OS100: A Benchmark Set of 100 Digitized UV-Visible Spectra and Derived Experimental Oscillator Strengths

Astrid S. Tarleton^a, Jorge C. Garcia-Alvarez^a, Anah Wynn^a, Cade M. Awbrey^a, Tomas P. Roberts^a,
Samer Gozem^{a*}

^aDepartment of Chemistry, Georgia State University, Atlanta, GA 30302, United States.

*To whom correspondence should be addressed: sgozem@gsu.edu.

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ABSTRACT

Excited-state quantum chemical calculations typically report excitation energies and oscillator strengths, f , for each electronic transition. On the other hand, UV-visible spectrophotometric experiments report energy-dependent molar extinction/attenuation coefficients, $\epsilon(\nu)$, that determine the absorption band line shapes. $\epsilon(\nu)$ and f are related, but this relation is complicated by various broadening and solvation effects. We fit and integrated experimental UV-visible spectra to obtain f_{exp} values for absorption bands and estimated the uncertainty in the fitting. We derived 164 f_{exp} values from 100 organic molecules ranging in size from 6-34 atoms. The corresponding computed oscillator strengths (f_{comp}) were obtained with time-dependent density functional theory and a polarizable continuum solvent model. By expressing experimental and computed absorption strengths using a common quantity, we directly compared f_{comp} and f_{exp} . While f_{comp} and f_{exp} are well correlated (linear regression $R^2=0.921$), f_{comp} in most cases significantly overestimates f_{exp} (regression slope=1.34). The agreement between absolute f_{comp} and f_{exp} values was substantially improved by accounting for a solvent refractive index factor, as suggested in some derivations in the literature. The 100 digitized UV-visible spectra are included as plain text files in the supporting information to aid in benchmarking computational or machine-learning approaches that aim to simulate realistic UV-visible absorption spectra.

INTRODUCTION

UV-visible spectrophotometry reports the range of frequencies of light absorbed by a sample and the strength of that absorbance. The former may be reported as energies, frequencies (ν), wavelengths (λ), or wavenumbers ($\tilde{\nu}$). The latter, the absorption strength, is typically reported using the molar attenuation coefficient (ϵ), an intensive property that appears in the Beer-Lambert law,¹ or the closely related photoabsorption cross section.

Excited-state quantum chemical methods have reached an evident level of maturity in predicting excitation energies. The effort to improve these predictions continues, but hundreds of studies indicate that it is possible to predict energy of maximal absorption to a fraction of an eV.² For instance, an extensive benchmark of time-dependent density functional theory (TD-DFT) vertical excitation energies indicates typical errors of ~ 0.15 - 0.25 eV for $\pi \rightarrow \pi^*$ transitions in organic dyes.³ These errors can be reduced to chemical accuracy (< 1 kcal/mol or < 0.043 eV) by going beyond the vertical approximation and using high-level excited-state *ab initio* methods.³⁻⁶

In comparison, there is a limited understanding of how well quantum chemical calculations can predict absorption strengths. This is not due to a lack of interest; predicting strengths is arguably as essential as predicting energies, with important applications in the design of dyes and in the identification and quantification of analytes, for instance.⁷⁻¹¹ However, comparing computed and experimental absorption strengths is not straightforward. In computations, transition strengths for each electronic transition are often represented by a single value (typically, an oscillator strength or a transition dipole moment). On the other hand, due to broadening effects, molecules absorb light at a range of frequencies. Often, experiments report the point of highest absorbance for each absorption band (ϵ_{max}) and the corresponding frequency (ν at ϵ_{max}). However, the values of ϵ_{max} and ν at ϵ_{max} are affected by broadening and solvent effects that modulate the width, and therefore also the height, of the absorption bands (see **Fig. 1**).^{12, 13}

Figure 1. Line broadening in absorption spectra. Top panels show schematic UV-visible absorption spectra, while the bottom diagrams illustrate the corresponding transitions. In gas-phase atoms (left), where broadening is caused by lifetime, Doppler, and pressure effects, absorption lines typically appear sharp. Molecular spectra (center) are additionally broadened by vibrational and rotational energy levels, but the vibronic peaks may still be resolved, particularly in rigid gas-phase systems. In conformationally flexible or condensed-phase systems (right) each transition in the absorption spectrum appears as a broad band. In all cases, the total probability of the transition occurring is related to the area under the band for that transition (represented using f_1 and f_2 for each band).

The total probability for a molecule to get promoted to an electronically excited state is related to the integral of the attenuation coefficient over the full range of wavenumbers for that band. A single-valued experimental oscillator strength (f_{exp}) for each band in the UV-visible spectrum can be obtained by integrating $\epsilon(\tilde{\nu})$ over the range of wavenumbers, $\tilde{\nu}$, for the band, giving the area under that band (**Fig. 1**):¹⁴

$$f_{exp} = \frac{10^3 \ln(10) m_e c^2}{N_A \pi e^2} \int \epsilon(\tilde{\nu}) d\tilde{\nu} = (4.319 \times 10^{-9} \text{ M cm}^2) \int \epsilon(\tilde{\nu}) d\tilde{\nu} \quad (2)$$

In equation (2), m_e is the mass of the electron, c the speed of light in vacuum, N_A is Avogadro's constant, and e is the elementary charge. The numerical value in the second equality can be used when $\epsilon(\tilde{\nu})$ and $\tilde{\nu}$ are in units of $\text{M}^{-1}\text{cm}^{-1}$ and cm^{-1} , respectively. The limits of integration should go over the range of wavenumbers for the band of interest. This is trivial for well-defined and separated bands like those shown in Fig. 1, but for overlapping bands where multiple transitions

contribute to absorbance at a common wavenumber, it becomes necessary to find a way to perform the integration in equation (2) for a specified band. This is discussed further in the Methodology section.

The oscillator strength can also be derived from quantum mechanically computed transition dipole moments:¹⁵

$$f_{comp} = \frac{4\pi m_e \nu}{3\hbar} |\langle \psi_I | \mathbf{r} | \psi_F \rangle|^2 \quad (3)$$

In equation (3), ν is the frequency for the transition, $\hbar$ is the reduced Planck constant, and $\langle \psi_I | \mathbf{r} | \psi_F \rangle$ is the transition dipole moment connecting the initial (ψ_I) and final (ψ_F) electronic state wave functions. When multiple transitions contribute to a band in a UV-visible spectrum, it is possible to sum equation (3) for several final state transitions.

Equations (2) and (3) give experimental and computed oscillator strengths, respectively, in a common quantity that is directly comparable. However, very few experimental studies report f_{exp} , while even fewer report the protocol used to derive f_{exp} from the UV-visible absorption spectrum. Therefore, most existing benchmark studies employ high-level *ab initio* methods as the reference, rather than using an experimental reference.² There is still limited understanding of how computed oscillator strength calculations compare to experimental ones.

Compounding the difficulty in comparing computations and experiments is that equations (2) and (3) were derived for systems *in vacuo* and are not exact for molecules in solution. Specifically, accounting for the refractive index of the solvent (n) is necessary in one or in both equations. How to do that is a topic of debate starting from the 1930s¹⁶ that remains unresolved. For instance, reports in the literature often use equation (2) as-is,¹⁷⁻²⁰ while others have multiplied equation (2) by factors of n^{-2} ,^{21, 22} n^{-1} ,^{23, 24} n ,²⁵⁻²⁷ or some more complicated function of n .²⁸⁻³² In this manuscript, we start with the assumption that calculations using a polarizable continuum model (PCM) to account for the effect of solvation on vertical excitation already account for the effect of refractive index on oscillator strength (see Methodology). We also initially use equation (2) as-is to derive the experimental oscillator strengths. We then discuss the effect of the refractive index after presenting the results.

In a 2013 review on TD-DFT benchmarks, Laurent and Jacquemin cited several studies that included oscillator strength benchmarks up to that time.² Most of these studies focused on a few molecules, and compared computed oscillator strengths with other theoretical results, or a mix of theory and experiments. A number of studies since then have focused on comparing TD-DFT

calculations with high-level *ab-initio* calculations for small molecules.^{33, 34} The most extensive validation against experiments, to our knowledge, was published by Jacquemin *et al.*³⁵ for a series of thirty related anthraquinones.³⁶

We collected and digitized one-hundred solution-phase UV/visible spectra of organic molecules ranging in size from 6-34 atoms. The systems range in type from simple unsaturated hydrocarbons to larger heteroatomic chromophores like substituted azobenzenes. This includes a few sulfur, phosphorous, and halogen-containing molecules (no heavier than bromine). Out of the 100 molecules, 19 are molecular anions and 12 are molecular cations. We refer to the benchmark set as OS100. We note that there is no relation to the GW100 benchmark of ionization potentials and electron affinities,³⁷ only that both sets of benchmarks include 100 molecules. The 100 UV-visible spectra were all obtained from a common source, the UV Atlas of organic compounds.³⁸ The UV Atlas is one of the resources used by the NIST online database, and reports experimental details including the solvent, concentration at which the spectra were taken, and spectral resolution for the all the measurements. 164 f_{exp} values were derived from well-defined bands appearing in these spectra. The following sections introduce the benchmark set and describe the fitting and scoring system. TD-DFT calculations are presented with a popular functional, B3LYP, to provide a preliminary comparison of f_{exp} and f_{comp} . More extensive benchmarking with other functionals and wave function methods is left to future work. The TD-B3LYP f_{comp} values are well-correlated with f_{exp} (linear regression $R^2=0.921$), but they systematically overestimate the oscillator strength (regression slope=1.34). This large slope could potentially be explained by a refractive index factor missing in equations (2) and/or (3).

METHODOLOGY

Figure 2. A schematic figure of the protocol used to derive oscillator strengths from experimental UV/vis spectra. See text for details.

The protocol to obtain f_{exp} from UV-visible spectra is schematically shown in **Fig. 2**. The UV-visible spectra were digitized (panel **B**) and numerically integrated using the midpoint method (panel **C**) to find the areas under each band. The limits of the numerical integration were set as the minima in ϵ at the low and high energy range of each band when a band can be distinctly identified. Bands with an oscillator strength below 0.01 were not considered. From here on, we refer to values of f_{exp} obtained by numerical integration as $f_{exp,n}$. In cases of incomplete or overlapping bands (like the example in **Fig. 2**), numerical integration does not correctly treat the overlap region; it accounts for spillover from nearby bands and/or misses part of the band that is outside of the numerical integration window. This error is in addition to numerical errors associated with finite-width

midpoint rule integration. However, in case of well-separated bands (like those in **Fig. 1** right), $f_{exp,n}$ is expected to be a good approximation for f_{exp} .

