.05799	-0.04042	0.16428	0.11012	0.09619	0.09778	0.12155	0.11744
1592	-0.11611	-0.06791	-0.07038	-0.05375	-0.06600	-0.05159	0.15380	0.10228	0.08646	0.08505	0.11304	0.10988
1593	-0.11667	-0.06803	-0.07753	-0.05777	-0.06888	-0.05514	0.14055	0.09531	0.07586	0.07162	0.10787	0.09934
1594	-0.12791	-0.07993	-0.08880	-0.06759	-0.07904	-0.06546	0.12340	0.08006	0.06354	0.06223	0.09458	0.08695
1595	-0.15474	-0.10528	-0.10707	-0.08380	-0.09769	-0.08375	0.10474	0.05737	0.04878	0.05382	0.07431	0.07530
1596	-0.18229	-0.12528	-0.12404	-0.09833	-0.11487	-0.09804	0.08994	0.03781	0.03140	0.03681	0.06028	0.06770
1597	-0.20734	-0.14146	-0.14153	-0.11396	-0.12998	-0.11024	0.07831	0.02538	0.01332	0.01592	0.05249	0.06058
1598	-0.23412	-0.16710	-0.16667	-0.13876	-0.14830	-0.13003	0.06539	0.01816	-0.00272	0.00305	0.04267	0.04705
1599	-0.26140	-0.19877	-0.19416	-0.16503	-0.17053	-0.15441	0.04893	0.00472	-0.01832	-0.00803	0.02863	0.02974
1600	-0.28901	-0.22932	-0.21820	-0.18463	-0.19684	-0.17830	0.02787	-0.02587	-0.03690	-0.02884	0.01054	0.01370
1601	-0.33352	-0.26954	-0.25711	-0.22060	-0.23483	-0.21383	0.00164	-0.06259	-0.06124	-0.05751	-0.01313	-0.00486
1602	-0.40040	-0.32442	-0.31967	-0.28572	-0.28509	-0.26703	-0.02889	-0.09196	-0.09129	-0.08811	-0.04250	-0.02916
1603	-0.44692	-0.36564	-0.36478	-0.33446	-0.32060	-0.31035	-0.05910	-0.11250	-0.11902	-0.11429	-0.07183	-0.05304
1604	-0.46351	-0.38791	-0.38163	-0.35156	-0.33802	-0.33619	-0.08846	-0.13123	-0.14331	-0.13735	-0.09899	-0.07546
1605	-0.52382	-0.44378	-0.43783	-0.40326	-0.39086	-0.38873	-0.12590	-0.16726	-0.17956	-0.17366	-0.13120	-0.10899
1606	-0.64277	-0.54541	-0.54670	-0.50552	-0.48928	-0.47763	-0.17286	-0.22336	-0.23224	-0.22570	-0.17200	-0.15650
1607	-0.74440	-0.64199	-0.63761	-0.59476	-0.57715	-0.55844	-0.21916	-0.27853	-0.28805	-0.27501	-0.21801	-0.20540
1608	-0.79752	-0.70471	-0.68634	-0.64531	-0.63081	-0.60920	-0.25558	-0.31828	-0.32990	-0.31102	-0.25837	-0.24279
1609	-0.81932	-0.73150	-0.71652	-0.67203	-0.66147	-0.63395	-0.27639	-0.33772	-0.34193	-0.33309	-0.27837	-0.25889
