Supplementary Material

The complex internal dynamics of diphenylether and its aggregates with water

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Contents

S1 Experimental Methods

S1.1 R2PI and IR/R2PI technique

The experimental setup for the IR/UV experiments is described in detail elsewhere,[1,2] thus only a short description of the method is given here. The R2PI technique offers the possibility to obtain different vibrational frequencies in the excited state of a specific conformer. In the IR/R2PI method the R2PI process generates a constant ion signal. If a tunable IR laser excites a vibration and arrives prior to the UV laser(s), the ground state is depopulated and less molecules are electronically excited and ionized. This leads to a depletion of the ion signal. In order to obtain IR/R2PI spectra the IR laser was fired 50 ns prior to the UV laser.

S1.2 ILSR and IGSR spectroscopy

The vibrational spectra of Raman active vibrations can be studied by monitoring the Raman-induced depletion/increase of the ion signal as a function of the wavelength of the respective tuneable laser beams. The ground state is depopulated by a pump photon (υ_p) which pumped the molecules from the ground state to a virtual level. Hereon a tunable photon (υ_s) dumped the molecules to an electronically excited state of the ground state. After the Stimulated Raman process the ionization takes place. In case of the ILSR method the ionization occurs from the ground state, in case of the IGSR method from an excited vibrational level of the ground state. By using the Loss method the Raman active vibrations are measured as a depletion of a constant ion signal. By using the IGSR method no ion signal can be observed because the energy of the UV photons is too low to exceed the ionization potential. The ionization process can only occur when the sum of the energy of the vibration (υ_p-υ_s) and the energy of the UV photons is sufficient to exceed the ionization potential. Thus the IGSR measurements were carried out against a zero baseline and show a clearly better signal to noise ratio than the results by ILSR spectroscopy. However it always depends on the investigated system which of the two methods can be applied.

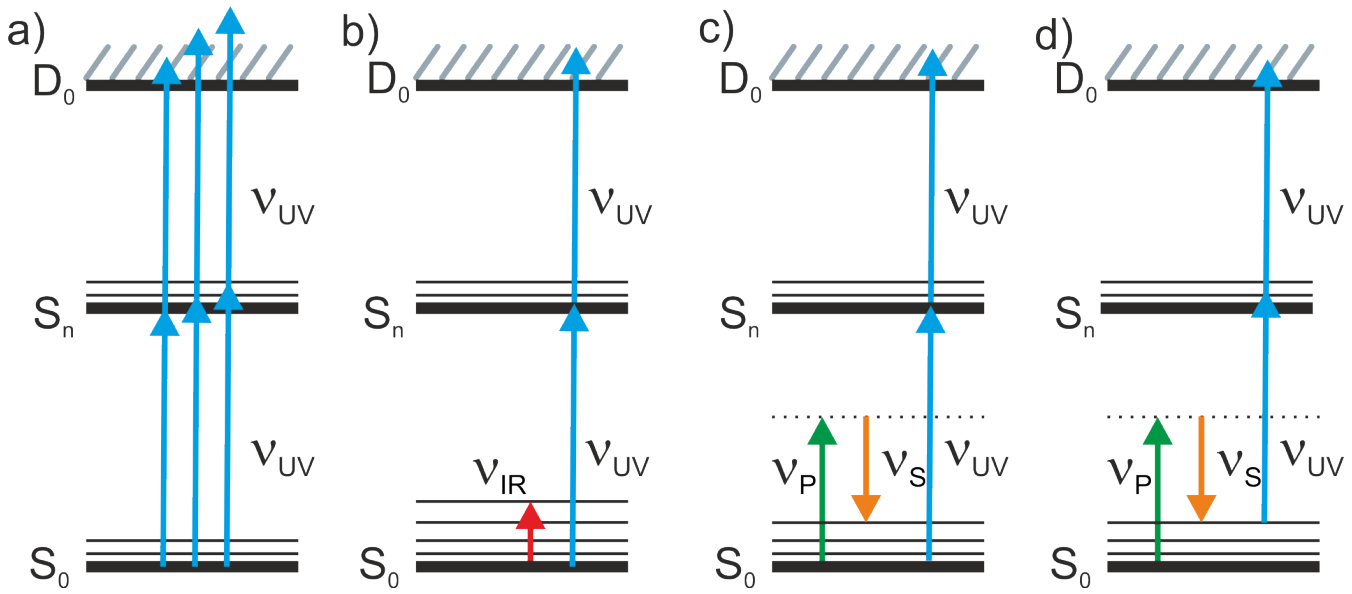

Fig. S1 Schemes for different methods a) one-color resonant two-photon ionization (R2PI), b) InfraRed/resonant two-photon ionization (IR/R2PI), c) Ionization Loss Stimulated Raman Spectroscopy (ILSRS) and the c) Ionization Gain Stimulated Raman Spectroscopy (IGSRS).

S2 Correction of Raman Intensities

According to Refs. 3 and 4 the Raman activities (S_i) which were calculated by the Gaussian package are converted to Raman intensities (I_i) by using the following formula:

$$I_i = \frac{f(\tilde{\nu}_0 - \tilde{\nu}_i)^4 S_i}{\tilde{\nu}_i \left(1 - \exp\left(\frac{hc\tilde{\nu}_i}{k_B T}\right)\right)}$$

with

- f = normalization factor of all peak intensities,
- $\tilde{\nu}_0$ = exciting wavenumber [cm^{-1}],
- $\tilde{\nu}_i$ = vibrational wavenumber [cm^{-1}],
- h = Planck constant,
- c = speed of light,
- k_B = Boltzmann constant,
- T = temperature [K]

S3 Molecular symmetry of DPE

The redundant set of generators for DPE molecular symmetry group $G_{16}(\mathrm{DPE})$ is:

- C_2-axis, which is the b-axis of the molecule, that swaps two phenyle groups,
- C_2^a and C_2^b – rotations of the first and second phenyle groups by 180°,
- E^* is the inversion.

The mapping of the resulting group onto the original $G_{16}(\mathrm{N_2H_4})$ group for Hydrazine[5] to $G_{16}(\mathrm{DPE})$ is given in Figure S2.