In addition to numerical integration, the UV-visible spectra were analytically integrated after curve fitting. Since multiple factors contribute to broadening of UV-visible spectra, neither a single Voigt function nor a single Gaussian function could accurately fit the absorption bands. Therefore, initially, the spectra were fit using a minimal number of Gaussian curves to describe overlap regions between bands (see panels **D**, **E1**, and **E2**). Then, for each band, the area under the curve was fit using an increasing number of Gaussian curves while freezing the fits for the nearby overlapping bands, until convergence (panels **F1** and **F2**). Convergence was monitored using the normalized root-mean-square deviation (%nRMSD, defined in Sources of Error). In most cases, %nRMSD was kept below 0.5%. In difficult to converge cases, a system was considered converged when %nRMSD does not change upon adding Gaussian curves. Bands that did not converge were discarded from the benchmark set (i.e., are not included among the 164 transitions). The area under the curve was obtained by analytical integration of the Gaussian functions included in fitting that band, excluding the spillover from nearby bands. Oscillator strengths derived in this way are labelled $f_{exp,g}$.

In cases of strongly overlapping bands where the bands could not be reliably deconvoluted, the bands were included in a single integration and assigned one oscillator strength value, which can be compared to the sum of the computed oscillator strengths for the bands.

Steps **B-F** were repeated a second time for each molecule, by a different person, using a different resolution for the digitization. This ensured reproducibility and provided an estimate of errors introduced during each of the digitization, numerical integration, and fitting processes. Ultimately, two sets of $f_{exp,n}$ and $f_{exp,g}$ values for each transition were produced, labeled $f_{exp,n1}$, $f_{exp,n2}$, $f_{exp,g1}$, and $f_{exp,g2}$. The higher resolution data are labeled $f_{exp,n1}$ and $f_{exp,g1}$ while the lower resolution data are labeled $f_{exp,n2}$ and $f_{exp,g2}$. The $f_{exp,n}$ and $f_{exp,g}$ data reported in this work are the averages of the two trials. The quality of the integration was then scored (see Sources of Error section), and each band was assigned a score indicating confidence in the integration process (panel **G**). This process was repeated for the 100 molecules.

Quantum chemical geometry optimizations were carried out at the density functional theory (DFT) level of theory using the B3LYP functional^{39, 40} and 6-31+G* basis set for all molecules. Frequency calculations were carried out at the same level of theory to ensure that exclusively

positive frequencies are obtained for all molecules. TD-DFT calculations were carried out using the same functional and basis set. The the integral equation formalism of PCM (IEF-PCM) was used to account for the solvent effect.⁴¹ The dielectric constant and optical dielectric for each solvent are obtained from the Minnesota solvent descriptor database based on the solvent used in the corresponding experiment.⁴² The list of solvent and solvent descriptors used are listed in Table S1 in the Supporting Information document. The IEF-PCM solvation was performed using a non-equilibrium linear response formalism to account for the effect of solvation on the excitations.⁴³

The geometry optimizations and TD-DFT calculations were performed by two different individuals, to check for consistency. Differences between the two trials could be easily reconciled and one final set of computational data was produced, labeled f_{comp} .

The TD-DFT calculations included 30 singlet states. For all molecules, the 30th excited state was higher in energy than the upper limit of the experimental spectrum (ν_{max}). To compare computed (f_{comp}) and derived from experiment (f_{exp}) oscillator strengths, it is necessary to assign computed transitions to UV-visible absorption bands. In many cases, the computed transition energies fall within the range of the experimental band energies, between ν_{min} and ν_{max} , where the ν_{min} and ν_{max} limits are the same limits used for the numerical integration (see **Fig. 2** panel **C** for a schematic representation). Specifically, ν_{min} and ν_{max} are defined as the lower and upper wavenumber limits where the molar extinction coefficient is at a minimum. In some cases, multiple computed transitions fall within a band. In these cases, f_{comp} is the sum of the oscillator strengths of those transitions. Plots of the digitized UV-visible spectra, their Gaussian fitting functions, and computed TD-B3LYP/6-31+G* IEF-PCM transition stick spectra are included as a supporting document (SIplots).

In some cases, there is a high confidence in the assignment of computed transitions to bands, since there is only one transition per band in the near-UV and visible range. However, there are also cases where the assignment is not straightforward, particularly if multiple transitions appear close to an overlap region between two bands. Therefore, while categorizing transitions based on whether their energies fall within the experimental ν_{min} and ν_{max} is a practical approach, it is not foolproof. For instance, by reviewing the SIplots, five exceptions were recognized where the computed transitions fall outside of the experimental band but can be assigned with a high degree of confidence to that band, or where a transition falls within one band but can be assigned to another. Those five exceptions are labeled in SIplots and have been used to update the

corresponding f_{comp} values. For more extensive benchmarking, however, a more reliable and fully automated approach is necessary for assigning the computed transitions.

WebPlotDigitizer was used to digitize the UV-visible spectra⁴⁴ and Excel’s Solver plugin was used to fit the spectra using the nonlinear generalized reduced gradient algorithm.⁴⁵ Regression and confidence interval analyses were carried out in Mathematica.⁴⁶ The two sets of computations were carried out using the random phase approximation formulation of TD-DFT⁴⁷ in Q-Chem⁴⁸ and using the default TD-DFT formulation in Gaussian 16,⁴⁹ respectively. The latter are the ones reported for f_{comp} .

SOURCES OF ERROR

When using experimental data as a benchmark, it is important to recognize sources of experimental errors. These include errors introduced by instrumentation, experimental design, sample quality (impurities, uncertainties in concentration, concentration-dependent aggregation effects, etc.), and human error. Some of these issues have been discussed at length in the literature, but it remains difficult to quantify the magnitude of the errors.⁵⁰⁻⁵² One concern raised for experimental oscillator strengths derived from photoabsorption spectroscopy and the Beer-Lambert law is that errors introduced by line-saturation effects could result in the underestimation of the experimentally measured f_{exp} relative to the “true” strength f .^{34, 53} This problem is clearly described by Chan *et al.*⁵² However, it appears that such issues are particularly problematic for narrow bands (e.g., well-resolved gas-phase spectra where there are vibronic peaks with full-width at half-maxima that are on the order of hundreds of cm^{-1}). The severity of these errors is reduced for broad absorption bands that are thousands of cm^{-1} across, like most of the bands used in this work.

We do not attempt to quantify the errors in f_{exp} , although we recognize that they exist. However, the uncertainty in f_{exp} is yet another motivation for an extensive benchmark study comparing experimental and computed oscillator strengths. By determining random or systematic errors against computations, particularly for high-level quantum chemical calculations, errors in the experimental measurements could be better understood.⁵⁴

Errors in f_{comp} exist when the transition dipole moment in equation (3) is computed using approximate rather than exact wave functions. This error can be quantified by systematically moving towards high-level quantum chemical methods,^{2, 33-35} but this limits benchmarking to small

molecules where these methods are affordable. Calculations of f_{comp} in this work also neglect nuclear motion, which can often be justified for rigid molecules within the Born-Oppenheimer and Condon approximations⁵⁵ but does not consider variations of oscillator strength with changes in the conformation of flexible molecules. Finally, approximate PCM solvation models may not correctly capture the effect of solvation on f_{comp} . The magnitudes of all these errors are difficult to quantify as well, which is why extensive benchmarking against experimental oscillator strengths is needed.

Here, we focus on uncertainties introduced in the fitting procedure itself, which we identify using four metrics:

- **%gn**: The percentage difference between $f_{exp,g}$ and $f_{exp,n}$. In practice, we compute two sets of %gn values then take the average:

$$\%gn = \frac{1}{2} \left(\frac{|f_{exp,g1} - f_{exp,n1}|}{f_{exp,g1}} + \frac{|f_{exp,g2} - f_{exp,n2}|}{f_{exp,g2}} \right) \quad (4)$$

Values of %gn ranged from 0.0% to 32.7%, with an average of 6.0%, a first quartile of 1.5%, median of 4.5%, and third quartile of 7.5%.

- **%gg**: The percentage difference between $f_{exp,g1}$ and $f_{exp,g2}$. This as an indicator of the reproducibility of the Gaussian fitting procedure performed by two different persons:

$$\%gg = \frac{2|f_{exp,g1} - f_{exp,g2}|}{(f_{exp,g1} + f_{exp,g2})} \quad (5)$$

Values of %gg ranged from 0.0% to 37.9%, with an average of 4.2%, a first quartile of 0.9%, median of 2.6%, and third quartile of 5.1%.

- **%nn**: The percentage difference between $f_{exp,n1}$ and $f_{exp,n2}$. Since the original spectra were plotted on a logarithmic scale, this exacerbates errors in the digitization of the UV-visible spectra, particularly for intense bands. Therefore, %nn reflects the uncertainty introduced by both the digitization and numerical integration procedures. %nn is computed in the same way as %gg in equation (5) but using the numerical $f_{exp,n1}$ and $f_{exp,n2}$. Values of %nn ranged from 0.0% to 7.0%, with an average of 1.4%, a first quartile of 0.5%, median of 1.1%, and third quartile of 1.8%.
- **%nRMSD**: The normalized root-mean-square deviation between the digitized UV-visible spectrum and the Gaussian deconvoluted spectrum. The %nRMSD is computed using:

$$\%nRMSD = \frac{\sqrt{\sum_{i=1}^n \frac{(\epsilon_{i,fit} - \epsilon_i)^2}{n}}}{\epsilon_{max} - \epsilon_{min}} \quad (6)$$

In equation (6), for each point i in the digitized spectrum, ϵ_i is the experimental attenuation coefficient at that point, $\epsilon_{i,fit}$ is the corresponding value at that point obtained from the sum of the Gaussian curves used in the fitting of the band, and n is the total number of points used in the digitized spectrum. The numerator in equation (6) is the RMSD, but since RMSD is not informative on its own (it is typically larger for high intensity bands, smaller for low intensity bands), we divide the RMSD by the range of attenuation coefficients spanned by the UV-visible spectra ($\epsilon_{max} - \epsilon_{min}$). The final %nRMSD reported is an average from the two trials. Values of %nRMSD ranged from 0.2% to 6.0%, with an average of 0.7%, a first quartile of 0.4%, median of 0.5%, and third quartile of 0.8%.

