Appendix A
The Discrete Dipole Approximation (DDA)

The discrete dipole approximation (DDA) is a computational method used to calculate the scattering, absorption, and extinction cross sections of particles of arbitrary size, shape, and material. The method was first proposed by Purcell and Pennypacker in 1973 to study light scattering by interstellar dust [1], but in recent years it has been found particularly well-suited to study the optical properties of non-spherical metal particles of all kinds [2–4]. The method has been implemented, reviewed and extended to 2-D periodic structures by Draine, Goodman, and Flatau [5, 6].

The main premise of the DDA is that any nanoparticle can be accurately represented by a cubic lattice of N point dipoles at positions, $\overrightarrow{r_i}\{i = 1, 2, \ldots, N\}$, each characterized by a polarizability α_i. The dipoles are subject to an incident monochromatic plane wave, $\vec{E}_{inc,i}(\vec{r}_i, t) = \vec{E}_0 e^{i\left(\vec{k}\cdot\vec{r}_i - \omega t\right)}$, and to the induced fields, $\vec{E}_{dip,i}(\vec{r}_i, t)$, from all other $N - 1$ dipoles. The local field at each dipole position is given by Eq. A.1.

$$\vec{E}_{loc,i}(\vec{r}_i, t) = \vec{E}_{inc,i}(\vec{r}_i, t) + \vec{E}_{dip,i}(\vec{r}_i, t) = \vec{E}_0 e^{i\vec{k}\cdot\vec{r}_i} - \sum_{i\neq j}^{N}\left(\vec{A}_{ij}\cdot\vec{P}_j\right) \tag{A.1}$$

$\vec{P}_j$ is the dipole moment of the jth dipole and $\vec{A}_{ij}$ is the Maxwellian interaction matrix describing the electromagnetic interaction of dipoles j and i. The product of these is given by Eq. A.2.

$$\vec{A}_{ij}\cdot\vec{P}_j = \frac{e^{i\vec{k}\cdot\vec{r}_{ij}}}{\left|\vec{r}_{ij}\right|^3}\left\{\left|\vec{k}\right|^2\vec{r}_{ij}\times\left(\vec{r}_{ij}\times\vec{P}_j\right) + \frac{1 - i\vec{k}\cdot\vec{r}_{ij}}{\left|\vec{r}_{ij}\right|^2}\left[\left|\vec{r}_{ij}\right|^2\vec{P}_j - 3\vec{r}_{ij}\left(\vec{r}_{ij}\cdot\vec{P}_j\right)\right]\right\} i \neq j \tag{A.2}$$

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The dipole moment of the *i*-th dipole is determined by the local electric field and the polarizability (Eq. A.3).

$$\vec{P}_i = \alpha_i \vec{E}_{loc,i}(\vec{r}_i, t) \tag{A.3}$$

Once the induced dipole moment of each dipole is found, the extinction, scattering and absorption cross sections of that particle can be calculated using well-established optical theorems (Eq. A.4) [7].

$$\begin{aligned} C_{ext} &= \frac{4\pi\left|\vec{k}\right|}{\left|\vec{E}_0\right|^2} \sum_{i=1}^{N} Im\left(\vec{E}_{inc,i} \cdot \vec{P}_i\right) \\ C_{abs} &= \frac{4\pi\left|\vec{k}\right|}{\left|\vec{E}_0\right|^2} \sum_{i=1}^{N} \left\{ Im\left(\frac{\vec{P}_i}{\alpha_i} \cdot \vec{P}_i\right) - \frac{2k^3}{3}\left|\vec{P}_i\right|^2 \right\} \\ C_{scat} &= C_{ext} - C_{abs} \end{aligned} \tag{A.4}$$

These equations constitute a set of $3N$ complex coupled linear equations that are solvable only by a numerical iterative approach. We will not go further into the computational details used to solve the equations, as these are described and reviewed elsewhere [3, 6, 8]. It is, however, appropriate to mention that we use the publicly available software package "DDSCAT ver. 7.3" developed and maintained by Draine and Flatau [9].

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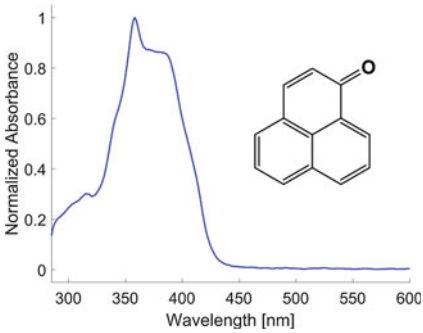
Appendix B
Sensitizers and Probes

This appendix provides an overview of the photophysical parameters of the chemical compounds used in this work. All absorbance spectra are recorded in toluene solution, except the spectrum of ADA which is recorded in phosphate-buffered D_2O.