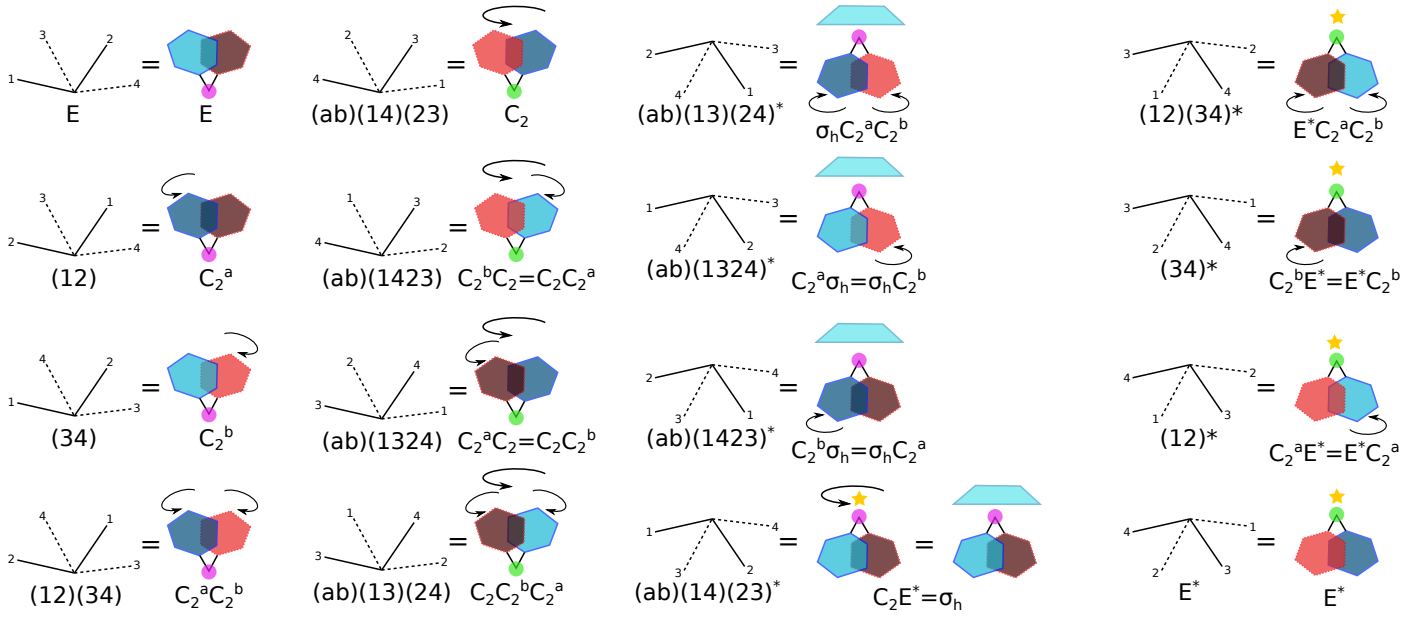

Fig. S2 Mapping of $G_{16}(\mathrm{N_2H_4})$ to $G_{16}(\mathrm{DPE})$.

The action of the symmetry elements on DPE internal rotation angles (θ_1, θ_2) is exactly the same as given in Ref.[6], and it is given in Table S1. The irreducible representations of $G_{16}(\mathrm{N_2H_4})$ and $G_{16}(\mathrm{DPE})$ groups are given in Table S2. The torsion states arise from the splitting $A_g^+ \oplus A_g^- \oplus A_u^+ \oplus A_u^- \oplus E_g \oplus E_u$ and dipole moment component along b-axis is A_u^+-symmetric. The correspondence to the C_4 representations is given in Table S3.

Due to C_2-symmetry of the equilibrium geometry of the DPE the G_{16} in the full case also can be reduced to $G_8 = C_4 \otimes E, \sigma_h$ (see Figure S4). In case of the irreducible representations this would lead to disappearance of all B-symmetric representations.

Table S1 Action of the symmetry elements of G_{16}(DPE) on DPE internal rotation angles (θ_1, θ_2) with $0 \leq \theta_i < 2\pi$.

E	(θ_1, θ_2)
$C_2^a C_2^b$	$(\theta_1+\pi, \theta_2+\pi) \mod 2\pi$
C_2^a	$(\theta_1+\pi, \theta_2) \mod 2\pi$
C_2^b	$(\theta_1, \theta_2+\pi) \mod 2\pi$
C_2	(θ_2, θ_1)
$C_2^a C_2^b C_2$	$(\theta_2+\pi, \theta_1+\pi) \mod 2\pi$
$C_2 C_2^a$	$(\theta_2, \theta_1+\pi) \mod 2\pi$
$C_2 C_2^b$	$(\theta_2+\pi, \theta_1) \mod 2\pi$
E^*	$(2\pi-\theta_1, 2\pi-\theta_2)$
$E^* C_2^a C_2^b$	$(2\pi, 2\pi) - ((\theta_1+\pi, \theta_2+\pi) \mod 2\pi)$
$E^* C_2^a$	$(2\pi, 2\pi) - ((\theta_1+\pi, \theta_2) \mod 2\pi)$
$E^* C_2^b$	$(2\pi, 2\pi) - ((\theta_1, \theta_2+\pi) \mod 2\pi)$
$\sigma_h = C_2 E^*$	$(2\pi-\theta_2, 2\pi-\theta_1)$
$\sigma_h C_2^a C_2^b$	$(2\pi, 2\pi) - ((\theta_2+\pi, \theta_1+\pi) \mod 2\pi)$
$\sigma_h C_2^b$	$(2\pi, 2\pi) - ((\theta_2+\pi, \theta_1) \mod 2\pi)$
$\sigma_h C_2^a$	$(2\pi, 2\pi) - ((\theta_2, \theta_1+\pi) \mod 2\pi)$

Table S2 Irreducible representations of group G_{16}. The naming of the representations of DPE are named according to elements C_2 (A/B), E^* (u/g) and C_2^a/C_2^b (+/-).