The above percentages are associated with uncertainties in the fitting process and are not errors. For instance, $f_{exp,g}$ and $f_{exp,n}$ are usually different, particularly for incomplete or overlapping bands, yielding large %gn. A large %gn is therefore an indicator of uncertainty (i.e., an incomplete band causes uncertainty in how to fit it). %gg is also an important indicator of uncertainty; if the same band is fit differently by two different individuals, it indicates a lower confidence in the fitting. Thus, we have developed a scoring system to indicate confidence in the analytical integration. The scores are based on the four metrics listed above, with the relative weights based on the ratio of the first quartiles:

$$\%gn : \%gg : \%nn : \%nRMSD = 1.5 : 0.9 : 0.5 : 0.4 \approx 9 : 6 : 3 : 2$$

Each transition is scored out of 20 points (9+6+3+2). Integer scores are assigned by deducting points for each 1% introduced in each of %gn, %gg, %nn, and %nRMSD, up to the maximum score for that category. E.g., a score of 20 is obtained if all four metrics have a value <1%. A spreadsheet is included for the score calculations in the SI (see the SI file named megatable). Molecules are categorized as “very high” confidence if the score is a perfect 20, “high” confidence for a score in the upper quartile (17-19), “medium” confidence for a score in the second quartile (12-16), “low” confidence for a in the third quartile (8-11), and “very low” confidence for a score in the lowest quartile (0-7).

RESULTS

Out of 164 transitions, 14 scored as “very high” confidence, 29 scored as “high”, 42 scored as “medium”, 42 scored as “low”, and 37 as “very low.” A list of the 100 molecule names and solvent information (**Table S1**), f_{comp} , $f_{\text{exp},g1}$, $f_{\text{exp},g2}$, $f_{\text{exp},n1}$, $f_{\text{exp},n2}$, and scores for the 164 transitions (**Table S2**), and ν_{min} , ν_{max} , ϵ_{max} , and ν at ϵ_{max} (**Table S3**) are included in the SI. Plain text files with the digitized UV-visible spectra, spreadsheets used for the numerical integration and gaussian deconvolution for $f_{\text{exp},n1}$ and $f_{\text{exp},g1}$, ChemDraw chemical structures, and B3LYP/6-31+G*/PCM geometry-optimized structures for the 100 organic molecules are also included in the SI.

Figure 3. Left: f_{comp} vs. $f_{\text{exp},g}$ for 164 transitions. The points are colored by confidence level, as indicated in the legend. The blue line is a linear regression (see comment⁵⁶). The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands. **Right:** f_{comp} and $f_{\text{exp},g}$ for each transition ordered by increasing strength of $f_{\text{exp},g}$. The lines connecting the points represent the absolute differences.

Fig. 3 shows the correlation between $f_{\text{exp},g}$ and f_{comp} . The linear regression analysis ($R^2=0.921$) indicates a strong correlation between experimental and computed oscillator strengths. However, the slope of the plot (1.34) indicates a clear systematic error; The computations substantially overestimate the oscillator strength. The mean absolute error (MAE) between f_{comp} and $f_{\text{exp},g}$ is 0.133.

Some of the “very low confidence” points appear well outside of the 95% confidence intervals in Fig. 3 left. If we exclude all “very low confidence” points from the plot and the analysis, the R^2 value increases to 0.935, the slope becomes 1.354 (see SI **Fig. S1**), but the MAE increases slightly to 0.137.

If plots used ϵ_{max} instead of $f_{\text{exp},g}$ as the reference, the R^2 value for f_{comp} vs. ϵ_{max} would be 0.77 (see SI **Fig. S2**). Therefore, ϵ_{max} is correlated with f_{comp} , as expected, but this correlation is weaker than f_{comp} with the area under the band.

The large slope in Fig. 3 left (1.34) appears on the order of magnitude of a refractive index factor, since refractive indices for most common solvents are in the range of 1.3-1.5. Indeed, so far, we have assumed that the PCM solvation model employed in calculations correctly capture the effect of the solvent on the oscillator strength, and that equation (2) is a valid equation for deriving experimental oscillator strengths for a molecule in solution. The question of how to correctly account for the effect of the solvent on oscillator strength has been a topic of debate for both experiments (equation 2), and theory (equation 3).²¹⁻³² To test whether a refractive index factor improves the agreement between theory and experiment, we show in Fig. 4 the correlation between $n \times f_{exp,g}$ and f_{comp} (i.e., we multiply the experimentally derived oscillator strength by the refractive index n).

Figure 4. Left: f_{comp} vs. $n \times f_{exp,g}$ for 164 transitions, where n is the solvent refractive index. The points are colored by confidence level, as indicated in the legend. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands. Right: f_{comp} and $n \times f_{exp,g}$ for each transition ordered by increasing magnitude of $n \times f_{exp,g}$. The lines connecting the points represent the absolute differences.

For f_{comp} against $n \times f_{exp,g}$, the R^2 increased slightly to 0.923, but the slope (0.988) indicates a stronger quantitative agreement between computed and experimental oscillator strengths after accounting for a refractive index factor. Indeed, the MAE is reduced significantly to 0.075. Removing “very low confidence” data (Fig. S3) improves the agreement further; without “very low confidence” points, the slope is 0.999, The R^2 is 0.937, and the MAE is 0.069.

On the other hand, dividing $f_{exp,g}$ in equation (2) by n , as suggested in some literature, significantly reduces the agreement between computations and experimental oscillator strengths. Not only is the slope (1.808) and MAE (0.207) larger, the R^2 between f_{comp} and $n^{-1} \times f_{exp,g}$ also decreases (0.917), as shown in Fig. S4.

Given the structural diversity of the molecules in the OS100 set, it would be informative to

check if certain types of molecules can account for most of the outliers. In Fig. S5, we plot the $f_{exp,g}$ vs. f_{comp} and color the points according to the molecule type instead of confidence score. We find that almost half of the outliers outside the 95% confidence interval be attributed to the azo benzene derivatives. This is not surprising, since these are among the largest molecules included in the benchmark set and their transitions often involve charge transfer character. In Fig. S6, we plot $f_{exp,g}$ vs. f_{comp} and color the points according to the total molecular charge. The correlation between $f_{exp,g}$ and f_{comp} for charged molecules do not appear to be worse than for neutral molecules. In fact, most of the outliers outside the 95% confidence interval are neutral molecules.

CONCLUSIONS

Using a benchmark set of 164 transitions from 100 molecules, we have compared quantum chemically computed oscillator strengths with oscillator strengths we derived from experimental UV-visible absorption spectra. Using equation (2) to obtain experimental oscillator strengths, the discrepancy between experimental and computed oscillator strengths is large (slope 1.34). One reason for this discrepancy could be the refractive index. Reports in the literature disagree on how equations (2) and (3) must be modified for absorption of molecules in solvent.¹⁶⁻³² Our benchmark cannot conclusively resolve this debate, although the discrepancy between experiments and computations can be largely reconciled by a factor of n (either multiplying $f_{exp,g}$ by n or dividing f_{comp} as computed in the TD-DFT IEF-PCM non-equilibrium linear response formalism^{43, 49} by n). This conclusion would be better supported through continued benchmarking, such as by expanding this benchmark set to include additional “high” and “very high” confidence data and performing additional computations to determine the sensitivity of the f_{comp} and $f_{exp,g}$ plot on the quantum chemical level of theory used.

An important next step would be to quantify the accuracy of continuum or explicit solvent models in predicting solvent effects oscillator strengths.⁵⁷ Both implicit and explicit models appear to successfully predict trends in oscillator strengths for the same molecule in different environments,^{58,59} but it is not yet clear if such predictions are quantitative. Preparing a benchmark set of experimental oscillator strengths gas-phase UV-visible spectra would also be valuable towards this end, but it is also more challenging since gas-phase spectra tend to have well-resolved vibronic transitions that are difficult to fit accurately.

Finally, while one way to compare experiments and theory directly is by deriving easily

computable quantities from experimental data, as done in this work, another approach is to continue to develop computational methods that simulate realistic spectra through combined quantum and (semi-)classical methods or machine learning approaches.⁶⁰⁻⁶⁸ To aid in benchmarking for such efforts, we have provided the digitized UV-visible data and optimized molecular geometries for the 100 molecules in the SI.

SUPPORTING INFORMATION

- Supporting.pdf: Information about the 100 molecules in the OS100 set and the solvent descriptors used (Table S1), f_{comp} , $f_{\text{exp,g1}}$, $f_{\text{exp,g2}}$, $f_{\text{exp,g}}$, $f_{\text{exp,n1}}$, $f_{\text{exp,n2}}$, $f_{\text{exp,n}}$, and total score for each of the 164 transitions (Table S2), ν_{min} , ν_{max} , ϵ_{max} , and ν at ϵ_{max} for each of the 164 transitions (Table S3), plot and linear regression for f_{comp} vs. $f_{\text{exp,g}}$ after excluding 37 “very low confidence” points (Fig. S1), plot and linear regression for f_{comp} vs. ϵ_{max} (Fig. S2), plot and linear regression for f_{comp} vs. $n \times f_{\text{exp,g}}$ after excluding 37 “very low confidence” points (Fig. S3), plots and linear regression for f_{comp} vs. $n^{-1} \times f_{\text{exp,g}}$, plots and linear regression for f_{comp} vs. $f_{\text{exp,g}}$ colored by molecule type (Fig. S5) and total molecule charge (Fig. S6).

- Supporting.zip: SIplots.pdf, with plots and deconvolutions of all digitized spectra for the $f_{\text{exp,g1}}$ data, chemical structures, and TD-B3LYP/6-31+G* stick spectra, ChemDraw Structures for the 100 molecules, Excel files of digitized spectra where numerical and Gaussian fitting was performed for $f_{\text{exp,g1}}$ and $f_{\text{exp,n1}}$, plain text files of the UV-visible spectra used for $f_{\text{exp,g1}}$ and $f_{\text{exp,n1}}$ data, B3LYP/6-31+G*/PCM geometry-optimized structures for the 100 molecules, tables S1, S2, and S3 in Excel format, an Excel file (megatable.xlsx) of f_{comp} , $f_{\text{exp,g1}}$, $f_{\text{exp,g2}}$, $f_{\text{exp,g}}$, $f_{\text{exp,n1}}$, $f_{\text{exp,n2}}$, and $f_{\text{exp,n}}$, digitization and fitting statistics, sources of uncertainty, and scoring functions.