1-Phenalenone (PN)



Solvent	Φ_Δ	ε (λ_{max})/$M^{-1}cm^{-1}$
Toluene	0.92 ± 0.03[a]	10,360 (358 nm)[b]
Acetonitrile	1.00 ± 0.03[a]	
Cyclohexane	0.91 ± 0.03[a]	
Ethanol	0.92 ± 0.03[a]	
Dichloromethane	0.96 ± 0.08[a]	

[a]From Marti et al. [2]
[b]From Arnbjerg et al. [4]

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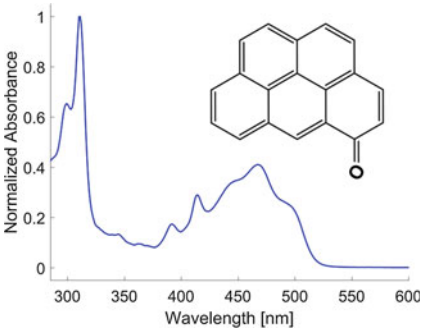
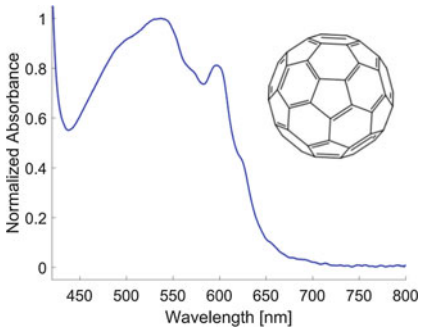
Benzo[*cd*]pyren-5-one (BP)



Solvent	Φ_Δ	ε (λ_{max})/$M^{-1}cm^{-1}$
Toluene	0.96 ± 0.05[a]	13,030 (467 nm)[a]
Acetonitrile	0.92 ± 0.06[a]	

[a]From Arnbjerg et al. [4]

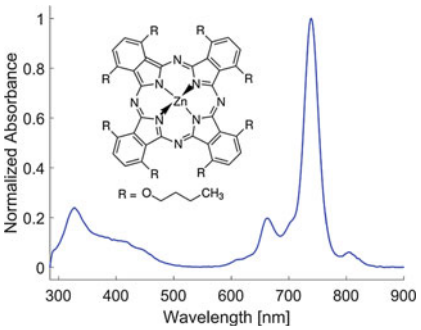
Buckminster Fullerene (C_{60})



Solvent	Φ_Δ (λ_{exc})	ε (λ_{max})/$M^{-1}cm^{-1}$
Benzene	0.76 (355 nm)[a] 0.96 (532 nm)[a] 0.98 (340 nm)[b] 0.92 (530 nm)[b]	3400 (535 nm)[a]
Toluene	1.01 (510 nm)[c]	

[a]From Arbogast et al. [3]
[b]From Terazima et al. [7]
[c]From Hung and Gabrowski [10]

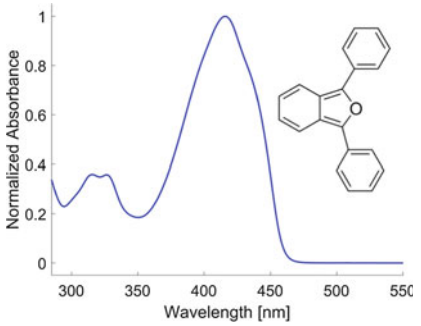
Zinc 1,4,8,11,15,18,22,25-octabutoxy-29*H*,31*H*-phthalocyanine ($ZnPc(oBu)_8$)



Solvent	Φ_Δ	ε (λ_{max})/$M^{-1}cm^{-1}$
Benzene	0.45 ± 0.05[a]	190,000 (739 nm)[a]
Benzene-d_6	0.50 ± 0.05[a]	
Toluene	0.60 ± 0.05[b]	
Acetonitrile	0.68 ± 0.05[b]	

[a]From Ford et al. [1]
[b]From Bregnhøj et al. [5]

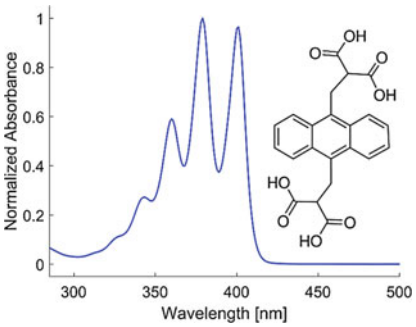
1,3-Diphenylisobenzofuran (DPBF)



Solvent	k_{rxn} (10^7 $M^{-1}s^{-1}$)	k_{trap} (10^7 $M^{-1}s^{-1}$)
Toluene	78 ± 4[a]	80.7 ± 1.2[a] 89[b] 67[c] 81[d]
Acetonitrile	136 ± 9[a]	158 ± 4[a] 110[c] 130[e]

[a]From Bregnhøj et al. [5]
[b]From Gorman et al. [6]
[c]From Gorman et al. [9]
[d]From Gorman et al. [12]
[e]From Peters and Rodgers [13]

9,10-Anthracenediyl-bis(methylene)dimalonic acid (ADA)