N_2H_4		E	$(12)(34)$	$\underbrace{(12)\quad(34)}$	$\underbrace{(ab)(14)(23)\quad(ab)(13)(24)}$	$\underbrace{(ab)(1423)\quad(ab)(1324)}$	E^*	$(12)(34)^*$	$\underbrace{(12)^*\quad(34)^*}$	$\underbrace{(ab)(14)(23)^*\quad(ab)(13)(24)^*}$	$\underbrace{(ab)(1324)^*\quad(ab)(1423)^*}$
	DPE	E	$C_2^a C_2^b$	C_2^b C_2^a	$C_2^a C_2^b C_2$ C_2	$C_2 C_2^b$ $C_2 C_2^a$	E^*	$E^* C_2^a C_2^b$	$E^* C_2^b$ $E^* C_2^a$	$\sigma_h C_2^a C_2^b$ σ_h	$\sigma_h C_2^a$ $\sigma_h C_2^b$
A_1^+	A_g^+	1	1	1	1	1	1	1	1	1	1
A_2^+	B_g^-	1	1	-1	-1	1	1	1	-1	-1	1
B_1^+	B_g^+	1	1	1	-1	-1	1	1	1	-1	-1
B_2^+	A_g^-	1	1	-1	1	-1	1	1	-1	1	-1
E^+	E_u	2	-2	0	0	0	2	-2	0	0	0
A_1^-	A_u^+	1	1	1	1	1	-1	-1	-1	-1	-1
A_2^-	B_u^-	1	1	-1	-1	1	-1	-1	1	1	-1
B_1^-	B_u^+	1	1	1	-1	-1	-1	-1	-1	1	1
B_2^-	A_u^-	1	1	-1	1	-1	-1	-1	1	-1	1
E^-	E_g	2	-2	0	0	0	-2	2	0	0	0

Table S3 Irreducible representations of group C_4.

C_4	E	$C_4 = C_2^a \sigma_h$	$C_4^2 = C_2^a C_2^b$	$C_4^3 = C_2^b \sigma_h$	G_{16}(DPE) representation
A	1	1	1	1	$A_g^+ \oplus B_g^- \oplus A_u^- \oplus B_u^+$
B	1	-1	1	-1	$A_g^- \oplus B_g^+ \oplus A_u^+ \oplus B_u^-$
E	1	i	-1	$-i$	$E_g \oplus E_u$
	1	$-i$	-1	i	

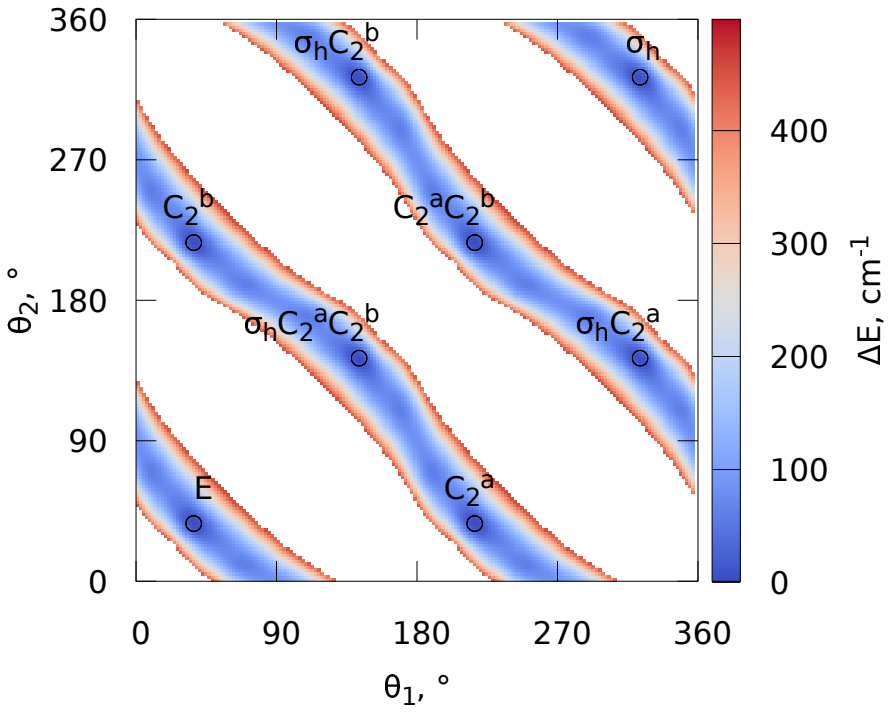

Fig. S3 Action of G_8 group on the positions of the DPE equilibrium structures.

S4 Internal rotation PES of DPE

The kinetic coefficients matrix B_{ij} had the following values estimated from the equilibrium structure of DPE optimized at B3LYP-D3/def2-TZVPP level:

$$\begin{cases} B_{11} = B_{22} = 0.351645 \ [\mathrm{cm}^{-1} \cdot \mathrm{Rad}^2] \ , \\ B_{12} = B_{21} = -0.144906 \ [\mathrm{cm}^{-1} \cdot \mathrm{Rad}^2] \ . \end{cases}$$

The PES were approximated as

$$V(\theta_1, \theta_2) = \sum_n V_n f_n(\theta_1, \theta_2)$$

using following basis functions:

- $f_n = \cos(n_1\theta_1) \cdot \cos(n_2\theta_2)$ (denoted as "0 n_1 0 n_2"),
- $f_n = \sin(n_1\theta_1) \cdot \cos(n_2\theta_2)$ (denoted as "1 n_1 0 n_2"),
- $f_n = \cos(n_1\theta_1) \cdot \sin(n_2\theta_2)$ (denoted as "0 n_1 1 n_2"),
- $f_n = \sin(n_1\theta_1) \cdot \sin(n_2\theta_2)$ (denoted as "1 n_1 1 n_2"),

where θ_i $(i = 1,2)$ are the internal rotation angles for phenyle groups. Approximations were constructed to yield fully symmetric representation of G_{16}.