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Declaration of competing financial interests

The authors declare no competing financial interests.

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Supporting Information for:

OS100: A Benchmark Set of 100 Digitized UV-Visible Spectra and Derived Experimental Oscillator Strengths

Astrid S. Tarleton^a, Jorge Garcia-Alvarez^a, Anah Wynn^a, Cade Awbrey^a, Tomas Roberts^a,
Samer Gozem^{a*}

^aDepartment of Chemistry, Georgia State University, Atlanta, GA 30302, United States.

Contents:

Tables S1: Information about the 100 molecules in the OS100 set and their solvent information.

Tables S2: f_{comp} , $f_{\text{exp.g1}}$, $f_{\text{exp.g2}}$, $f_{\text{exp.g}}$, $f_{\text{exp.n1}}$, $f_{\text{exp.n2}}$, $f_{\text{exp.n}}$, and total score for each of the 164 transitions.

Tables S3: v_{min} , v_{max} , ϵ_{max} , and v at ϵ_{max} for each of the 164 transitions.

Fig. S1: Plot and linear regression for f_{comp} vs. $f_{\text{exp.g}}$ after excluding 37 “very low confidence” points.

Fig. S2: Plot and linear regression for f_{comp} vs. ϵ_{max} .

Fig. S3: Plot and linear regression for f_{comp} vs. $n \times f_{\text{exp.g}}$ after excluding 37 “very low confidence” points.

Fig. S4: Plots and linear regression for f_{comp} vs. $n^{-1} \times f_{\text{exp.g}}$.

Fig. S5: Plot and linear regression for f_{comp} vs. $f_{\text{exp.g}}$ colored by molecule type.

Fig. S6: Plot and linear regression for f_{comp} vs. $f_{\text{exp.g}}$ colored by total molecule charge.

Additional Supporting Files

A Supporting.zip file containing the following:

- A pdf file (SIplots.pdf) with plots and deconvolutions of all digitized spectra for the $f_{\text{exp.g1}}$ data, chemical structures, and TD-B3LYP/6-31+G* stick spectra.
- ChemDraw Structures for the 100 molecules.
- Excel files of digitized spectra where numerical and Gaussian fitting was performed for $f_{\text{exp.g1}}$ and $f_{\text{exp.n1}}$.
- Plain text files of the UV-visible spectra used for $f_{\text{exp.g1}}$ and $f_{\text{exp.n1}}$ data.
- B3LYP/6-31+G*/PCM geometry-optimized structures for the 100 molecules.
- Tables S1, S2, and S3 in Excel format.
- An Excel file (megatable.xlsx) of f_{comp} , $f_{\text{exp.g1}}$, $f_{\text{exp.g2}}$, $f_{\text{exp.g}}$, $f_{\text{exp.n1}}$, $f_{\text{exp.n2}}$, and $f_{\text{exp.n}}$, digitization and fitting statistics, sources of uncertainty, and scoring functions.

Table S1: 100 molecules for which UV-visible spectra are digitized and processed in this work. The original spectra were all obtained from the UV Atlas of Organic Compounds.¹ The molecules are assigned IDs from 000–099 which are used throughout the rest of the supporting information. The table includes the chemical names, reference IDs from Ref. 1, solvent in which the spectra were obtained, solvent dielectric, and solvent refractive indices at 20°C. The solvent dielectric constants and refractive indices were obtained from the Minnesota Solvent Descriptor Database.²

ID	Molecule name	Reference ¹	Solvent	Solvent Dielectric	Refractive Index (n)
000	cis -1, 2-Dichloroethylene	A1/4	Heptane	1.9113	1.3878
001	trans-1,2-Dichloroethylene	A1/5	Heptane	1.9113	1.3878
002	Trichloroethylene	A1/6	Heptane	1.9113	1.3878
003	Tetrachloroethylene	A1/7	Heptane	1.9113	1.3878
004	Penta-1,3-diene	A3/1	Heptane	1.9113	1.3878
005	2,5-dimethylhexa-2,4-diene	A3/2	Heptane	1.9113	1.3878
006	Cycloocta-1,3-diene	A3/4	Hexane	1.8819	1.3749
007	1-(cyclohexen-1-yl)cyclohexene	A3/5	Heptane	1.9113	1.3878
008	cis-Hex-3-en-1-yne	A4/1	Ethanol	24.852	1.3611
009	trans-Hex-3-en-1-yne	A4/2	Ethanol	24.852	1.3611
010	1,6-Dihydroazulene	A15/3	Hexane	1.8819	1.3749
011	p-Benzoquinone	B8/23	Hexane	1.8819	1.3749
012	Hydroxy-p-benzoquinone	B8/24	CCl ₄	2.228	1.4601
013	Methoxy-p-benzoquinone	B8/25	Hexane	1.8819	1.3749
014	2-Sulfinylhexahydro-1,3-benzodithiole	B16/3	Ethanol	24.852	1.3611
015	Thiourea	B17/6	Water	78.355	1.3328
016	S-ethyl thioacetate	B21/1	Heptane	1.9113	1.3878
017	Nitromethane	C4/1	Hexane	1.8819	1.3749
018	t-Butyl nitrite	C4/3	Hexane	1.8819	1.3749
019	Isopentyl nitrite	C4/4	Hexane	1.8819	1.3749
020	N-Benzylideneaniline	C6/1	Ethanol	24.852	1.3611
021	4- Nitro-N-benzylideneaniline	C6/2	Ethanol	24.852	1.3611
022	N-Benzylidene-4-dimethylaminoaniline	C6/3	Ethanol	24.852	1.3611
023	Tetramethylazodicarboxamide	C7/2	Dioxane	2.2099	1.4224
024	Phenylazoformate (anion)	C7/3	Ethanol	24.852	1.3611
025	Dimethyl [(E)-phenyldiazenyl]phosphonate	V7/4	Dioxane	2.2099	1.4224
026	trans-Azobenzene	C7/5	Hexane	1.8819	1.3749
027	4-(Dimethylamino)azobenzene (cation)	C7/7	H ₂ SO ₄ (aq)	78.355	1.3328
028	4-Dimethylamino-4'-nitroazobenzene	C7/8	Ethanol	24.852	1.3611
029	1-Ethyl-2-(phenylazo)-pyridinium (cation)	C7/10	Acetonitrile	35.688	1.3442
030	1-Phenyl-2-(phenylthio)diazene	C7/12	Dioxane	2.2099	1.4224
031	1-Phenyl-2-(phenylsulfonyl)diazene	C7/13	Dioxane	2.2099	1.4224
032	N,N,N',N'-Tetramethylformamidine (cation)	C8/1	Ethanol	24.852	1.3611
033	N-[3-(Dimethylamino)allylidene]-N-methylmethanaminium (cation)	C8/2	Ethanol	24.852	1.3611
034	2,4-Cyclopentadien-1-ylidenehydrazine	C9/1	Hexane	1.8819	1.3749
035	Cyclohexanone semicarbazone	C9/2	Ethanol	24.852	1.3611
036	1-Isopropylidene-2-p-nitrophenyl-hydrazine	C9/3	Ethanol	24.852	1.3611
037	1-Ethylidene-2-(2,4-dinitrophenyl)-hydrazine	C9/4	CHCl ₃ /Ethanol	24.852	1.3611
038	1-Ethylidene-2-(2,4-dinitrophenyl)-hydrazone (anion)	C9/5	CHCl ₃ /Ethanol	24.852	1.3611
039	Crotonaldehyde 2,4-dinitrophenylhydrazone	C9/6	CHCl ₃ /Ethanol	24.852	1.3611
040	N,N'-Di(2-hydroxybenzylidene)hydrazine	C9/10	Methanol	32.613	1.3288
041	o-Xylene	D2/5	Heptane	1.9113	1.3878
042	m-Xylene	D2/6	Heptane	1.9113	1.3878
043	p-Xylene	D2/7	Heptane	1.9113	1.3878
044	2,3,5,6,7,8-hexahydro-1H-benz(f)indene	D3/5	Petroleum Ether	1.89	1.3715
045	1,2,3,4,5,6,7,8-octahydroanthracene	D3/6	Petroleum Ether	1.89	1.3715
046	Phenol	D5/5	Water	78.355	1.3328