1610	-0.83602	-0.74423	-0.74319	-0.69121	-0.68438	-0.65364	-0.29631	-0.35451	-0.34913	-0.35483	-0.29322	-0.27178
1611	-0.87523	-0.77578	-0.77539	-0.71918	-0.71577	-0.69536	-0.33759	-0.39431	-0.39269	-0.39416	-0.33103	-0.31052
1612	-0.94276	-0.83474	-0.82611	-0.77279	-0.76668	-0.75842	-0.38496	-0.44072	-0.44741	-0.43785	-0.37704	-0.35847
1613	-1.02901	-0.91285	-0.90080	-0.85720	-0.83834	-0.82779	-0.41246	-0.46585	-0.47061	-0.46414	-0.40440	-0.38621
1614	-1.09692	-0.97341	-0.96359	-0.92469	-0.89818	-0.87737	-0.41727	-0.47034	-0.46784	-0.47214	-0.41367	-0.39415
1615	-1.11866	-0.98880	-0.98325	-0.93722	-0.91847	-0.89020	-0.40492	-0.46162	-0.45507	-0.46674	-0.41072	-0.38972
1616	-1.11477	-0.98023	-0.97494	-0.92698	-0.91257	-0.88446	-0.38613	-0.44374	-0.43955	-0.45278	-0.39474	-0.37666
1617	-1.10275	-0.96638	-0.95559	-0.91826	-0.89525	-0.87414	-0.36640	-0.42159	-0.42401	-0.43294	-0.36925	-0.35828
1618	-1.07774	-0.94416	-0.92946	-0.89647	-0.86997	-0.85317	-0.33955	-0.40253	-0.40543	-0.40596	-0.34793	-0.33817
1619	-1.03735	-0.90827	-0.89458	-0.85397	-0.83744	-0.81875	-0.30466	-0.38303	-0.38013	-0.37227	-0.32978	-0.31464
1620	-0.98555	-0.85419	-0.84347	-0.79778	-0.79640	-0.77511	-0.26902	-0.34627	-0.34474	-0.33499	-0.29456	-0.27978
1621	-0.92337	-0.78539	-0.78089	-0.73356	-0.74372	-0.72414	-0.23430	-0.29622	-0.30206	-0.29718	-0.24490	-0.23718
1622	-0.85057	-0.71275	-0.72134	-0.66572	-0.67657	-0.66610	-0.19689	-0.25422	-0.26003	-0.26141	-0.20324	-0.19998
1623	-0.78506	-0.65081	-0.66468	-0.60695	-0.61167	-0.61028	-0.15598	-0.22183	-0.22311	-0.22788	-0.17431	-0.16998
1624	-0.74869	-0.61225	-0.60529	-0.56944	-0.57062	-0.56757	-0.11358	-0.18920	-0.19262	-0.19485	-0.15058	-0.14186
1625	-0.71674	-0.58432	-0.56141	-0.52900	-0.52955	-0.52283	-0.07882	-0.15270	-0.16390	-0.15756	-0.11709	-0.10973
1626	-0.65983	-0.54837	-0.54800	-0.46124	-0.46144	-0.46065	-0.05877	-0.11306	-0.13185	-0.11396	-0.06508	-0.07115
1627	-0.60820	-0.50427	-0.52538	-0.40304	-0.40379	-0.40901	-0.03987	-0.07847	-0.09941	-0.07855	-0.02433	-0.03892
1628	-0.58873	-0.45893	-0.46569	-0.38446	-0.38827	-0.38962	-0.01102	-0.05498	-0.07035	-0.06209	-0.01632	-0.02226