Table S4 DPE PES approximated from B3LYP-D3/def2-TZVPP calculations

```
#############################################################################
  Basis Function   Coefficient V_i, cm^{-1}
  0  0  0  0       853.259
  0  2  0  0       -24.466
  0  0  0  2       -24.466
  0  4  0  0       -32.106
  0  0  0  4       -32.106
  0  6  0  0        -9.326
  0  0  0  6        -9.326
  0  8  0  0        -8.727
  0  0  0  8        -8.727
  0 10  0  0       -10.157
  0  0  0 10       -10.157
  0 12  0  0        -5.036
  0  0  0 12        -5.036
  0  2  0  2       808.053
  0  4  0  4       126.318
  0  6  0  6        27.110
  0  8  0  8        -1.286
  0 10  0 10        -3.468
  0 12  0 12        -3.308
  1  2  1  2      -931.869
  1  4  1  4      -127.267
  1  6  1  6       -20.466
  1  8  1  8         3.784
  1 10  1 10         9.427
  0  4  0  2       137.716
  0  2  0  4       137.716
  1  4  1  2      -167.193
  1  2  1  4      -167.193
  0  6  0  2         5.883
  0  2  0  6         5.883
  1  6  1  2       -17.479
  1  2  1  6       -17.479
  0  8  0  2        -0.349
  0  2  0  8        -0.349
  1  8  1  2       -10.316
  1  2  1  8       -10.316
  0 10  0  2        -3.004
  0  2  0 10        -3.004
  1 10  1  2        -3.813
  1  2  1 10        -3.813
  0 12  0  2        -1.764
  0  2  0 12        -1.764
  0  6  0  4        39.020
  0  4  0  6        39.020
  1  6  1  4       -35.803
  1  4  1  6       -35.803
  0  8  0  4        15.957
  0  4  0  8        15.957
  1  8  1  4       -10.713
  1  4  1  8       -10.713
  0 10  0  4         9.706
  0  4  0 10         9.706
```

```
  1 10  1  4        -4.069
  1  4  1 10        -4.069
  0 12  0  4         3.622
  0  4  0 12         3.622
  0  8  0  6        11.827
  0  6  0  8        11.827
  1  8  1  6        -6.954
  1  6  1  8        -6.954
  0 10  0  6         9.549
  0  6  0 10         9.549
  1 10  1  6        -5.660
  1  6  1 10        -5.660
  0 12  0  6         3.135
  0  6  0 12         3.135
  0 10  0  8         2.859
  0  8  0 10         2.859
  1 10  1  8        -0.375
  1  8  1 10        -0.375
  0 12  0  8         3.934
  0  8  0 12         3.934
#############################################################################
```