Solvent	k_{rxn} (10^7 $M^{-1}s^{-1}$)	k_{trap} (10^7 $M^{-1}s^{-1}$)
D_2O-PBS[a]	5.6 ± 0.3[b] 5.5 ± 0.5[c] 1.3[d]	6.0 ± 0.4[b] 0.55[d]

[a]Phosphate buffer solution of D_2O
[b]From Bregnhøj et al. [5]
[c]From Lybech et al. [8]
[d]From Lebrun et al. [11]

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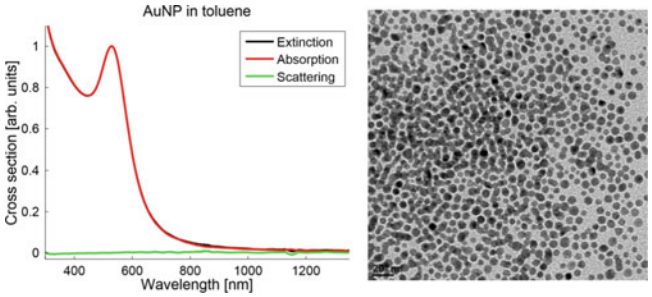
Appendix C
Nanoparticles

This appendix provides an overview of our arsenal of nanoparticles. All spectra are recorded in chloroform solution, except for sample 1 which is recorded in toluene.

Sample 1: Gold nanoparticles (AuNP1)



Sample #	1
Name	AuNP1
Solvent	Toluene
Diameter	≈5 nm
λ_{max}	529 nm
η	0.0004

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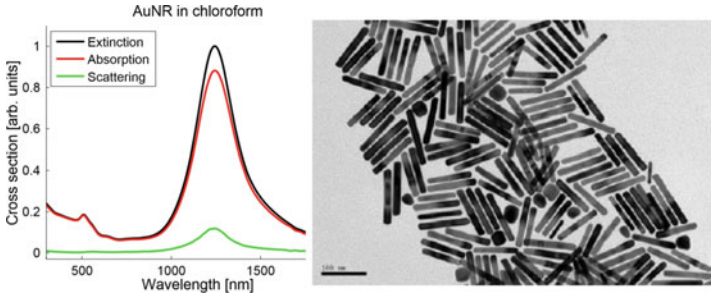
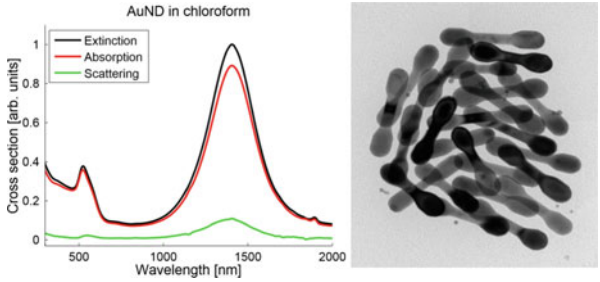
Sample 2: Gold nanorods (AuNR1)



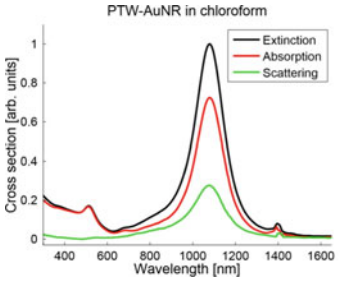
Sample #	2
Name	AuNR1
Solvent	Chloroform and toluene
Length	107.4 ± 12.9 nm
Diameter	14.9 ± 1.5 nm
λ_{max}	1244 nm
η	0.12

Sample 3: Gold nanodumbbells (AuND)



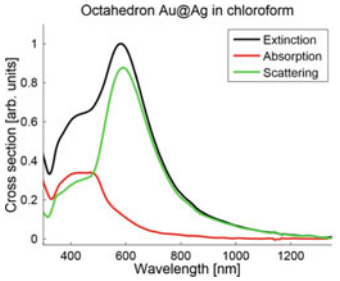
Sample #	3
Name	AuND
Solvent	Chloroform
Length	≈ 130 nm
Diameter	≈ 20 nm
λ_{max}	1408 nm
η	0.11

Sample 4: Penta-twinned gold nanorods (PTW-AuNR)



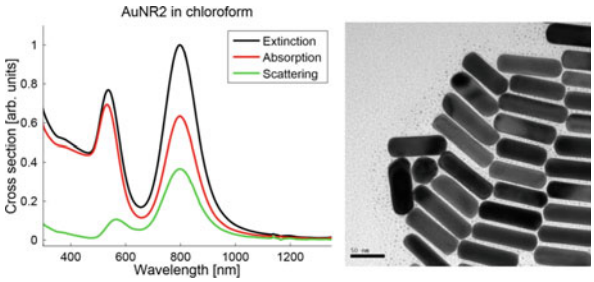
Sample #	4
Name	PTW-AuNR
Solvent	Chloroform
Length	132.7 ± 9.6 nm
Diameter	27.6 ± 2.4 nm
λ_{max}	1079 nm
η	0.28