047	Phenolate (anion)	D5/6	NaOH (aq)	78.355	1.3328
048	N,N-Diethylaniline	D6/2	Heptane	1.9113	1.3878
049	Nitrobenzene	D8/6	Petroleum Ether	1.89	1.3715
050	o-Chlorotoluene	D9/25	Heptane	1.9113	1.3878
051	p-Chlorotoluene	D9/26	Heptane	1.9113	1.3878
052	p-Bromofluorobenzene	D9/27	Heptane	1.9113	1.3878
053	o-Nitrophenol	D9/29	Water	78.355	1.3328
054	m-Nitrophenol	D9/30	Water	78.355	1.3328
055	p-Nitrophenol	D9/31	Water	78.355	1.3328
056	p-Nitrophenolate (anion)	D9/32	NaOH (aq)	78.355	1.3328
057	o-Acetylphenol	D9/33	Ethanol	24.852	1.3611
058	o-Methoxyacetophenone	D9/34	Ethanol	24.852	1.3611
059	o-Hydroxybenzaldehyde	D9/35	Ethanol	24.852	1.3611
060	o-Methoxybenzaldehyde	D9/36	Ethanol	24.852	1.3611
061	o-Aminobenzaldehyde	D9/37	Ethanol	24.852	1.3611
062	p-Hydroxybenzaldehyde	D9/39	Ethanol	24.852	1.3611
063	p-Dimethylaminobenzaldehyde	D9/41	Cyclohexane	2.0165	1.4266
064	p-Cyanobenzaldehyde	D9/42	Cyclohexane	2.0165	1.4266
065	Hydrogen phthalate (anion)	D9/45	Water	78.355	1.3328
066	p-Nitrophenylhydrazine	D9/47	Methanol	32.613	1.3288
067	2,3-Dimethylphenolate (anion)	D9/49	KOH(aq)	78.355	1.3328
068	4-Methyl-2-nitroaniline	D9/50	Methanol	32.613	1.3288
069	Cinnamaldehyde	D10/40	Methanol	32.613	1.3288
070	Benzylideneacetone	D10/41	Ethanol	24.852	1.3611
071	Benzophenone	D11/9	Ethanol	24.852	1.3611
072	4-Methylbenzophenone	D11/10	Cyclohexane	2.0165	1.4266
073	4-Aminobenzophenone	D11/13	Ethanol	24.852	1.3611
074	4-(N,N-Dimethylamino)-benzophenone	D11/14	Cyclohexane	2.0165	1.4266
075	4-Hydroxybenzophenone	D11/15	Hexane	1.8819	1.3749
076	Diphenylamine	D11/19	Ethanol	24.852	1.3611
077	2-Nitrodiphenylamine	D11/20	Methanol	32.613	1.3288
078	4-Nitrodiphenylamine	D11/21	Methanol	32.613	1.3288
079	Thiobenzophenone	D11/23	Methanol	32.613	1.3288
080	1-Naphthol	E1/6	Methanol	32.613	1.3288
081	1-Naphtholate (anion)	E1/7	0.1 M KOH	78.355	1.3328
082	2-Naphtholate (anion)	E1/9	0.1 M KOH	78.355	1.3328
083	1-Naphthoic acid	E1/10	Methanol	32.613	1.3288
084	2-Naphthaldehyde	E1/11	Methanol	32.613	1.3288
085	1,5-Dinitronaphthalene	E1/14	Methanol	32.613	1.3288
086	Thiazole	G2/1	Heptane	1.9113	1.3878
087	2-Mercaptothiazole	G2/2	Water	78.355	1.3328
088	Pyridinium (cation)	G5/7	H2SO4 (aq)	78.355	1.3328
089	2-Methoxypyridine	G5/8	Heptane	1.9113	1.3878
090	2-Chloro-6-ethoxypyridine	G5/9	Heptane	1.9113	1.3878
091	cis-1,2-Di-(3'-pyridyl)ethylene	G11/15	Heptane	1.9113	1.3878
092	Deprotonated 2-Hydroxyquinoline (anion)	H1/13	1 M NaOH	78.355	1.3328
093	4-Hydroxyquinolynium (cation)	H1/15	0.1 M HCl	78.355	1.3328
094	Deprotonated 4-Hydroxyquinoline (anion)	H1/16	0.01 M KOH	78.355	1.3328
095	5-Hydroxyquinoline	H1/17	Methanol	32.613	1.3288
096	5-Hydroxyquinolynium (cation)	H1/18	0.1 M HCl	78.355	1.3328
097	Deprotonated 5-Hydroxyquinoline (anion)	H1/19	0.1 M NaOH	78.355	1.3328
098	3-Hydroxyphthalamide	H12/2	Ethanol	24.852	1.3611
099	3-Amino-1-methylphthalamide	H12/5	Ethanol	24.852	1.3611

Table S2: A table of $f_{\text{comp}}, f_{\text{exp,g1}}, f_{\text{exp,g2}}, f_{\text{exp,g}}, f_{\text{exp,n1}}, f_{\text{exp,n2}}, f_{\text{exp,n}}$, total score (out of 20) and category (VL, L, M, H, and VH) for each of the 164 transitions.

ID	Band	f_{comp}	$f_{\text{exp,g1}}$	$f_{\text{exp,g2}}$	$f_{\text{exp,g}}$	$f_{\text{exp,g1/n}}$	$f_{\text{exp,g1} \times n}$	$f_{\text{exp,n1}}$	$f_{\text{exp,n2}}$	$f_{\text{exp,n}}$	Score	Category
000	1	3.89E-01	2.97E-01	2.98E-01	2.98E-01	2.14E-01	4.13E-01	2.64E-01	2.60E-01	2.62E-01	10	L
001	1	3.63E-01	3.06E-01	2.99E-01	3.03E-01	2.18E-01	4.20E-01	2.77E-01	2.83E-01	2.80E-01	9	L
002	1	4.16E-01	3.28E-01	3.30E-01	3.29E-01	2.37E-01	4.56E-01	3.07E-01	3.07E-01	3.07E-01	14	M
003	1	5.36E-01	4.20E-01	4.00E-01	4.10E-01	2.95E-01	5.69E-01	3.87E-01	3.81E-01	3.84E-01	9	L
004	1	8.99E-01	7.15E-01	7.07E-01	7.11E-01	5.12E-01	9.87E-01	6.79E-01	6.69E-01	6.74E-01	13	M
005	1	1.10E+00	7.65E-01	7.04E-01	7.35E-01	5.29E-01	1.02E+00	7.06E-01	6.96E-01	7.01E-01	9	L
006	1	2.63E-01	1.75E-01	1.87E-01	1.81E-01	1.32E-01	2.49E-01	1.83E-01	1.87E-01	1.85E-01	10	L
007	1	7.24E-01	4.79E-01	5.01E-01	4.90E-01	3.53E-01	6.80E-01	5.05E-01	5.13E-01	5.09E-01	11	L
008	1	4.32E-01	3.60E-01	3.43E-01	3.51E-01	2.58E-01	4.78E-01	3.25E-01	3.25E-01	3.25E-01	9	L
009	1	5.07E-01	3.95E-01	3.99E-01	3.97E-01	2.92E-01	5.41E-01	3.60E-01	3.61E-01	3.60E-01	11	L
010	1	1.34E-01	1.14E-01	1.09E-01	1.11E-01	8.10E-02	1.53E-01	8.88E-02	8.80E-02	8.84E-02	7	VL
011	2	4.37E-01	5.10E-01	5.14E-01	5.12E-01	3.72E-01	7.04E-01	4.80E-01	4.80E-01	4.80E-01	14	M
012	1	2.97E-02	3.30E-02	3.30E-02	3.30E-02	2.26E-02	4.83E-02	3.25E-02	3.23E-02	3.24E-02	19	H
012	2	3.35E-01	1.99E-01	1.84E-01	1.92E-01	1.31E-01	2.80E-01	1.43E-01	1.36E-01	1.40E-01	2	VL
013	1	3.15E-02	2.69E-02	2.62E-02	2.66E-02	1.93E-02	3.65E-02	2.66E-02	2.64E-02	2.65E-02	18	H
013	2	3.12E-01	2.40E-01	2.36E-01	2.38E-01	1.73E-01	3.27E-01	2.21E-01	2.21E-01	2.21E-01	12	M
014	1	3.04E-01	1.98E-01	2.08E-01	2.03E-01	1.49E-01	2.77E-01	2.08E-01	2.03E-01	2.05E-01	11	L
014	2	9.29E-02	1.12E-01	1.03E-01	1.08E-01	7.90E-02	1.46E-01	9.74E-02	9.08E-02	9.41E-02	2	VL
015	1	3.49E-01	2.09E-01	2.07E-01	2.08E-01	1.56E-01	2.77E-01	2.29E-01	2.38E-01	2.33E-01	8	L
015	2	1.65E-01	5.09E-01	4.24E-01	4.67E-01	3.50E-01	6.22E-01	3.26E-01	3.12E-01	3.19E-01	2	VL
016	1	9.02E-02	7.93E-02	7.96E-02	7.95E-02	5.73E-02	1.10E-01	7.73E-02	7.59E-02	7.66E-02	16	M
017	2	2.03E-01	1.36E-01	1.37E-01	1.37E-01	9.93E-02	1.88E-01	1.17E-01	1.17E-01	1.17E-01	11	L
018	2	8.52E-02	9.68E-02	8.07E-02	8.88E-02	6.46E-02	1.22E-01	8.46E-02	8.42E-02	8.44E-02	6	VL
019	2	1.14E-01	8.11E-02	7.06E-02	7.59E-02	5.52E-02	1.04E-01	6.04E-02	6.05E-02	6.05E-02	5	VL
020	1+2	1.00E+00	5.87E-01	6.01E-01	5.94E-01	4.36E-01	8.09E-01	5.93E-01	5.96E-01	5.95E-01	18	H
021	1+2	1.07E+00	7.05E-01	6.58E-01	6.82E-01	5.01E-01	9.28E-01	6.80E-01	6.79E-01	6.80E-01	11	L
022	1	7.92E-01	4.67E-01	4.66E-01	4.67E-01	3.43E-01	6.35E-01	4.59E-01	4.60E-01	4.59E-01	19	H
022	2	6.53E-01	6.81E-01	6.52E-01	6.66E-01	4.89E-01	9.07E-01	6.04E-01	5.96E-01	6.00E-01	6	VL
023	2	5.65E-02	8.81E-02	8.40E-02	8.61E-02	6.05E-02	1.22E-01	8.34E-02	8.34E-02	8.34E-02	13	M
024	2	2.96E-01	3.10E-01	3.19E-01	3.14E-01	2.31E-01	4.28E-01	3.28E-01	3.33E-01	3.31E-01	12	M
025	2	5.87E-01	3.78E-01	3.87E-01	3.82E-01	2.69E-01	5.44E-01	3.23E-01	3.26E-01	3.24E-01	8	L
026	2	9.52E-01	5.77E-01	5.84E-01	5.80E-01	4.22E-01	7.98E-01	5.71E-01	5.77E-01	5.74E-01	17	H
026	3	2.08E-01	2.49E-01	2.49E-01	2.49E-01	1.81E-01	3.42E-01	2.58E-01	2.56E-01	2.57E-01	16	M
027	1	1.26E+00	7.24E-01	7.10E-01	7.17E-01	5.38E-01	9.55E-01	7.31E-01	7.14E-01	7.22E-01	17	H
027	2+3	2.43E-01	5.05E-01	4.96E-01	5.01E-01	3.76E-01	6.67E-01	4.83E-01	4.77E-01	4.80E-01	14	M
028	1	1.03E+00	5.76E-01	5.66E-01	5.71E-01	4.19E-01	7.77E-01	5.84E-01	5.75E-01	5.80E-01	17	H
029	1	3.57E-02	1.36E-02	1.39E-02	1.38E-02	1.02E-02	1.85E-02	1.17E-02	1.15E-02	1.16E-02	7	VL
029	2	8.81E-01	5.98E-01	6.01E-01	6.00E-01	4.46E-01	8.06E-01	5.69E-01	5.74E-01	5.71E-01	16	M
030	1	5.08E-01	2.90E-01	2.76E-01	2.83E-01	1.99E-01	4.02E-01	2.80E-01	2.77E-01	2.79E-01	14	M
030	2	4.02E-01	2.48E-01	3.02E-01	2.75E-01	1.93E-01	3.91E-01	2.53E-01	2.57E-01	2.55E-01	3	VL
031	2	7.99E-01	4.07E-01	4.11E-01	4.09E-01	2.88E-01	5.82E-01	4.28E-01	4.28E-01	4.28E-01	16	M
032	1	4.78E-01	3.36E-01	3.36E-01	3.36E-01	2.47E-01	4.57E-01	3.13E-01	3.11E-01	3.12E-01	13	M
033	1	1.03E+00	7.42E-01	7.46E-01	7.44E-01	5.47E-01	1.01E+00	7.42E-01	7.46E-01	7.44E-01	20	VH
033	2	5.26E-02	2.94E-02	2.91E-02	2.93E-02	2.15E-02	3.98E-02	2.75E-02	2.75E-02	2.75E-02	14	M
034	1+2+3	5.18E-01	3.54E-01	3.52E-01	3.53E-01	2.57E-01	4.85E-01	3.54E-01	3.52E-01	3.53E-01	20	VH
035	1	6.57E-01	2.48E-01	2.57E-01	2.53E-01	1.86E-01	3.44E-01	2.99E-01	3.07E-01	3.03E-01	6	VL
036	1	7.27E-01	5.00E-01	4.89E-01	4.95E-01	3.63E-01	6.73E-01	5.05E-01	4.91E-01	4.98E-01	16	M
036	2	3.56E-01	3.19E-01	2.99E-01	3.09E-01	2.27E-01	4.20E-01	3.37E-01	3.26E-01	3.32E-01	4	VL
037	1	6.39E-01	5.37E-01	5.54E-01	5.46E-01	4.01E-01	7.43E-01	5.44E-01	5.54E-01	5.49E-01	16	M
038	1+2	8.61E-01	5.06E-01	4.87E-01	4.97E-01	3.65E-01	6.76E-01	5.34E-01	5.31E-01	5.32E-01	10	L
039	1	7.90E-01	6.46E-01	6.61E-01	6.54E-01	4.80E-01	8.90E-01	6.50E-01	6.59E-01	6.55E-01	17	H