Table S5 DPE PES approximated from DLPNO(TightPNO)-CCSD(T)/def2-TZVPP calculations

```
#############################################################################
  Basis Function   Coefficient V_i, cm^{-1}
  0  0  0  0       872.871
  0  2  0  0        68.947
  0  0  0  2        68.947
  0  4  0  0       -46.559
  0  0  0  4       -46.559
  0  6  0  0       -13.720
  0  0  0  6       -13.720
  0  8  0  0       -13.481
  0  0  0  8       -13.481
  0 10  0  0       -15.182
  0  0  0 10       -15.182
  0 12  0  0        -7.458
  0  0  0 12        -7.458
  0  2  0  2       857.702
  0  4  0  4       155.659
  0  6  0  6        31.836
  0  8  0  8        -0.895
  0 10  0 10        -4.609
  0 12  0 12        -5.019
  1  2  1  2     -1034.408
  1  4  1  4      -165.497
  1  6  1  6       -30.189
  1  8  1  8         3.596
  1 10  1 10        12.490
  0  4  0  2       152.044
  0  2  0  4       152.044
  1  4  1  2      -191.808
  1  2  1  4      -191.808
  0  6  0  2         1.145
  0  2  0  6         1.145
  1  6  1  2       -21.031
  1  2  1  6       -21.031
```

```
  0  8  0  2        -5.034
  0  2  0  8        -5.034
  1  8  1  2       -12.030
  1  2  1  8       -12.030
  0 10  0  2        -9.562
  0  2  0 10        -9.562
  1 10  1  2        -5.175
  1  2  1 10        -5.175
  0 12  0  2        -3.953
  0  2  0 12        -3.953
  0  6  0  4        46.466
  0  4  0  6        46.466
  1  6  1  4       -46.176
  1  4  1  6       -46.176
  0  8  0  4        15.242
  0  4  0  8        15.242
  1  8  1  4       -12.073
  1  4  1  8       -12.073
  0 10  0  4         7.484
  0  4  0 10         7.484
  1 10  1  4        -4.110
  1  4  1 10        -4.110
  0 12  0  4         2.939
  0  4  0 12         2.939
  0  8  0  6        13.553
  0  6  0  8        13.553
  1  8  1  6       -10.799
  1  6  1  8       -10.799
  0 10  0  6         9.422
  0  6  0 10         9.422
  1 10  1  6        -7.645
  1  6  1 10        -7.645
  0 12  0  6         1.810
  0  6  0 12         1.810
  0 10  0  8         3.473
  0  8  0 10         3.473
  1 10  1  8        -2.571
  1  8  1 10        -2.571
  0 12  0  8         4.588
  0  8  0 12         4.588
###############################################################################
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S5 Fitted rotational constants for the isotopologues of DPE monomer

Table S6 Experimental rotational constants of ^{13}C for diphenylether. Quartic centrifugal distortion constants (Δ_J , Δ_{JK}, δ_J and δ_K) are kept fixed to the parent species. The fits are obtained by only fitting the center frequencies (see main text for more detail).

	Parent-center	^{13}C1,1"	^{13}C2,2"	^{13}C3,3"
A (MHz)	2362.07003(92)	2359.2155(11)	2350.26829(61)	2336.99122(90)
B (MHz)	437.98867(21)	437.47283(53)	437.05073(19)	435.17343(29)
C (MHz)	412.44316(22)	411.90452(37)	411.70069(17)	409.66408(26)
Δ_J (kHz)	0.02706(77)	[0.027062287]	[0.027062287]	[0.027062287]
Δ_{JK} (kHz)	1.0058(78)	[1.005806182]	[1.005806182]	[1.005806182]