Sample 5: Gold octahedrons with silver coating (Octa-Au@Ag)



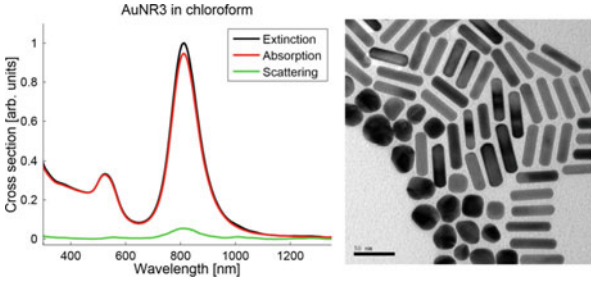
Sample #	5
Name	Octa-Au@Ag
Solvent	Chloroform
Diameter	94.0 ± 5.0 nm
Shell thickness	≈16 nm
λ_{max}	581 nm
η	0.88

Sample 6: Gold nanorods 2 (AuNR2)



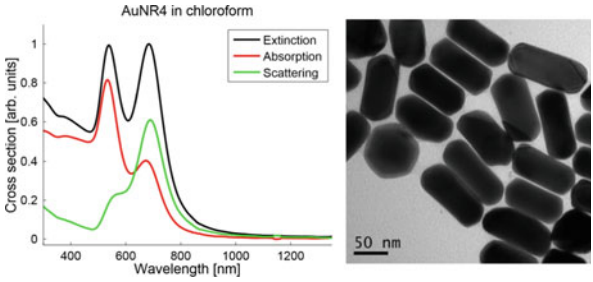
Sample #	6
Name	AuNR2
Solvent	Chloroform
Length	91.4 ± 9.0 nm
Diameter	27.0 ± 2.3 nm
λ_{max}	798 nm
η	0.37

Sample 7: Gold nanorods 3 (AuNR3)



Sample #	7
Name	AuNR3
Solvent	Chloroform
Length	53.6 ± 3.7 nm
Diameter	13.8 ± 1.1 nm
λ_{max}	812 nm
η	0.055

Sample 8: Gold nanorods 4 (AuNR4)



Sample #	8
Name	AuNR4
Solvent	Chloroform
Length	97.5 ± 6.7 nm
Diameter	43.8 ± 3.3 nm
λ_{max}	684 nm
η	0.61

Appendix D
Data Compilation on $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g^+)$

The tables below are by no means an exhaustive compilation of all published data, but they represent what we believe are the most accurately known values to date at room-temperature. The data have been critically compiled from publications that have the dedicated purpose of investigating the effects of solvent on the photophysics of $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g^+)$ (Tables D.1, D.2, D.3 and D.4).

Table D.1 The lifetime of $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g^+)$

Solvent	τ_Δ (μs)	τ_Σ (ps)
Water	3.5 ± 0.1[a]	8.2 ± 0.8[h]
Water-d_2 (D_2O)	68.9 ± 1.4[a]	42 ± 4.2[h]
Methanol	9.9 ± 0.3[a]	18 ± 1.8[h]
Methanol-*d* (CH_3OD)	31.4 ± 0.6[a]	–
Methanol-d_4 (CD_3OD)	276 ± 6[a]	94 ± 9.4[h]
Ethanol	15.3 ± 0.8[d]	–
Ethanol-*d*	30.5 ± 0.5[d]	–
Ethanol-d_6	23[d]	–
1-propanol	15.9 ± 0.3[a]	–
2-propanol	22.1 ± 1.1[d]	–
2-methyl-2-propanol	30.8 ± 1.5[d]	–
2-methyl-1-propanol	21.1 ± 1.1[d]	–
1-butanol	17.5 ± 0.9[d]	–
2-butanol	19.7 ± 1.0[d]	–
1-pentanol	17.8 ± 0.9[d]	–
1-hexanol	17.9 ± 0.9[d]	–
Cyclohexanol	15.1 ± 0.8[d]	–
1-heptanol	18.1 ± 0.9[d]	–

(continued)

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Table D.1 (continued)