1629	-0.57581	-0.42515	-0.41293	-0.37264	-0.38372	-0.37584	0.01721	-0.03745	-0.04471	-0.05325	-0.01189	-0.00948
1630	-0.55340	-0.40684	-0.39391	-0.34572	-0.36532	-0.34966	0.03665	-0.02182	-0.02400	-0.04172	0.00678	0.00729
1631	-0.53875	-0.39012	-0.38211	-0.32114	-0.33927	-0.32372	0.05022	-0.00957	-0.01329	-0.02622	0.02139	0.02249
1632	-0.53364	-0.36958	-0.36260	-0.30560	-0.31429	-0.30467	0.06006	-0.00313	-0.01013	-0.01191	0.02356	0.03263
1633	-0.51769	-0.35225	-0.34152	-0.28798	-0.29747	-0.28783	0.06587	-0.00489	-0.00300	-0.00987	0.02210	0.03851
1634	-0.49549	-0.34071	-0.32057	-0.26770	-0.28546	-0.27205	0.06851	-0.00797	0.00713	-0.01529	0.02679	0.04202
1635	-0.49095	-0.33290	-0.29770	-0.25340	-0.26780	-0.25960	0.06960	0.00027	0.00965	-0.01165	0.04503	0.04549
1636	-0.49837	-0.32548	-0.28221	-0.24713	-0.25057	-0.25103	0.06801	0.01143	0.00827	-0.00288	0.06095	0.04944
1637	-0.49837	-0.31611	-0.28594	-0.24609	-0.24640	-0.24617	0.06237	0.00944	0.01259	-0.00215	0.05212	0.05356
1638	-0.49558	-0.31238	-0.29509	-0.24214	-0.24832	-0.24709	0.06031	0.00676	0.01584	-0.00524	0.03836	0.05897
1639	-0.50057	-0.32165	-0.29283	-0.22998	-0.24578	-0.25401	0.06858	0.01875	0.01014	-0.00358	0.04556	0.06654
1640	-0.51042	-0.33467	-0.28966	-0.22402	-0.24405	-0.25633	0.07677	0.02808	0.00857	0.00158	0.05831	0.07378
1641	-0.52217	-0.34239	-0.29619	-0.23445	-0.24895	-0.25020	0.07679	0.02234	0.02038	0.00761	0.06025	0.07813
1642	-0.54147	-0.34715	-0.30546	-0.24777	-0.25736	-0.25614	0.07800	0.02315	0.03121	0.01469	0.05953	0.07895
1643	-0.56681	-0.35181	-0.31358	-0.25453	-0.26413	-0.27801	0.08593	0.03941	0.03369	0.02162	0.06360	0.07883
1644	-0.58213	-0.35675	-0.32644	-0.25879	-0.26330	-0.28450	0.09477	0.04881	0.03893	0.02423	0.07168	0.08517
1645	-0.58232	-0.35726	-0.33578	-0.25694	-0.25531	-0.26782	0.10137	0.04700	0.04968	0.02487	0.08111	0.09702
1646	-0.57609	-0.34334	-0.31726	-0.23576	-0.24754	-0.25102	0.10712	0.05326	0.05700	0.03337	0.08820	0.10366
1647	-0.55743	-0.31294	-0.27758	-0.19937	-0.23606	-0.23874	0.11402	0.06537	0.05852	0.04779	0.09477	0.10517
1648	-0.51181	-0.27171	-0.24619	-0.16563	-0.20955	-0.22008	0.12357	0.06541	0.05794	0.05758	0.10594	0.10987
1649	-0.46319	-0.23472	-0.22265	-0.14437	-0.17676	-0.19254	0.13054	0.06261	0.06071	0.06326	0.11582	0.11713
1650	-0.44722	-0.21817	-0.19357	-0.13774	-0.15430	-0.15983	0.12926	0.07637	0.07153	0.07069	0.11580	0.12236
1651	-0.44260	-0.21491	-0.16866	-0.12974	-0.13931	-0.13374	0.13351	0.09616	0.08552	0.07991	0.11740	0.12788
1652	-0.41942	-0.21127	-0.15990	-0.10550	-0.12417	-0.12356	0.15477	0.10584	0.09550	0.08891	0.13274	0.13673
1653	-0.39484	-0.20168	-0.15526	-0.07968	-0.11033	-0.11807	0.16864	0.10996	0.09904	0.09574	0.14807	0.14503
1654	-0.38988	-0.18662	-0.14434	-0.06817	-0.10110	-0.10757	0.15644	0.11495	0.09707	0.09974	0.15047	0.14942
1655	-0.40717	-0.17705	-0.13501	-0.07225	-0.09898	-0.09827	0.13521	0.11976	0.09617	0.10332	0.14451	0.15187