δ_J (kHz)	−0.00210(11)	[−0.002107759133]	[−0.002107759133]	[−0.002107759133]
δ_K (kHz)	0.602(35)	[0.602186104]	[0.602186104]	[0.602186104]
No. of lines	52	15	19	20
σ (kHz)	6.1	7.5	4.7	7.1

	^{13}C4,4"	^{13}C5,5"	^{13}C6,6"
A (MHz)	2355.9728(11)	2355.95377(71)	2345.29321(78)
B (MHz)	432.93371(17)	433.26928(20)	435.91124(17)
C (MHz)	407.78631(21)	408.32952(19)	410.39673(18)
Δ_J (kHz)	[0.027062287]	[0.027062287]	[0.027062287]
Δ_{JK} (kHz)	[1.005806182]	[1.005806182]	[1.005806182]
δ_J (kHz)	[−0.002107759133]	[−0.002107759133]	[−0.002107759133]
δ_K (kHz)	[0.602186104]	[0.602186104]	[0.602186104]
No. of lines	20	23	22
σ (kHz)	6.9	6.1	6.1

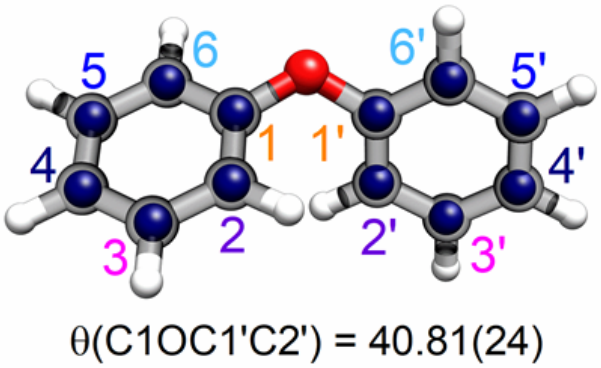


Fig. S4 The experimental structure of the DPE monomer ($r_m^{(1)}$ fit, blue spheres) is shown (from Figure 2), in comparison to the underlying grey structure computed at the B3LYP-D3(BJ)/def2-TZVP level of theory.

S6 R2PI spectrum of DPE

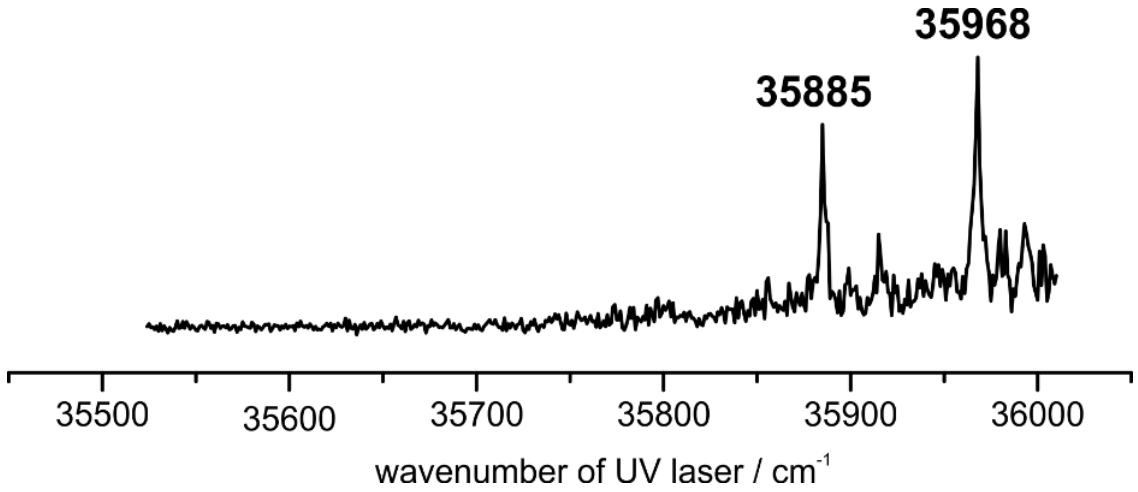


Fig. S5 R2PI spectrum of DPE in the range of 35500-36000 cm^{-1} (carrier gas helium).

S7 ILSR and IGSR spectra of DPE and DPE(H_2O)

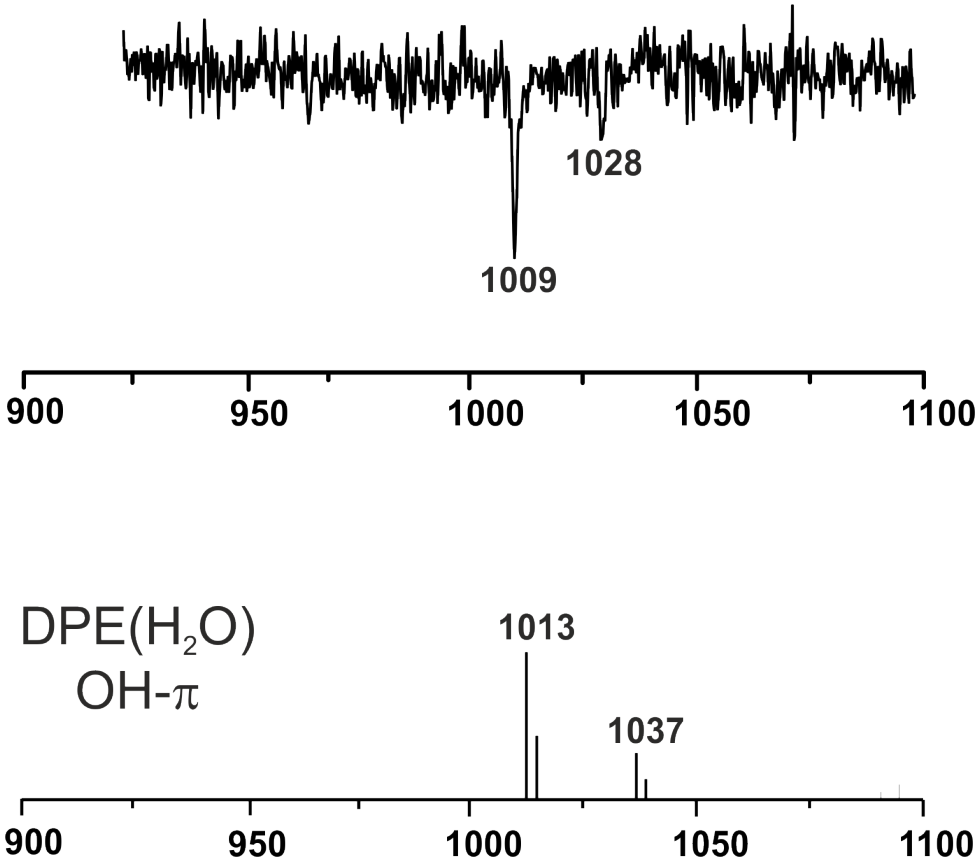


Fig. S6 Comparison of the ILSR spectrum of the CH bending region (top trace, helium) and quantum chemical calculations of the DPE (H_2O) aggregate (bottom trace, scaling factor 0.99). The spectrum is recorded on the mass of DPE(H_2O).

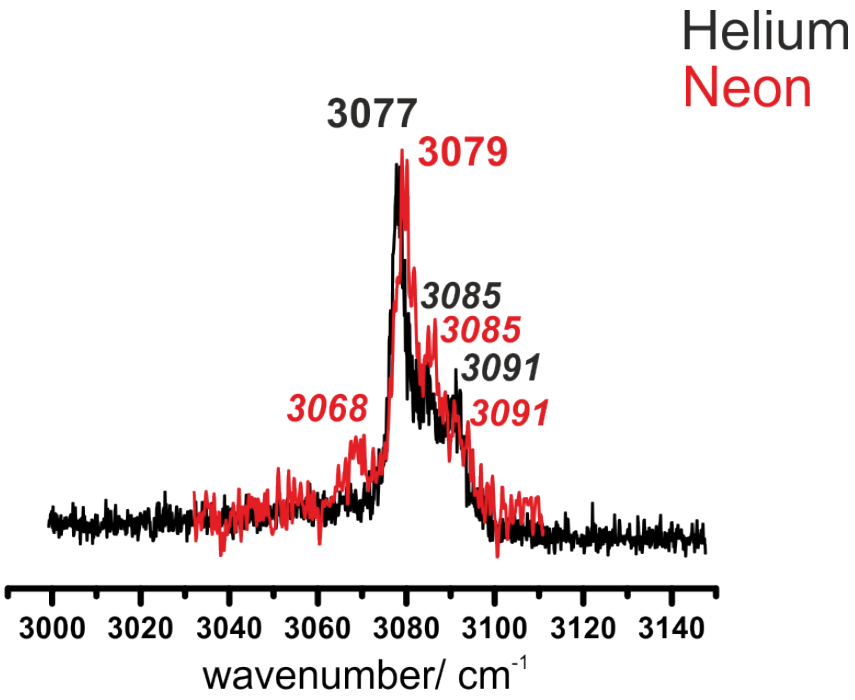


Fig. S7 IGSR spectra: Comparison between two different carrier gases (neon and helium) of the DPE monomer in the CH-stretching region. The colder condition in a neon expansion leads to a clearly structured spectrum with an additional transition at 3068 cm^{-1} . This transition may arise from fragmentation of aggregates with water moieties (see manuscript). The most prominent transition at 3077 cm^{-1} in helium is only slightly shifted to 3079 cm^{-1} in neon.

S8 Calculated harmonic vibrational frequencies with Raman intensities and spectra of DPE monomer, DPE(H_2O) and DPE(H_2O)$_2$

Table S7 List of calculated harmonic vibrational frequencies (scaled and unscaled) of DPE at the B3LYP-D3(BJ)/def2-TZVP level (scaling factor 0.96). All values are given in cm^{-1}.

unscaled	scaled
3170.87	3044.0352
3171.03	3044.1888
3178.84	3051.6864
3178.94	3051.7824
3192.51	3064.8096
3192.74	3065.0304
3199.94	3071.9424
3200.26	3072.2496
3203	3074.8800
3203.38	3075.2448

Table S8 List of calculated harmonic vibrational frequencies (scaled and unscaled) of DPE at the B3LYP-D3(BJ)/def2- TZVP level (scaling factor 0.99). All values are given in cm^{-1}.

unscaled	scaled	unscaled	scaled	unscaled	scaled	unscaled	scaled
2.86	2.8314	639.71	633.3129	970.99	961.2801	1338.78	1325.3922
44.34	43.8966	703.27	696.2373	1023.78	1013.5422	1355.03	1341.4797
88.69	87.8031	707.95	700.8705	1024.31	1014.0669	1356.29	1342.7271
216.67	214.5033	764.49	756.8451	1047.35	1036.8765	1488.24	1473.3576
239.26	236.8674	765.9	758.241	1047.82	1037.3418	1496.93	1481.9607
318.28	315.0972	808.56	800.4744	1099.73	1088.7327	1524.04	1508.7996