040	1	8.09E-01	3.91E-01	4.10E-01	4.00E-01	3.01E-01	5.32E-01	4.22E-01	4.26E-01	4.24E-01	10	L
040	2	6.17E-01	5.55E-01	5.22E-01	5.38E-01	4.05E-01	7.15E-01	5.15E-01	5.09E-01	5.12E-01	9	L
041	2+3	1.50E+00	1.08E+00	1.05E+00	1.06E+00	7.67E-01	1.48E+00	9.85E-01	9.53E-01	9.69E-01	7	VL
042	2	2.21E-02	1.12E-01	1.16E-01	1.14E-01	8.22E-02	1.58E-01	1.14E-01	1.12E-01	1.13E-01	14	M
042	3	1.35E+00	9.37E-01	9.00E-01	9.18E-01	6.62E-01	1.27E+00	8.33E-01	8.35E-01	8.34E-01	8	L
043	2	7.44E-02	1.35E-01	1.33E-01	1.34E-01	9.67E-02	1.86E-01	1.27E-01	1.24E-01	1.26E-01	10	L
043	3	1.32E+00	9.71E-01	9.50E-01	9.61E-01	6.92E-01	1.33E+00	8.81E-01	8.69E-01	8.75E-01	9	L
044	1	8.67E-02	3.35E-02	3.37E-02	3.36E-02	2.46E-02	4.59E-02	3.34E-02	3.34E-02	3.34E-02	18	H
044	2+3	1.31E+00	1.06E+00	1.05E+00	1.06E+00	7.74E-01	1.44E+00	9.96E-01	9.92E-01	9.94E-01	14	M
045	1	4.77E-02	1.86E-02	1.79E-02	1.83E-02	1.34E-02	2.49E-02	1.87E-02	1.78E-02	1.83E-02	12	M
045	2+3	1.26E+00	1.03E+00	1.01E+00	1.02E+00	7.47E-01	1.39E+00	9.67E-01	9.58E-01	9.63E-01	13	M
046	1	4.50E-02	1.96E-02	1.94E-02	1.95E-02	1.46E-02	2.60E-02	1.97E-02	1.98E-02	1.98E-02	18	H
046	2	5.66E-02	1.46E-01	1.34E-01	1.40E-01	1.05E-01	1.86E-01	1.02E-01	1.01E-01	1.01E-01	5	VL
047	1	8.52E-02	3.85E-02	3.91E-02	3.88E-02	2.91E-02	5.17E-02	3.87E-02	3.91E-02	3.89E-02	18	H
047	2	3.96E-01	2.01E-01	1.91E-01	1.96E-01	1.47E-01	2.61E-01	1.86E-01	1.86E-01	1.86E-01	11	L
048	1	5.05E-02	3.13E-02	3.39E-02	3.26E-02	2.35E-02	4.52E-02	3.33E-02	3.35E-02	3.34E-02	10	L
048	2	4.69E-01	2.95E-01	2.87E-01	2.91E-01	2.10E-01	4.04E-01	2.85E-01	2.82E-01	2.83E-01	16	M
048	3	7.59E-01	4.20E-01	4.62E-01	4.41E-01	3.18E-01	6.12E-01	4.72E-01	4.76E-01	4.74E-01	7	VL
049	1+2	3.02E-01	2.45E-01	2.43E-01	2.44E-01	1.79E-01	3.33E-01	2.44E-01	2.43E-01	2.44E-01	20	VH
050	2	6.43E-02	1.14E-01	1.14E-01	1.14E-01	8.20E-02	1.58E-01	1.10E-01	1.08E-01	1.09E-01	15	M
050	3	1.30E+00	8.30E-01	7.90E-01	8.10E-01	5.84E-01	1.12E+00	7.68E-01	7.61E-01	7.64E-01	10	L
051	2	1.66E-01	1.66E-01	1.56E-01	1.61E-01	1.16E-01	2.24E-01	1.50E-01	1.52E-01	1.51E-01	7	VL
051	3	1.18E+00	7.45E-01	8.00E-01	7.73E-01	5.57E-01	1.07E+00	7.72E-01	7.63E-01	7.68E-01	8	L
052	1	2.22E-02	1.23E-02	1.13E-02	1.18E-02	8.50E-03	1.64E-02	1.13E-02	1.10E-02	1.12E-02	5	VL
052	2	1.83E-01	1.58E-01	1.52E-01	1.55E-01	1.12E-01	2.15E-01	1.34E-01	1.27E-01	1.31E-01	3	VL
052	3	7.65E-01	7.21E-01	6.76E-01	6.99E-01	5.03E-01	9.69E-01	6.46E-01	6.33E-01	6.39E-01	4	VL
053	1	6.40E-02	6.78E-02	7.01E-02	6.90E-02	5.17E-02	9.19E-02	6.99E-02	7.21E-02	7.10E-02	12	M
053	2	2.79E-01	1.66E-01	1.69E-01	1.68E-01	1.26E-01	2.23E-01	1.64E-01	1.68E-01	1.66E-01	17	H
054	1	3.69E-02	3.94E-02	4.10E-02	4.02E-02	3.02E-02	5.36E-02	3.76E-02	3.69E-02	3.73E-02	9	L
054	2	2.18E-01	1.52E-01	1.50E-01	1.51E-01	1.13E-01	2.01E-01	1.42E-01	1.45E-01	1.44E-01	14	M
054	3	9.35E-02	9.33E-02	9.62E-02	9.48E-02	7.11E-02	1.26E-01	1.26E-01	1.25E-01	1.26E-01	7	VL
054	4	3.10E-01	2.91E-01	2.65E-01	2.78E-01	2.08E-01	3.70E-01	2.65E-01	2.66E-01	2.66E-01	8	L
055	1	3.83E-01	2.81E-01	2.78E-01	2.79E-01	2.10E-01	3.72E-01	2.82E-01	2.82E-01	2.82E-01	19	H
055	2	4.72E-02	1.68E-01	1.76E-01	1.72E-01	1.29E-01	2.29E-01	1.50E-01	1.48E-01	1.49E-01	6	VL
056	1	5.88E-01	3.78E-01	3.80E-01	3.79E-01	2.84E-01	5.05E-01	3.84E-01	3.85E-01	3.84E-01	19	H
057	1	1.01E-01	6.74E-02	6.74E-02	6.74E-02	4.95E-02	9.18E-02	6.75E-02	6.77E-02	6.76E-02	20	VH
057	2	2.56E-01	1.40E-01	1.40E-01	1.40E-01	1.03E-01	1.91E-01	1.42E-01	1.42E-01	1.42E-01	19	H
058	1	5.58E-02	7.08E-02	6.86E-02	6.97E-02	5.12E-02	9.49E-02	7.06E-02	6.97E-02	7.02E-02	16	M
058	2	2.30E-01	1.44E-01	1.45E-01	1.45E-01	1.06E-01	1.97E-01	1.43E-01	1.42E-01	1.42E-01	19	H
059	1	8.07E-02	6.79E-02	6.76E-02	6.78E-02	4.98E-02	9.22E-02	6.83E-02	6.80E-02	6.82E-02	20	VH
059	2	2.79E-01	1.56E-01	1.56E-01	1.56E-01	1.15E-01	2.13E-01	1.60E-01	1.59E-01	1.60E-01	18	H
060	1	1.28E-01	7.88E-02	7.90E-02	7.89E-02	5.80E-02	1.07E-01	7.99E-02	8.01E-02	8.00E-02	19	H
060	2	2.43E-01	1.74E-01	1.76E-01	1.75E-01	1.29E-01	2.38E-01	1.75E-01	1.75E-01	1.75E-01	19	H
061	1	1.16E-01	9.24E-02	9.21E-02	9.23E-02	6.78E-02	1.26E-01	9.23E-02	9.19E-02	9.21E-02	20	VH
061	2	6.01E-02	6.43E-02	6.13E-02	6.28E-02	4.61E-02	8.55E-02	6.72E-02	6.52E-02	6.62E-02	8	L
061	3	3.86E-01	3.92E-01	4.29E-01	4.10E-01	3.01E-01	5.59E-01	4.28E-01	4.28E-01	4.28E-01	10	L
062	1	4.49E-01	3.74E-01	3.76E-01	3.75E-01	2.75E-01	5.10E-01	3.75E-01	3.78E-01	3.76E-01	20	VH
062	2	2.27E-01	2.23E-01	2.14E-01	2.18E-01	1.60E-01	2.97E-01	2.04E-01	2.07E-01	2.06E-01	11	L
063	1	6.79E-01	5.06E-01	4.95E-01	5.01E-01	3.51E-01	7.14E-01	5.06E-01	4.99E-01	5.03E-01	17	H
063	2	1.55E-01	1.63E-01	1.57E-01	1.60E-01	1.12E-01	2.28E-01	1.67E-01	1.65E-01	1.66E-01	13	M
064	1	4.51E-02	2.50E-02	2.82E-02	2.66E-02	1.87E-02	3.79E-02	2.60E-02	2.69E-02	2.65E-02	6	VL
064	2+3	5.99E-01	4.59E-01	4.44E-01	4.51E-01	3.16E-01	6.44E-01	4.33E-01	4.37E-01	4.35E-01	13	M
065	1	6.00E-04	1.99E-02	1.96E-02	1.98E-02	1.48E-02	2.63E-02	1.86E-02	1.81E-02	1.84E-02	10	L
065	2+3	1.63E+00	1.21E+00	1.24E+00	1.22E+00	9.17E-01	1.63E+00	1.04E+00	1.02E+00	1.03E+00	8	L
066	1	5.18E-01	3.72E-01	3.72E-01	3.72E-01	2.80E-01	4.94E-01	3.75E-01	3.76E-01	3.76E-01	20	VH