Table III. Global analysis data for 3HF and 3HTC. The collective spectral data for each compound at each frequency over time (0.2-10 ps) were fit using Nonlinear Curve Fit-Global Fitting in Origin with 5 cm^{-1} resolution. Output consists of a static profile (A_0) and a shorter-lived profile (A_1) which follows a monoexponential decay at a constant value determined by the fit (t_1).

Global Analysis	3HF						3HTC					
Frequency (cm^{-1})	A_0 Value	A_0 Std. Error	A_1 Value	A_1 Std. Error	t_1 Value	t_1 Std. Error	A_0 Value	A_0 Std. Error	A_1 Value	A_1 Std. Error	t_1 Value	t_1 Std. Error
1245	0.34030	0.00433	0.04064	0.00967	1073.77666	70.90087	0.22195	0.00547	0.01226	0.00856	3207.06984	173.88538
1250	0.32395	0.00432	0.02302	0.00965	1073.77666	70.90087	0.22313	0.00548	0.02813	0.00856	3207.06984	173.88538
1255	0.31447	0.00432	0.03384	0.00966	1073.77666	70.90087	0.21560	0.00551	0.04462	0.00857	3207.06984	173.88538
1260	0.32193	0.00432	0.03489	0.00966	1073.77666	70.90087	0.19964	0.00552	0.04872	0.00857	3207.06984	173.88538
1265	0.31946	0.00432	0.01871	0.00965	1073.77666	70.90087	0.18969	0.00553	0.05178	0.00857	3207.06984	173.88538
1270	0.33694	0.00432	0.01139	0.00965	1073.77666	70.90087	0.19188	0.00554	0.05622	0.00857	3207.06984	173.88538
1275	0.34522	0.00432	0.00613	0.00964	1073.77666	70.90087	0.21300	0.00548	0.02488	0.00856	3207.06984	173.88538
1280	0.38232	0.00432	-0.02102	0.00965	1073.77666	70.90087	0.22424	0.00547	-0.02101	0.00856	3207.06984	173.88538
1285	0.44166	0.00432	-0.03372	0.00966	1073.77666	70.90087	0.21572	0.00553	-0.05034	0.00857	3207.06984	173.88538
1290	0.51981	0.00434	-0.06149	0.00969	1073.77666	70.90087	0.19885	0.00558	-0.06796	0.00858	3207.06984	173.88538
1295	0.55842	0.00434	-0.05823	0.00969	1073.77666	70.90087	0.25379	0.00569	-0.09527	0.00860	3207.06984	173.88538
1300	0.54709	0.00433	-0.04163	0.00967	1073.77666	70.90087	0.40775	0.00595	-0.14101	0.00866	3207.06984	173.88538
1305	0.48115	0.00432	-0.01346	0.00965	1073.77666	70.90087	0.59093	0.00636	-0.19449	0.00874	3207.06984	173.88538
1310	0.38861	0.00432	0.01920	0.00965	1073.77666	70.90087	0.68492	0.00646	-0.20664	0.00877	3207.06984	173.88538
1315	0.29482	0.00433	0.04902	0.00967	1073.77666	70.90087	0.63772	0.00601	-0.14950	0.00867	3207.06984	173.88538
1320	0.23247	0.00434	0.06349	0.00970	1073.77666	70.90087	0.56471	0.00565	-0.08550	0.00859	3207.06984	173.88538
1325	0.23272	0.00434	0.05607	0.00968	1073.77666	70.90087	0.57006	0.00554	-0.05391	0.00857	3207.06984	173.88538
1330	0.29174	0.00432	0.03341	0.00966	1073.77666	70.90087	0.60027	0.00553	-0.05322	0.00857	3207.06984	173.88538
1335	0.36292	0.00432	-0.01089	0.00965	1073.77666	70.90087	0.58140	0.00551	-0.04306	0.00857	3207.06984	173.88538
1340	0.40432	0.00432	-0.03215	0.00966	1073.77666	70.90087	0.45131	0.00546	-0.00506	0.00856	3207.06984	173.88538
1345	0.37934	0.00432	-0.02985	0.00966	1073.77666	70.90087	0.29866	0.00551	0.04227	0.00857	3207.06984	173.88538
1350	0.31442	0.00432	-0.00358	0.00964	1073.77666	70.90087	0.19339	0.00561	0.07653	0.00859	3207.06984	173.88538
1355	0.18208	0.00443	0.12974	0.00986	1073.77666	70.90087	0.12983	0.00564	0.08432	0.00859	3207.06984	173.88538
1360	0.17436	0.00439	0.10314	0.00978	1073.77666	70.90087	0.14973	0.00570	0.09688	0.00860	3207.06984	173.88538
1365	0.17707	0.00435	0.07293	0.00971	1073.77666	70.90087	0.18634	0.00576	0.10955	0.00862	3207.06984	173.88538
1370	0.20077	0.00432	0.02667	0.00965	1073.77666	70.90087	0.22940	0.00594	0.13980	0.00865	3207.06984	173.88538
1375	0.20668	0.00432	0.00453	0.00964	1073.77666	70.90087	0.27572	0.00604	0.15409	0.00867	3207.06984	173.88538
1380	0.15831	0.00432	0.03296	0.00966	1073.77666	70.90087	0.29743	0.00593	0.13796	0.00865	3207.06984	173.88538
1385	0.11927	0.00433	0.04869	0.00967	1073.77666	70.90087	0.33905	0.00557	0.06499	0.00858	3207.06984	173.88538
1390	0.08197	0.00434	0.06295	0.00969	1073.77666	70.90087	0.33703	0.00548	0.02503	0.00856	3207.06984	173.88538
1395	0.05865	0.00434	0.06375	0.00970	1073.77666	70.90087	0.34261	0.00547	-0.01882	0.00856	3207.06984	173.88538
1400	0.02532	0.00434	0.05792	0.00969	1073.77666	70.90087	0.34356	0.00551	-0.04458	0.00857	3207.06984	173.88538
1405	-0.03278	0.00433	0.04877	0.00967	1073.77666	70.90087	0.27589	0.00552	-0.04949	0.00857	3207.06984	173.88538
1410	-0.11323	0.00432	0.03300	0.00966	1073.77666	70.90087	0.13850	0.00549	-0.03435	0.00856	3207.06984	173.88538