387.82	383.9418	838.94	830.5506	1102.93	1091.9007	1531.01	1515.6999
421.63	417.4137	843.28	834.8472	1180.74	1168.9326	1629.1	1612.809
426.27	422.0073	889.43	880.5357	1181.39	1169.5761	1633.53	1617.1947
488.94	484.0506	914.22	905.0778	1188.21	1176.3279	1637.72	1621.3428
510.82	505.7118	921.11	911.8989	1190.01	1178.1099	1650.52	1634.0148
581.93	576.1107	960.95	951.3405	1226.75	1214.4825		
619.15	612.9585	962.04	952.4196	1270.42	1257.7158		
634.29	627.9471	969.63	959.9337	1317.72	1304.5428		

Table S9 Comparison of the experimental transitions and the calculated harmonic frequencies of DPE at the B3LYP-D3(BJ)/def2-TZVP level. Scaling factor 0.99 (C-O stretching region) and 0.96 (CH stretching region).

Exp.	DPE monomer	
[cm^{-1}]	unscaled [cm^{-1}]	scaled [cm^{-1}]
1009	1023.78	1013.54
1028	1047.35	1036.87
1207	1226.75	1214.48
3077	3203.38	3075.25
3085		
3091		

Table S10 Description of the calculated vibrations of DPE (DFT/B3LYP-D3/TZVP); Scaling factor 0.96.

wavenumber/cm^{-1}	
1014	CH „breathing“ vibration of both phenylrings
1037	CH „wagging“ vibration of both phenylrings
1214	CO stretching vibration
3052	asym. CH stretching vibrations of both phenylrings
3075	sym. CH stretching vibrations of both phenylrings

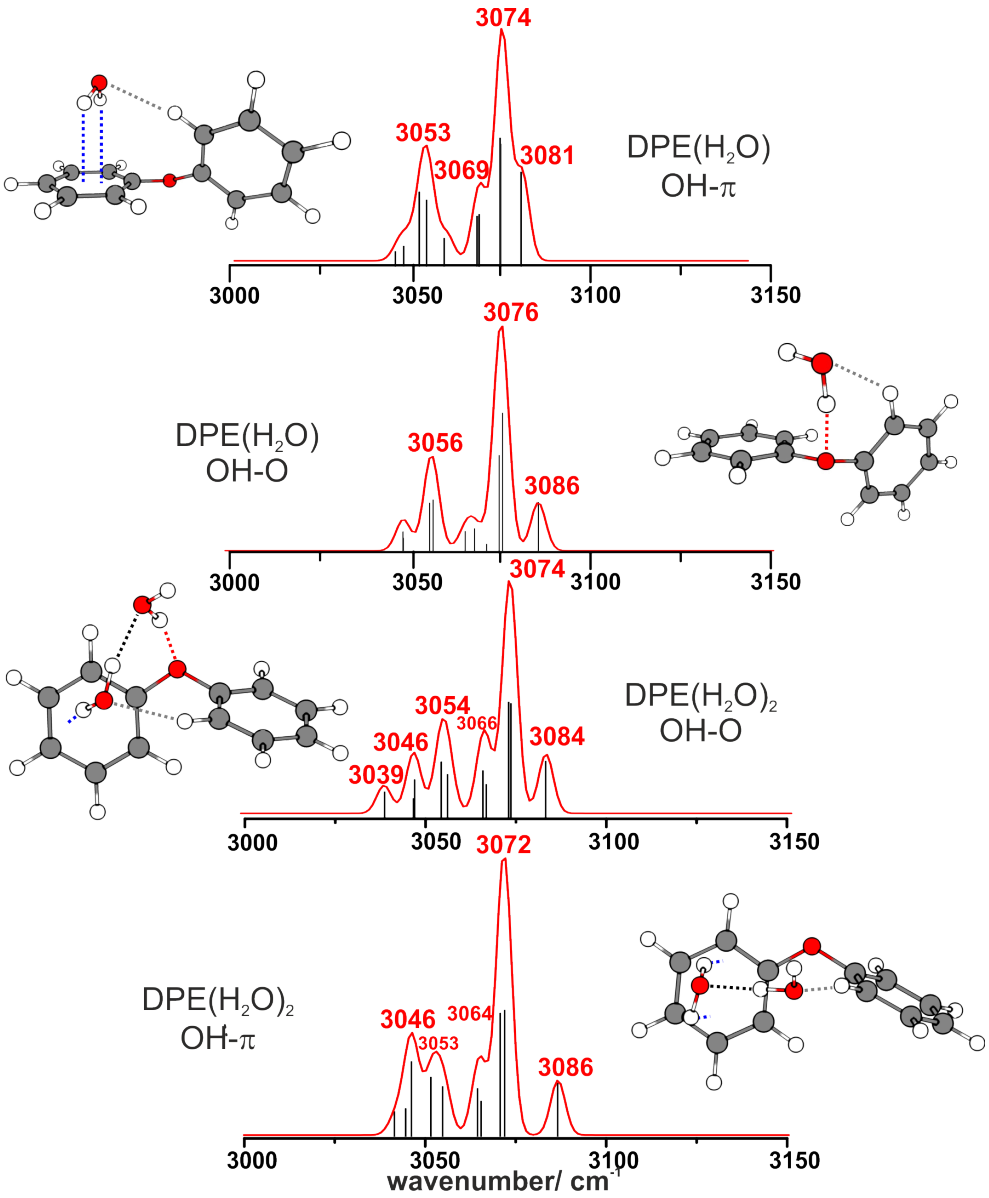


Fig. S8 Calculated harmonic vibrational frequencies with Raman intensities of the DPE-(H_2O) and DPE-(H_2O)$_2$ cluster at the B3LYP-D3(BJ)/def2-TZVP level. Scaling factor 0.96.

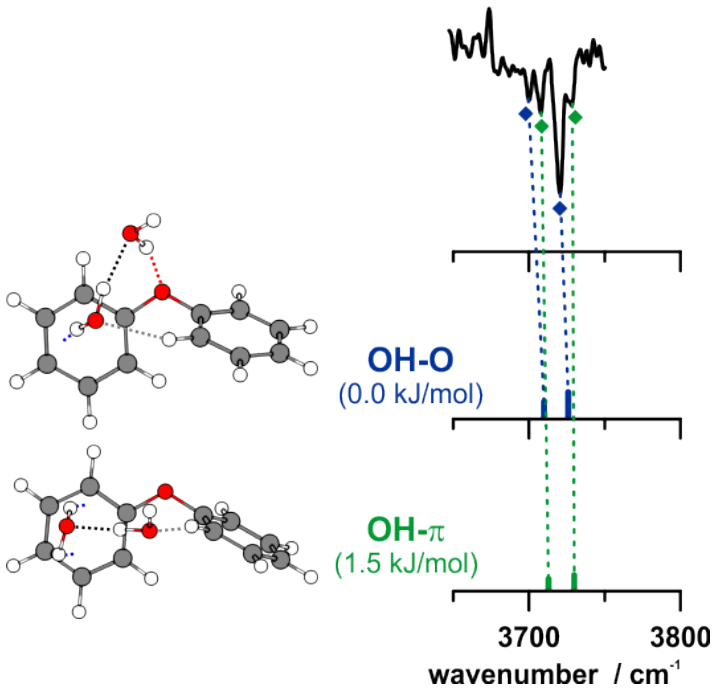


Fig. S9 IR/R2PI spectrum of DPE-$(H_2O)_2$ via the UV excitation energy of 3590 cm^{-1} using the carrier gas neon, compared to calculated vibrational frequencies for the two most stable clusters calculated at the B3LYP-D3(BJ)/def2-TZVP level: Region of the OH stretching frequencies. In order to get a better comparison, the chosen scaling factor is here 0.9677 as derived from calculations on pure water.

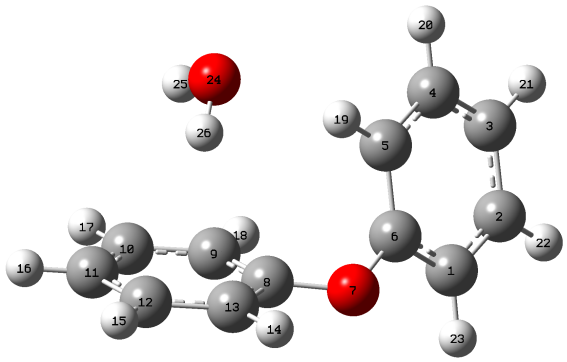
Table S11 Comparison of the experimental transitions and the calculated harmonic frequencies of DPE(H_2O) and DPE$(H_2O)_2$ at the B3LYP-D3(BJ)/def2-TZVP level. Scaling factor 0.99 (C-O stretching region) and 0.96 (CH stretching region). All values are given in cm^{-1}.

Exp.	DPE$(H_2O)_n$		DPE$(H_2O)_n$		DPE$(H_2O)_n$	
	n=1		n=2		n=2	
	OH-π		OH-O		OH-π	
	unscaled	unscaled	unscaled	scaled	unscaled	scaled
3068	3179.70 / 3181.70	3052.51 / 3054.51	3193.59 / 3194.56	3065.84 / 3066.78	3192.11 / 3193.15	3064.43 / 3065.42
3078	3203.04 / 3203.41	3074.92 / 3075.27	3200.99 / 3201.68	3072.95 / 3073.61	3198.92 / 3200.19	3070.96 / 3072.18
3085	3209.1	3080.74	3211.69	3083.22		
3091					3215.19	3086.58

S9 DPE-1w theoretical rotational constants and r_0 fit

Table S12 The results from quantum-chemical calculations for the DPE-1w structures at the B3LYP-D3(BJ)/def2-TZVP level of theory.

	OH-π	OH-O
A(MHz)	1416.46	1165.99
B(MHz)	407.09	427.99
C (MHz)	367.38	354.46
$\mu_a/\mu_b/\mu_c$ (D)	0.7/1.1/0.9	0.2/3.0/0.5



DPE-1w OH-π structure

Table S13 DPE-1w OH-π r_0 fit results. The atom numbering corresponds to the figure above.