Solvent	τ_Δ (μs)	τ_Σ (ps)
1-octanol	18.5 ± 0.3[a]	–
1-nonanol	18.6 ± 0.9[d]	–
1-decanol	17.8 ± 0.9[d]	–
2,2,2-trifluoroethanol	30.5 ± 1.0[a]	–
Acetone	45.6 ± 0.9[a]	123 ± 12[h]
Acetone-d_6	1039 ± 21[a]	294 ± 29[h]
Acetonitrile	81 ± 1.6[a]	134 ± 13[h]
Acetonitrile-d_3	1610 ± 32[a]	613 ± 61[h]
Benzonitrile	40.0 ± 0.8[a]	–
Benzene	30.4 ± 0.6[a]	135 ± 14[h]
Benzene-d_6	747 ± 15[a]	279 ± 28[h]
Toluene	30.5 ± 0.6[a]	–
Toluene-d_8	314 ± 6[a]	–
o-xylene	23.4 ± 0.5[a]	–
o-xylene-d_{10}	87 ± 2[b]	–
Mesitylene	16.9 ± 0.3[a]	–
Mesitylene-d_{12}	31.8 ± 0.6[b]	–
Ethylbenzene	26[d]	–
Butylbenzene	25[d]	–
Benzyl alcohol	14.4 ± 0.3[a]	–
Trifluorotoluene	61.7 ± 1.2[a]	–
Fluorobenzene	45.8 ± 2.5[d]	–
Chlorobenzene	43.6 ± 0.9[a]	–
Bromobenzene	42.5 ± 0.2[c]	–
Bromobenzene-d_5	1360 ± 20[e]	–
Iodobenzene	38.9 ± 0.8[a]	–
o-dichlorobenzene	57.0 ± 1.1[a]	–
1,2,4-trichlorobenzene	93.8 ± 1.9[a]	–
Hexafluorobenzene	35,000 ± 1000[g]	12,600 ± 1260[h]
Chloropentafluorobenzene	24,500 ± 2000[e]	–
Bromopentafluorobenzene	21,900 ± 1000[e]	–
Iodopentafluorobenzene	15,100 ± 1000[e]	–
Tetrahydrofuran (THF)	23.5 ± 4[d]	–
1,4-dioxane	26.7 ± 1.3[d]	–
Cyclohexane	24.0 ± 0.48[a]	83 ± 8.3 [h]
Cyclohexane-d_{12}	483 ± 10[a]	–
n-pentane	34.8 ± 0.7[a]	–
2,2,4-trimethylpentane (isooctane)	37.6 ± 1.9[d]	–
n-hexane	32.2 ± 0.6[a]	–
n-heptane	30.1 ± 0.6[a]	–

(continued)

Table D.1 (continued)

Solvent	τ_Δ (μs)	τ_Σ (ps)
n-octane	28.6 ± 0.6[a]	–
n-decane	26.5 ± 0.5[a]	–
Carbon tetrachloride	128,000 ± 12,800[f]	150,000 ± 15,000[h]
Chloroform	229 ± 12[f]	1180 ± 118[h]
Chloroform-*d*	9400 ± 500[g]	2220 ± 222[h]
Dichloromethane	95.7 ± 1[c]	–
Dichloromethane-d_2	120[d]	–
1,2-dichloroethane	63.2 ± 3.16[d]	–
Tetrachloroethylene	1250 ± 50[d]	200,000 ± 20,000[h]
Diiodomethane	55.5 ± 0.4[c]	–
Perchlorobutadiene	–	90,000 ± 9000[h]
Perfluorohexane	214,000 ± 21,400[f]	–
1-iodoperfluorohexane	53,000 ± 5300[f]	–
1,2-dibromotetrafluoroethane	111,000 ± 11,100[f]	–
1,1,2-trichloro-1,2,2-trifluoroethane	133,000 ± 13,300[f]	47,700 ± 4770[h]
Trichlorofluoromethane (Freon 11)	24,000 ± 1000[g]	–
Diethyl ether	30.4 ± 1.5[d]	–
Ethyl acetate	45[d]	–
Carbon disulfide	79,000 ± 7900[f]	300,000 ± 30,000[h]
Perfluorodecalin	309,000 ± 30,900[f]	–
N,N-dimethylformamide (DMF)	19.3 ± 4.5[d]	–

[a]From Bregnhøj et al. [1]
[b]Unpublished data
[c]From Bregnhøj et al. [2]
[d]From the database of Wilkinson et al. [3]. The given value is the average of selected entries in this compilation with the standard deviation given as the error
[e]From Schmidt [4]
[f]From Schmidt and Afshari [5]
[g]From Schmidt and Brauer [6]
[h]From Weldon et al. [7] and references therein

Table D.2 Spectral data for the $O_2(a^1\Delta_g) \rightarrow O_2(X^3\Sigma_g^-)$ transition