1415	-0.19779	0.00432	0.02005	0.00965	1073.77666	70.90087	-0.00803	0.00548	-0.02387	0.00856	3207.06984	173.88538
1420	-0.21309	0.00432	0.00984	0.00965	1073.77666	70.90087	-0.12322	0.00547	-0.01590	0.00856	3207.06984	173.88538
1425	-0.14117	0.00432	0.01261	0.00965	1073.77666	70.90087	-0.26071	0.00547	-0.02075	0.00856	3207.06984	173.88538
1430	-0.02601	0.00432	0.01206	0.00965	1073.77666	70.90087	-0.34670	0.00548	-0.02795	0.00856	3207.06984	173.88538
1435	0.08093	0.00432	0.00670	0.00964	1073.77666	70.90087	-0.26305	0.00548	-0.02700	0.00856	3207.06984	173.88538
1440	0.15361	0.00432	0.00151	0.00964	1073.77666	70.90087	-0.06596	0.00547	-0.01112	0.00856	3207.06984	173.88538
1445	0.17363	0.00432	-0.01181	0.00965	1073.77666	70.90087	0.10005	0.00546	-0.00442	0.00856	3207.06984	173.88538
1450	0.13607	0.00432	-0.02603	0.00965	1073.77666	70.90087	0.17759	0.00547	-0.01706	0.00856	3207.06984	173.88538
1455	0.11102	0.00433	-0.04809	0.00967	1073.77666	70.90087	0.21344	0.00553	-0.05093	0.00857	3207.06984	173.88538
1460	0.13998	0.00436	-0.08451	0.00973	1073.77666	70.90087	0.26083	0.00570	-0.09757	0.00860	3207.06984	173.88538
1465	0.18198	0.00440	-0.10899	0.00979	1073.77666	70.90087	0.29604	0.00597	-0.14348	0.00866	3207.06984	173.88538
1470	0.18648	0.00438	-0.09656	0.00976	1073.77666	70.90087	0.27571	0.00597	-0.14359	0.00866	3207.06984	173.88538
1475	0.13595	0.00432	-0.03732	0.00966	1073.77666	70.90087	0.21258	0.00578	-0.11254	0.00862	3207.06984	173.88538
1480	0.05655	0.00432	0.02319	0.00965	1073.77666	70.90087	0.13225	0.00562	-0.07996	0.00859	3207.06984	173.88538
1485	-0.00982	0.00433	0.04068	0.00967	1073.77666	70.90087	0.08348	0.00555	-0.05966	0.00858	3207.06984	173.88538
1490	-0.03796	0.00433	0.04579	0.00967	1073.77666	70.90087	0.09302	0.00552	-0.04581	0.00857	3207.06984	173.88538
1495	-0.03044	0.00433	0.04422	0.00967	1073.77666	70.90087	0.10171	0.00549	-0.03327	0.00856	3207.06984	173.88538
1500	-0.00448	0.00433	0.05332	0.00968	1073.77666	70.90087	0.10990	0.00548	-0.02244	0.00856	3207.06984	173.88538
1505	0.02445	0.00433	0.04398	0.00967	1073.77666	70.90087	0.11205	0.00547	-0.01711	0.00856	3207.06984	173.88538
1510	0.03515	0.00432	0.02975	0.00966	1073.77666	70.90087	0.08731	0.00547	-0.01381	0.00856	3207.06984	173.88538
1515	0.05035	0.00432	0.01801	0.00965	1073.77666	70.90087	0.06903	0.00547	-0.01381	0.00856	3207.06984	173.88538
1520	0.06426	0.00432	0.02507	0.00965	1073.77666	70.90087	0.05692	0.00546	-0.01000	0.00856	3207.06984	173.88538