066	2	1.10E-01	2.33E-01	2.38E-01	2.35E-01	1.77E-01	3.13E-01	2.09E-01	2.09E-01	2.09E-01	9	L
067	1	1.13E-01	4.27E-02	3.88E-02	4.08E-02	3.06E-02	5.43E-02	4.20E-02	4.12E-02	4.16E-02	10	L
067	2	2.72E-01	1.38E-01	1.33E-01	1.36E-01	1.02E-01	1.81E-01	1.33E-01	1.35E-01	1.34E-01	14	M
067	3	7.38E-01	5.92E-01	5.47E-01	5.69E-01	4.27E-01	7.59E-01	4.85E-01	4.76E-01	4.80E-01	3	VL
068	1	1.15E-01	9.50E-02	9.38E-02	9.44E-02	7.11E-02	1.25E-01	9.24E-02	9.28E-02	9.26E-02	18	H
068	2	2.23E-01	8.17E-02	8.63E-02	8.40E-02	6.32E-02	1.12E-01	6.80E-02	6.86E-02	6.83E-02	6	VL
068	3	5.98E-01	4.15E-01	4.12E-01	4.14E-01	3.11E-01	5.49E-01	4.36E-01	4.36E-01	4.36E-01	14	M
069	1	8.64E-01	5.77E-01	5.82E-01	5.79E-01	4.36E-01	7.70E-01	5.77E-01	5.81E-01	5.79E-01	20	VH
070	1	8.17E-01	5.78E-01	5.79E-01	5.79E-01	4.25E-01	7.88E-01	5.79E-01	5.79E-01	5.79E-01	20	VH
070	2	1.63E-01	1.67E-01	1.81E-01	1.74E-01	1.28E-01	2.37E-01	1.74E-01	1.77E-01	1.76E-01	10	L
071	2	5.34E-01	4.12E-01	4.19E-01	4.16E-01	3.05E-01	5.66E-01	4.07E-01	3.99E-01	4.03E-01	15	M
072	2	6.01E-01	4.29E-01	4.14E-01	4.21E-01	2.95E-01	6.01E-01	4.37E-01	4.35E-01	4.36E-01	14	M
073	1	4.56E-01	4.12E-01	4.11E-01	4.11E-01	3.02E-01	5.60E-01	4.04E-01	4.02E-01	4.03E-01	18	H
073	2	4.43E-01	2.88E-01	2.71E-01	2.80E-01	2.05E-01	3.81E-01	2.97E-01	2.95E-01	2.96E-01	9	L
074	1	5.11E-01	4.54E-01	4.54E-01	4.54E-01	3.18E-01	6.47E-01	4.58E-01	4.49E-01	4.53E-01	19	H
074	2	5.54E-01	3.83E-01	3.73E-01	3.78E-01	2.65E-01	5.39E-01	3.89E-01	3.83E-01	3.86E-01	15	M
075	2+3	5.85E-01	5.01E-01	5.03E-01	5.02E-01	3.65E-01	6.90E-01	4.90E-01	4.89E-01	4.90E-01	18	H
076	1	6.72E-01	4.56E-01	4.69E-01	4.63E-01	3.40E-01	6.30E-01	4.86E-01	4.89E-01	4.88E-01	13	M
077	1	2.10E-01	1.48E-01	1.44E-01	1.46E-01	1.10E-01	1.94E-01	1.45E-01	1.44E-01	1.44E-01	18	H
077	2+3	8.65E-01	7.39E-01	7.54E-01	7.46E-01	5.62E-01	9.92E-01	6.99E-01	6.91E-01	6.95E-01	10	L
078	1	7.60E-01	5.90E-01	5.77E-01	5.83E-01	4.39E-01	7.75E-01	5.86E-01	5.96E-01	5.91E-01	15	M
078	2	2.48E-01	3.17E-01	3.65E-01	3.41E-01	2.57E-01	4.53E-01	2.97E-01	3.02E-01	3.00E-01	3	VL
079	1	6.11E-01	4.28E-01	4.34E-01	4.31E-01	3.24E-01	5.72E-01	4.67E-01	4.66E-01	4.66E-01	11	L
080	1	1.31E-01	1.23E-01	1.22E-01	1.22E-01	9.22E-02	1.63E-01	1.22E-01	1.23E-01	1.22E-01	19	H
080	2+3	1.64E+00	1.35E+00	1.31E+00	1.33E+00	1.00E+00	1.77E+00	1.29E+00	1.29E+00	1.29E+00	13	M
081	1	2.43E-01	1.58E-01	1.62E-01	1.60E-01	1.20E-01	2.13E-01	1.47E-01	1.48E-01	1.47E-01	10	L
081	2	4.97E-01	3.70E-01	3.30E-01	3.50E-01	2.63E-01	4.67E-01	3.54E-01	3.70E-01	3.62E-01	3	VL
082	1	8.78E-02	4.07E-02	4.04E-02	4.06E-02	3.04E-02	5.41E-02	4.25E-02	4.30E-02	4.28E-02	14	M
082	2	1.05E-01	1.13E-01	1.08E-01	1.11E-01	8.29E-02	1.47E-01	9.69E-02	9.62E-02	9.66E-02	6	VL
082	3	1.35E+00	1.05E+00	9.65E-01	1.01E+00	7.58E-01	1.35E+00	9.19E-01	9.12E-01	9.15E-01	5	VL
083	1	1.50E-01	1.43E-01	1.42E-01	1.42E-01	1.07E-01	1.89E-01	1.42E-01	1.40E-01	1.41E-01	18	H
083	2	1.53E+00	1.13E+00	1.26E+00	1.20E+00	9.02E-01	1.59E+00	1.17E+00	1.16E+00	1.16E+00	8	L
084	1	7.57E-02	3.09E-02	2.63E-02	2.86E-02	2.15E-02	3.80E-02	2.54E-02	2.58E-02	2.56E-02	4	VL
084	2	1.10E-01	1.51E-01	1.72E-01	1.61E-01	1.22E-01	2.14E-01	1.62E-01	1.60E-01	1.61E-01	7	VL
085	1	2.88E-01	1.92E-01	2.09E-01	2.00E-01	1.51E-01	2.66E-01	1.92E-01	1.96E-01	1.94E-01	9	L
085	2	2.88E-01	4.37E-01	4.32E-01	4.34E-01	3.27E-01	5.77E-01	3.43E-01	3.56E-01	3.50E-01	7	VL
086	1	1.13E-01	5.40E-02	4.99E-02	5.20E-02	3.74E-02	7.21E-02	6.31E-02	6.08E-02	6.20E-02	2	VL
087	1	3.13E-01	1.94E-01	1.95E-01	1.94E-01	1.46E-01	2.59E-01	1.94E-01	1.95E-01	1.95E-01	20	VH
088	1	1.23E-01	7.37E-02	7.34E-02	7.36E-02	5.52E-02	9.80E-02	7.37E-02	7.36E-02	7.37E-02	20	VH
088	2	8.00E-04	4.66E-02	5.13E-02	4.90E-02	3.67E-02	6.53E-02	4.92E-02	4.74E-02	4.83E-02	5	VL
089	1	9.00E-02	5.70E-02	5.69E-02	5.70E-02	4.10E-02	7.90E-02	5.66E-02	5.62E-02	5.64E-02	20	VH
089	2	2.16E-01	1.51E-01	1.50E-01	1.50E-01	1.08E-01	2.09E-01	1.41E-01	1.37E-01	1.39E-01	10	L
090	1	1.39E-01	8.11E-02	8.18E-02	8.15E-02	5.87E-02	1.13E-01	8.22E-02	8.17E-02	8.19E-02	20	VH
090	2	2.33E-01	1.93E-01	1.89E-01	1.91E-01	1.38E-01	2.65E-01	1.79E-01	1.77E-01	1.78E-01	12	M
091	1	6.14E-01	3.93E-01	4.10E-01	4.02E-01	2.89E-01	5.57E-01	4.07E-01	4.13E-01	4.10E-01	13	M
092	1	1.22E-01	8.66E-02	8.80E-02	8.73E-02	6.55E-02	1.16E-01	8.59E-02	8.64E-02	8.62E-02	18	H
093	1	1.20E-01	1.48E-01	1.46E-01	1.47E-01	1.10E-01	1.96E-01	1.49E-01	1.46E-01	1.48E-01	17	H
093	2	1.36E+00	1.09E+00	1.05E+00	1.07E+00	8.04E-01	1.43E+00	9.42E-01	9.39E-01	9.41E-01	7	VL
094	1	2.12E-01	1.86E-01	1.80E-01	1.83E-01	1.37E-01	2.44E-01	1.82E-01	1.80E-01	1.81E-01	16	M
095	1	7.07E-02	8.28E-02	8.90E-02	8.59E-02	6.47E-02	1.14E-01	7.85E-02	7.84E-02	7.85E-02	6	VL
095	2	8.96E-01	5.61E-01	4.97E-01	5.29E-01	3.98E-01	7.03E-01	5.35E-01	5.41E-01	5.38E-01	7	VL
096	1+2	5.35E-02	7.42E-02	7.29E-02	7.36E-02	5.52E-02	9.80E-02	7.41E-02	7.24E-02	7.33E-02	16	M
097	1	1.89E-01	9.62E-02	9.36E-02	9.49E-02	7.12E-02	1.27E-01	9.24E-02	9.07E-02	9.16E-02	14	M
097	2	6.67E-01	5.08E-01	5.38E-01	5.23E-01	3.92E-01	6.97E-01	5.30E-01	5.24E-01	5.27E-01	11	L
098	1+2	1.54E-01	5.57E-02	5.36E-02	5.47E-02	4.01E-02	7.44E-02	5.32E-02	5.42E-02	5.37E-02	14	M