Solvent	ν_{max}^{aX} (cm^{-1})	$\Delta\nu_{FWHM}^{aX}$ (cm^{-1})	k_r^{aX} (s^{-1})
Gas-phase	7882.4[b]	–	2.3×10^{-4}[h]
Water	7849.1 ± 3[a]	108.4 ± 6[a]	0.16 ± 0.016[e,f]
Water-d_2 (D_2O)	7849.7 ± 1[a]	108.3 ± 2[a]	0.19 ± 0.019[e,f]
Methanol	7853.2 ± 1[a]	125.4 ± 2[a]	0.35 ± 0.035[e,f]
Methanol-d_4	7851.4 ± 1[a]	122.9 ± 4[a]	–
Ethanol	7856.8 ± 3[a,b]	119.8 ± 6[a,b]	0.55 ± 0.055[g]
Ethanol-d (CH_3CH_2OD)	–	–	0.35 ± 0.035[e]
Ethanol-d_6	7856.5 ± 1[a]	120.3 ± 2[a]	–
1-propanol	7855.6 ± 1[a]	111.7 ± 2[a]	0.47 ± 0.047[e]
2-propanol	–	–	0.47 ± 0.047[g]
1-butanol	7853.8 ± 1[a]	104.5 ± 2[a]	0.44 ± 0.044[e]
2-butanol	–	–	0.57 ± 0.057[e]
1-pentanol	7852.3 ± 1[a]	102.2 ± 2[a]	–
1-hexanol	7851.7 ± 1[a]	98.5 ± 2[a]	–
1-octanol	7851.2 ± 1[a]	96.8 ± 2[a]	–
1-nonanol	7850.4 ± 1[a]	95 ± 2[a]	–
1-decanol	7850.2 ± 1[a]	95.1 ± 2[a]	–
2,2,2-trifluoroethanol	7869.2 ± 1[a]	84.5 ± 2[a]	0.25 ± 0.025[e,f]
Acetone	7852.6 ± 1[a]	121.1 ± 2[a]	0.56 ± 0.056[e,f]
Acetone-d_6	7849.0 ± 1[a,b]	114 ± 5[a,b]	–
Acetonitrile	7851.5 ± 1[a]	125.3 ± 2[a]	0.45 ± 0.045[e]
Acetonitrile-d_3	7849.9 ± 1[a,b]	122.2 ± 4[a,b]	–
Benzonitrile	7836.3 ± 1[a]	106.3 ± 2[a]	1.80 ± 0.18[e]
1,1,1-trifluoro acetic acid	7873.2 ± 3[a]	86.9 ± 6[a]	–
1,1,1-trifluoro acetic acid-d_1	7870.8 ± 3[b]	90 ± 15[b]	–
Formic acid	–	–	0.25 ± 0.025[g]
Propionic acid	–	–	0.79 ± 0.079[g]
Benzene	7839.5 ± 1[a]	115.9 ± 2[a]	1.50 ± 0.15[e,f]
Benzene-d_6	7838.8 ± 2[a,b]	115.9 ± 1[a,b]	1.34 ± 0.13[f]
Toluene	7839.7 ± 1[a,c]	112.9 ± 2[a,c]	1.44 ± 0.14[e]
Toluene-d_8	7838.8 ± 1[b]	114 ± 5[b]	1.47 ± 0.15[g]
p-xylene	7840.6 ± 1[a]	109.6 ± 2[a]	1.70 ± 0.17[g]
Mesitylene	–	–	1.72 ± 0.17[g]
1,2,4-trimethylbenzene	–	–	2.00 ± 0.20[g]
Benzyl alcohol	7832.5 ± 2[a,b]	115.4 ± 9[a,b]	–
Trifluorotoluene	7856.2 ± 1[a]	94.5 ± 2[a]	1.14 ± 0.11[e]
1,3-dibromobenzene	–	–	2.72 ± 0.27[e]
Fluorobenzene	7844.4 ± 1[a]	107.2 ± 2[a]	1.28 ± 0.13[e]
Chlorobenzene	7839.6 ± 1[a]	109.6 ± 2[a]	1.68 ± 0.17[e]
Bromobenzene	7832.8 ± 1[a]	112.4 ± 2[a]	1.97 ± 0.20[e]

(continued)

Table D.2 (continued)