1525	0.05989	0.00432	0.01303	0.00965	1073.77666	70.90087	0.04929	0.00547	-0.01412	0.00856	3207.06984	173.88538
1530	0.06739	0.00432	0.01546	0.00965	1073.77666	70.90087	0.05909	0.00547	-0.01651	0.00856	3207.06984	173.88538
1535	0.05843	0.00432	0.02008	0.00965	1073.77666	70.90087	0.06176	0.00547	-0.01726	0.00856	3207.06984	173.88538
1540	0.03914	0.00432	0.00589	0.00964	1073.77666	70.90087	0.05942	0.00548	-0.02607	0.00856	3207.06984	173.88538
1545	-0.03115	0.00432	0.01620	0.00965	1073.77666	70.90087	0.21276	0.00550	0.03716	0.00856	3207.06984	173.88538
1550	-0.02474	0.00432	0.01115	0.00965	1073.77666	70.90087	0.23982	0.00549	0.03504	0.00856	3207.06984	173.88538
1555	-0.03595	0.00432	-0.00103	0.00964	1073.77666	70.90087	0.20979	0.00548	0.02251	0.00856	3207.06984	173.88538
1560	-0.05208	0.00432	-0.01013	0.00965	1073.77666	70.90087	0.18718	0.00546	0.00824	0.00856	3207.06984	173.88538
1565	-0.08246	0.00432	-0.00893	0.00965	1073.77666	70.90087	0.16875	0.00546	0.00017	0.00856	3207.06984	173.88538
1570	-0.12004	0.00432	-0.00475	0.00964	1073.77666	70.90087	0.11367	0.00546	0.00050	0.00856	3207.06984	173.88538
1575	-0.10659	0.00432	0.01012	0.00965	1073.77666	70.90087	0.09670	0.00546	0.00312	0.00856	3207.06984	173.88538
1580	-0.12170	0.00432	0.02751	0.00965	1073.77666	70.90087	0.09300	0.00547	0.01157	0.00856	3207.06984	173.88538
1585	-0.05547	0.00432	0.02328	0.00965	1073.77666	70.90087	0.13344	0.00547	0.01975	0.00856	3207.06984	173.88538
1590	-0.04213	0.00432	0.00235	0.00964	1073.77666	70.90087	0.11429	0.00546	0.01004	0.00856	3207.06984	173.88538
1595	-0.09238	0.00432	-0.01720	0.00965	1073.77666	70.90087	0.06667	0.00546	-0.00158	0.00856	3207.06984	173.88538
1600	-0.18945	0.00432	-0.03764	0.00966	1073.77666	70.90087	0.00523	0.00548	-0.02586	0.00856	3207.06984	173.88538
1605	-0.39375	0.00434	-0.05509	0.00968	1073.77666	70.90087	-0.12530	0.00551	-0.04527	0.00857	3207.06984	173.88538
1610	-0.67796	0.00435	-0.06834	0.00970	1073.77666	70.90087	-0.29033	0.00555	-0.06009	0.00858	3207.06984	173.88538
1615	-0.91675	0.00437	-0.08634	0.00974	1073.77666	70.90087	-0.39626	0.00556	-0.06087	0.00858	3207.06984	173.88538
1620	-0.79474	0.00434	-0.05475	0.00968	1073.77666	70.90087	-0.28951	0.00550	-0.03959	0.00857	3207.06984	173.88538
1625	-0.52902	0.00432	-0.03583	0.00966	1073.77666	70.90087	-0.11096	0.00548	-0.02723	0.00856	3207.06984	173.88538