098	3+4	5.01E-01	2.90E-01	4.26E-01	3.58E-01	2.63E-01	4.88E-01	3.48E-01	3.38E-01	3.43E-01	3	VL
099	1	1.27E-01	7.79E-02	8.42E-02	8.11E-02	5.95E-02	1.10E-01	8.02E-02	8.10E-02	8.06E-02	11	L
099	2+3+4	6.73E-01	5.32E-01	6.45E-01	5.88E-01	4.32E-01	8.01E-01	5.36E-01	5.41E-01	5.39E-01	6	VL

Table S3: A table of $\nu_{\min}$, $\nu_{\max}$, $\epsilon_{\max}$, and ν at $\epsilon_{\max}$ for each of the 164 transitions. Those were obtained from the higher resolution digitization used for the $f_{\text{exp,gl}}$ and $f_{\text{exp,nl}}$ data.

ID	Band	$\nu_{\min}$	$\nu_{\max}$	$\epsilon_{\max}$	ν at $\epsilon_{\max}$
000	1	42359	54873	10971	51860
001	1	41718	54825	10550	50128
002	1	39330	54832	10405	49851
003	1	37383	54918	11377	48914
004	1	39137	54853	25922	44827
005	1	36268	54846	24476	41154
006	1	36804	49535	5826	43960
007	1	37306	51108	18941	41819
008	1	40187	49711	13819	45323
009	1	39914	49308	14927	44941
010	1	23813	37857	3150	33568
011	2	37088	47612	20883	41743
012	1	20066	34864	1170	27443
012	2	34864	40627	10948	39539
013	1	22386	35775	1085	29223
013	2	35923	45191	10520	40300
014	1	24418	32775	10658	28702
014	2	32775	39935	5394	35294
015	1	34247	46141	11843	42548
015	2	46141	54542	12078	51122
016	1	34758	50043	3618	43277
017	2	41550	52933	4414	49486
018	2	31679	53032	1732	45441
019	2	32244	49046	1569	44719
020	1+2	25037	41830	16776	38158
021	1+2	22004	40218	13906	34582
022	1	20841	33406	17499	26659
022	2	33406	44993	20295	39530
023	2	25556	43304	1636	38001
024	2	28525	43657	10553	37804
025	2	24787	39897	11678	34329
026	2	26365	39890	22427	31644
026	3	39890	47019	14072	43743
027	1	16519	26079	46730	19410
027	2+3	26079	40228	12226	31332
028	1	14971	28398	25220	21288
029	1	17858	23207	652	21617
029	2	23207	39961	22689	28631
030	1	22068	33618	12007	29921
030	2	33618	40024	11615	38542
031	2	27095	40759	14084	33879
032	1	38085	50082	10943	44381
033	1	28584	41455	47744	32154
033	2	41591	47594	2779	46048
034	1+2+3	24175	42775	14306	32749
035	1	36108	47335	12845	43701

036	1	20047	35033	22313	25532
036	2	35033	46613	10467	40178
037	1	20175	34082	20584	27969
038	1+2	15176	30090	17957	23478
039	1	20054	32378	26560	26838
040	1	24620	31263	23796	28112
040	2	31263	38731	26817	34224
041	2+3	43506	54936	56160	52292
042	2	42969	48644	8384	47140
042	3	48644	54857	53151	51385
043	2	42913	48636	8458	47107
043	3	48636	54853	57646	51491
044	1	33529	41294	3121	34955
044	2+3	41294	54279	44732	49176
045	1	33825	40954	1977	34991
045	2+3	41103	54319	42242	48602
046	1	34662	41404	1481	37065
046	2	42179	49019	41503	52040
047	1	31659	38533	2566	34780
047	2	38533	46382	9968	42570
048	1	31058	35779	2276	33076
048	2	35779	44684	16149	38519
048	3	44684	53005	20297	49535
049	1+2	25184	44992	9055	39723
050	2	42474	48436	7810	46989
050	3	48436	54845	48055	51911
051	2	41842	48512	9536	45389
051	3	48512	54912	50474	51953
052	1	35218	40651	1006	36790
052	2	40651	48930	7453	47294
052	3	48930	54816	41871	52092
053	1	22342	31531	3048	28442
053	2	31531	40942	6260	35899
054	1	24482	31963	1907	30344
054	2	31963	40190	5848	36746
054	3	40190	45135	7604	43902
054	4	45135	51427	12252	47909
055	1	22944	39389	9214	31565
055	2	39389	47313	6428	44080
056	1	20947	33946	17404	24838
057	1	25763	36336	3374	30511
057	2	36471	43385	9168	39646
058	1	26754	37029	3490	32656
058	2	37029	43792	7883	40419
059	1	26179	36157	3564	30525
059	2	36157	43259	10597	39225
060	1	27505	35826	4583	31010
060	2	35826	43566	10104	39340
061	1	23041	35574	4927	27083
061	2	35574	40169	5914	38522
061	3	40169	46591	20988	43065
062	1	27338	41909	16172	35102
062	2	41909	47773	12574	44972
063	1	27443	38574	33667	30686
063	2	38574	46351	9054	42843

064	1	32243	36817	1926	34811
064	2+3	36817	45310	24078	40084
065	1	32465	37811	1293	35651
065	2+3	37811	54193	33155	51033
066	1	20402	35579	15065	26060
066	2	35579	46566	6689	43544
067	1	32050	38140	2865	34568
067	2	38140	44393	7879	41915
067	3	44393	50346	33980	49062
068	1	20419	31158	4293	24104
068	2	31158	37549	4285	35638
068	3	37549	48601	16045	43525
069	1	26025	42437	24024	35225
070	1	25959	42286	23482	34729
070	2	42286	47253	11654	45327
071	2	31948	44213	17292	39652
072	2	33079	43851	18643	39493
073	1	25704	36567	16381	29586
073	2	36567	44715	12977	41082
074	1	24930	37241	27024	30128
074	2	37241	45245	18013	41161
075	2+3	31884	42619	17938	37302
076	1	30422	40151	23786	34998
077	1	20110	30898	6578	23548
077	2+3	30898	46713	14234	38664
078	1	20998	35914	23553	26695
078	2	35914	46099	9778	43870
079	1	25043	37217	17069	31651
080	1	29950	39999	5045	33871
080	2+3	39999	52130	41771	47578
081	1	25979	36967	7434	29944
081	2	36967	43458	25409	40534
082	1	25637	32383	2846	28911
082	2	32639	38287	6056	35538
082	3	38287	46784	51149	41911
083	1	30454	40053	6825	35221
083	2	40053	49743	66586	44665
084	1	27022	31697	1928	29149
084	2	31697	38148	9826	35617
085	1	23735	37136	6508	30392
085	2	37260	44540	19058	42992
086	1	38057	45592	3492	42798
087	1	29024	38436	11992	31977
088	1	36467	45278	5371	39158
088	2	45430	51885	2900	49706
089	1	34250	42202	3734	36557
089	2	42202	50736	7197	46438
090	1	33459	40920	5581	36007
090	2	41077	49249	9389	44938
091	1	28984	42623	10984	37343
092	1	27387	34766	5355	30306
093	1	29594	39331	7099	33067
093	2	39331	49827	53283	43955
094	1	28481	38073	9784	31789
095	1	26931	37042	2891	31131

095	2	37042	44972	43790	41254
096	1+2	22004	36758	2207	26980
097	1	21954	34738	3162	27480
097	2	34738	44208	30740	39331
098	1+2	21138	34498	1607	29540
098	3+4	34498	48466	15362	45672
099	1	21847	31282	4220	25534
099	2+3+4	35018	47319	18945	44250

Figure S1. The plot of f_{comp} vs. $f_{exp,g}$ after excluding 37 “very low confidence” points from plot Fig. 3 left in the main manuscript. The points are colored by confidence level, as indicated in the legend. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands.

Figure S2. The plot of f_{comp} vs. ϵ_{max} for all 164 transitions. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands.

Figure S3. The plot of f_{comp} vs. $n \times f_{exp,g}$ for the 164 transitions, where n is the solvent refractive index, after excluding 37 “very low confidence” points from plot Fig. 4 left in the main manuscript. The points are colored by confidence level, as indicated in the legend. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands.

Figure S4. Left: f_{comp} vs. $n^{-1} \times f_{exp,g}$ for the 164 transitions, where n is the solvent refractive index. The points are colored by confidence level, as indicated in the legend. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands. **Right:** f_{comp} and $n^{-1} \times f_{exp,g}$ for each transition ordered by increasing strength of $n^{-1} \times f_{exp,g}$. The lines connecting the points are the absolute differences.

Figure S5. The plot of f_{comp} vs. $f_{exp,g}$ where the data points are colored according to the type of molecule. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands.

Figure S6. The plot of f_{comp} vs. $f_{exp,g}$ where the data points are colored according to the molecular charge. The blue line is a linear regression. The orange lines and area indicate 95% confidence bands for the data, while the green lines and area indicate the 95% mean confidence prediction bands.

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