Solvent	ν_{max}^{aX} (cm^{-1})	$\Delta\nu_{FWHM}^{aX}$ (cm^{-1})	k_r^{aX} (s^{-1})
Bromobenzene-d_5	–	–	2.07 ± 0.21[f]
Iodobenzene	7824.1 ± 1[a]	123.7 ± 2[a]	2.61 ± 0.26[e]
Hexafluorobenzene	7867.4 ± 1[b]	82.5 ± 5[b]	0.51 ± 0.051[f]
Chloropentafluorobenzene	7862.6 ± 1[b]	95.0 ± 5[b]	0.89 ± 0.089[f]
Bromopentafluorobenzene	7859.1 ± 1[b]	88.3 ± 5[b]	1.25 ± 0.13[f]
Iodopentafluorobenzene	7852.7 ± 1[b]	96.3 ± 5[b]	1.23 ± 0.12[f]
Anisole	–	–	1.80 ± 0.18[g]
p-chloroanisole	–	–	2.20 ± 0.22[g]
p-bromoanisole	–	–	1.90 ± 0.19[g]
1,3-dimethoxybenzene	–	–	1.90 ± 0.19[g]
Tetrahydrofuran (THF)	7848.1 ± 1[a]	118.5 ± 2[a]	0.62 ± 0.062[e]
1,4-dioxane	7841.6 ± 1[a]	119.3 ± 2[a]	0.56 ± 0.056[e]
Pyridine	7834.7 ± 1[c]	116.8 ± 2[c]	–
Pyridine-d_5	7831.6 ± 3[b]	117 ± 15[b]	–
1-methylnaphthalene	7825.5 ± 1[a]	116.7 ± 2[a]	2.77 ± 0.28[e]
1-bromonaphthalene	7824.4 ± 1[a]	112.0 ± 2[a]	3.11 ± 0.31[e]
2-ethylnaphthalene	–	–	2.03 ± 0.20[e]
Cyclohexane	7853.8 ± 1[a]	101.8 ± 2[a]	0.66 ± 0.066[e]
n-pentane	7859.8 ± 1[a]	97.1 ± 2[a]	0.47 ± 0.047[g]
n-hexane	7858.2 ± 1[a]	97.6 ± 2[a]	0.60 ± 0.060[g]
n-heptane	7856.8 ± 1[a]	96.0 ± 2[a]	0.66 ± 0.066[e]
n-octane	7858.0 ± 1[a]	94.1 ± 2[a]	–
n-nonane	7855.0 ± 1[a]	94.2 ± 2[a]	–
n-decane	7854.2 ± 1[a]	93.6 ± 2[a]	–
1-hexene	7855.2 ± 1[a]	102.4 ± 2[a]	–
Carbon tetrachloride (CCl_4)	7849.7 ± 1[a,b]	102.8 ± 4[a,b]	1.06 ± 0.11[e,f,g]
Chloroform	7848.1 ± 2[a,b]	106.8 ± 9[a,b]	1.05 ± 0.11[e,f]
Chloroform-d_1	7846.8 ± 1[b]	107.3 ± 5[b]	–
Dichloromethane	7837.0 ± 3[b]	125 ± 15[b]	0.75 ± 0.075[e]
Dichloromethane-d_2	7845.0 ± 1[b]	113.8 ± 5[b]	–
Dibromomethane	–	–	0.80 ± 0.080[g]
1,2-dichloroethane	–	–	0.75 ± 0.075[g]
Tetrachloroethylene	7847.0 ± 1[a,b]	93.2 ± 4[a,b]	1.89 ± 0.19[f]
Diiodomethane	7800[d]	–	4.08 ± 0.41[e]
1-iodopropane	–	–	1.44 ± 0.14[e]
Perchlorobutadiene	7844.2 ± 1[b]	92.5 ± 5[b]	1.85 ± 0.19[f]
Dibromodifluoromethane	7857.7 ± 1[b]	99.5 ± 5[b]	–
Perfluorohexane	7881.5 ± 1[b]	74.0 ± 5[b]	–
1-iodoperfluorohexane	–	–	1.41 ± 0.14[f]
1,2-dibromotetrafluoroethane	7863.5 ± 1[b]	94.5 ± 5[b]	1.40 ± 0.14[f]

(continued)

Table D.2 (continued)

Solvent	ν_{max}^{aX} (cm^{-1})	$\Delta\nu_{FWHM}^{aX}$ (cm^{-1})	k_r^{aX} (s^{-1})
1,1,2-trichloro-1,2,2-trifluoroethane	7865.4 ± 1[b]	92.5 ± 5[b]	–
Trichlorofluoromethane (Freon 11)	7859.4 ± 1[b]	99.5 ± 5[b]	–
Diethyl ether	–	–	0.62 ± 0.062[g]
Diphenyl ether	–	–	2.0 ± 0.20[g]
2-nitropropane	–	–	0.19 ± 0.019[g]
Acetic anhydride	–	–	0.53 ± 0.053[g]
Diphenyl sulfide	–	–	2.66 ± 0.27[e]
Carbon disulfide (CS_2)	7828.3 ± 1[a,b]	122.1 ± 4[a,b]	3.13 ± 0.31[e,f]
Perfluorodecalin	7882.2 ± 1[b]	68.0 ± 5[b]	–
Perfluoroperhydrophenanthrene	7881.8 ± 1[b]	63.5 ± 5[b]	–
N,N-dimethylformamide (DMF)	–	–	0.63 ± 0.063[g]

[a]From Wessel and Rodgers [8]
[b]From MacPherson and Truscott [9]
[c]From Dam et al. [10]
[d]From Ogilby [11]
[e]From Poulsen et al. [12] and references therein
[f]From Hild and Schmidt [13] and references therein
[g]From Darmanyan [14] and references therein
[h]From Schweitzer and Schmidt [15]

Table D.3 Spectral data for the $O_2(b^1\Sigma_g^+) \rightarrow O_2(a^1\Delta_g)$ transition