1630	-0.35598	0.00432	-0.03659	0.00966	1073.77666	70.90087	0.00510	0.00547	-0.02063	0.00856	3207.06984	173.88538
1635	-0.26959	0.00433	-0.04550	0.00967	1073.77666	70.90087	0.04109	0.00548	-0.02823	0.00856	3207.06984	173.88538
1640	-0.24862	0.00433	-0.05157	0.00968	1073.77666	70.90087	0.06377	0.00549	-0.03418	0.00856	3207.06984	173.88538
1645	-0.26462	0.00434	-0.06577	0.00970	1073.77666	70.90087	0.09222	0.00550	-0.03874	0.00856	3207.06984	173.88538
1650	-0.15055	0.00433	-0.04855	0.00967	1073.77666	70.90087	0.12724	0.00550	-0.03820	0.00856	3207.06984	173.88538
1655	-0.09698	0.00433	-0.04434	0.00967	1073.77666	70.90087	0.15965	0.00550	-0.03781	0.00856	3207.06984	173.88538

V. References

1. S. Gunduz, A. C. Goren and T. Ozturk, *Org. Lett*., 2012, **14**, 1576-1579.

2. F. Neese, F. Wennmohs, U. Becker and C. Riplinger, The ORCA quantum chemistry program package, *J. Chem. Phys*., 2020, **152**, 224108.

3. C. T. Lee, W. T. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys*., 1988, **37**, 785–789.

4. R. A. Kendall, T. H. Dunning, Jr. and R. J. Harrison, *J. Chem. Phys*., 1992, **96**, 6796.

5. D. E. Woon and T. H. Dunning, Jr., *J. Chem. Phys*., 1993, **98**, 1358.

6. F. Weigend, *Phys. Chem. Chem. Phys*., 2006, **8**, 1057.

7. S.Grimme, J.Antony, S.Ehrlich and H.Krieg, *J. Chem. Phys*., 2010, **132**, 154104.

8. S.Grimme, S.Ehrlich and L.Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.