Solvent	ν_{max}^{ab} (cm^{-1})	$\Delta\nu_{FWHM}^{ab}$ (cm^{-1})	ε_{max}^{ab} ($M^{-1}cm^{-1}$)	k_r^{ba} (s^{-1})
Gas-phase	5241[d]	–	–	0.0025[d]
Water-d_2 (D_2O)	5228 ± 6[a]	75 ± 4[a]	6 ± 2[a]	199 ± 67[a,b]
Methanol	5217 ± 4[b,c]	84 ± 8[b,c]	7 ± 3[b]	235 ± 93[b]
2-propanol	5208 ± 3[b]	62 ± 5[b]	12 ± 5[b]	356 ± 101[b]
1-octanol	5191 ± 3[b]	60 ± 5[b]	21 ± 6[b]	626 ± 146[b]
Acetone	5218 ± 3[b]	82 ± 5[b]	14 ± 3[b]	507 ± 120[b]
Acetonitrile	5223 ± 4[b,c]	81 ± 8[b,c]	16 ± 5[b]	528 ± 153[b]
Benzonitrile	5194 ± 2[b,c]	80 ± 4[b,c]	36 ± 5[b]	1413 ± 236[b]
Acetic acid	5223 ± 3[b]	79 ± 5[b]	10 ± 4[b]	373 ± 91[b]
Benzene	5197 ± 2[b,c]	76 ± 4[b,c]	32 ± 3[b]	1289 ± 187[b]
Toluene	5191 ± 2[b,c]	73 ± 4[b,c]	30 ± 4[b]	1146 ± 161[b]
o-xylene	5191 ± 3[b]	73 ± 5[b]	35 ± 5[b]	1396 ± 204[b]
p-xylene	5190 ± 1[c]	73 ± 2[c]	–	–
Mesitylene	5194 ± 3[b,c]	72 ± 5[b,c]	35 ± 5[b]	1378 ± 206[b]
Bromobenzene	5184 ± 3[b]	68 ± 5[b]	43 ± 5[b]	1671 ± 225[b]
Tetrahydropyran	5202 ± 1[c]	83 ± 2[c]	–	–
Tetrahydrofuran (THF)	5207 ± 1[c]	84 ± 2[c]	–	–
1,4-dioxane	5212 ± 1[c]	92 ± 2[c]	–	–
Cyclohexane	5193 ± 1[c]	73 ± 2[c]	–	–
n-hexane	5199 ± 2[b,c]	69 ± 4[b,c]	23 ± 4[b]	777 ± 146[b]
Carbon tetrachloride (CCl_4)	5195 ± 2[b,c]	71 ± 4[b,c]	26 ± 6[b]	854 ± 192[b]
1,1,2-trichloro-1,2, 2-trifluoroethane (Freon 113)	5209 ± 2[b,c]	62 ± 4[b,c]	26 ± 4[b]	659 ± 138[b]
Carbon disulfide (CS_2)	5168 ± 2[b,c]	89 ± 4[b,c]	49 ± 5[b]	2528 ± 324[b]

[a]From Andersen et al. [16]
[b]From Bregnhøj and Ogilby [17]
[c]From Dam et al. [10]
[d]From Noxon [18]

Table D.4 Spectral data for the $O_2(b^1\Sigma_g^+) \rightarrow O_2(X^3\Sigma_g^-)$ transition

Solvent[a]	ν_{max}^{Xb} (cm^{-1})	$\Delta\nu_{FWHM}^{Xb}$ (cm^{-1})	ε_{max}^{Xb} (10^{-4} $M^{-1}cm^{-1}$)	k_r^{bX} (s^{-1})
Gas-phase	13,120[b]	–	–	0.087[b]
Water-d_2 (D_2O)	13,084 ± 10	101 ± 10	13.4 ± 1.6	0.56 ± 0.10
Methanol	13,089 ± 10	117 ± 12	7.1 ± 0.8	0.34 ± 0.05
1-octanol	13,060 ± 12	119 ± 12	7.3 ± 1.7	0.41 ± 0.13
2,2,2-trifluoroethanol	13,113 ± 14	153 ± 12	7.0 ± 0.8	0.41 ± 0.06
Acetone	13,096 ± 10	113 ± 10	8.8 ± 1.0	0.43 ± 0.07
Acetonitrile	13,094 ± 12	122 ± 12	7.8 ± 0.9	0.40 ± 0.07
Benzonitrile	13,057 ± 10	131 ± 9	9.7 ± 1.5	0.69 ± 0.11
Toluene	13,045 ± 7	116 ± 7	17.5 ± 2.0	1.05 ± 0.14
Chlorobenzene	13,058 ± 17	135 ± 15	15.2 ± 1.7	1.10 ± 0.17
Bromobenzene	13,034 ± 12	165 ± 10	40.9 ± 4.7	3.78 ± 0.50
Iodobenzene	13,002 ± 20	237 ± 17	387 ± 48	55.2 ± 7.5
Cyclohexane	13,062 ± 9	111 ± 10	12.3 ± 1.4	0.65 ± 0.10
Carbon tetrachloride (CCl_4)	13,065 ± 7	114 ± 9	12.6 ± 1.4	0.71 ± 0.10
Dichloromethane	13,074 ± 12	128 ± 9	7.6 ± 1.1	0.46 ± 0.08
Diiodomethane	12,957 ± 24	284 ± 20	190 ± 61	37.2 ± 12.2
Carbon disulfide (CS_2)	13,011 ± 12	130 ± 12	14.7 ± 1.7	1.16 ± 0.17

[a]All solution phase data are from Bregnhøj et al. [2]
[b]From Ritter and Wilkerson [19]

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