```
 FINAL RESULTS OF LEAST SQUARES FIT:

     D(24,19, 5, 4) =   117.353665 +-  1.817773
        A(10, 9, 8) =   120.006348 +-  0.387508
           R(11,10) =     1.398957 +-  0.011241
           R(24,19) =     2.468553 +-  0.004815
           R(12,11) =     1.408895 +-  0.011875
           R( 3, 2) =     1.443057 +-  0.007777
           R( 2, 1) =     1.402507 +-  0.008476
           R( 7, 6) =     1.354473 +-  0.007130
     D( 9, 8, 7, 6) =    32.477764 +-  0.605877
     D( 8, 7, 6, 5) =    51.402854 +-  0.238964

          Chi-squared =        0.0765616681
       Deviation of fit =        0.048914
```

S10 Dihedral angles of DPE, DPE dimer and its aggregates

Table S14 Dihedral angles (θ1 and θ2) of DPE, DPE dimer and its aggregates with different alcohols and water as given in Refs. 7 and 8. The value in square bracket for the DPE+H2O OH-π cluster is determined from the r_0 fit. These values are compared with the dihedral angles of DPE-2w and DPE-3w. For consistency all the calculation are at the B3LYP-D3(BJ)/def2-TZVP level of theory.

Cluster	Isomer	θ1/$^\circ$	θ2/$^\circ$
DPE+H_2O	OH-O	11.7	75.0
	OH-π	52.2	30.7
		[51.40(23)]	[32.48(61)]
DPE+MeOH	OH-O	25.9	56.4
	OH-π	33.9	44.6
DPE+tBuOH	OH-O	37.5	43.3
	OH-π	23.1	51.8
DPE+AdOH	OH-O	34.6	47.0
	OH-π	62.0	11.8
DPE		37.0	37.0
DPE Dimer 1[b]	DPE1	20.0	84.9
	DPE2	19.1	53.4
DPE-2w		66.0	19.2
DPE-3w		86.2	-9.0

[b] M. Fatima, A. L. Steber, A. Poblotzki, C. Pérez, S. Zinn, M. Schnell, *Angew. Chem. Int. Ed.* **2019** , 58 , 3108.

S11 Structures of DPE-2w and DPE-3w

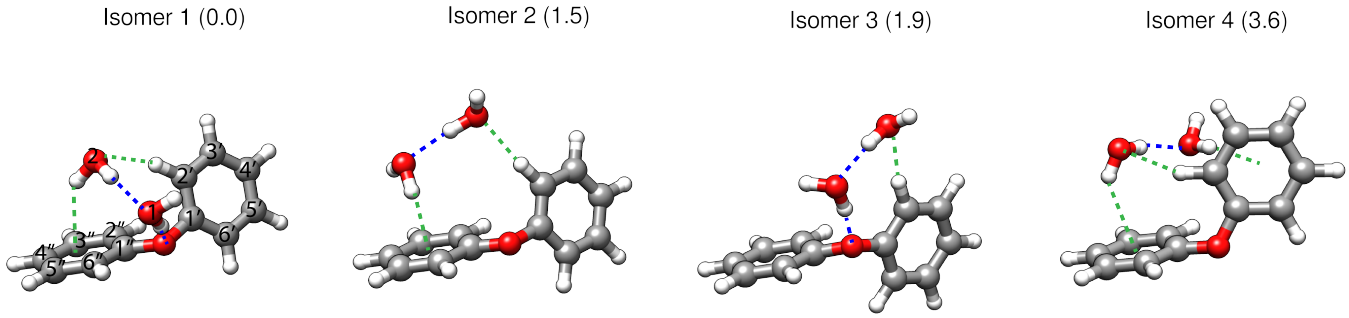


Fig. S10 The four lowest energy conformers of DPE-2w calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory. The values in the parentheses are zero point and BSSE corrected relative energies with respect to the lowest energy structure, Isomer 1 (OHO structure in the main text), in kJ mol^{-1}. OH-O hydrogen bonds are represented by blue dotted lines and CH-O or CH-π by green dotted lines.

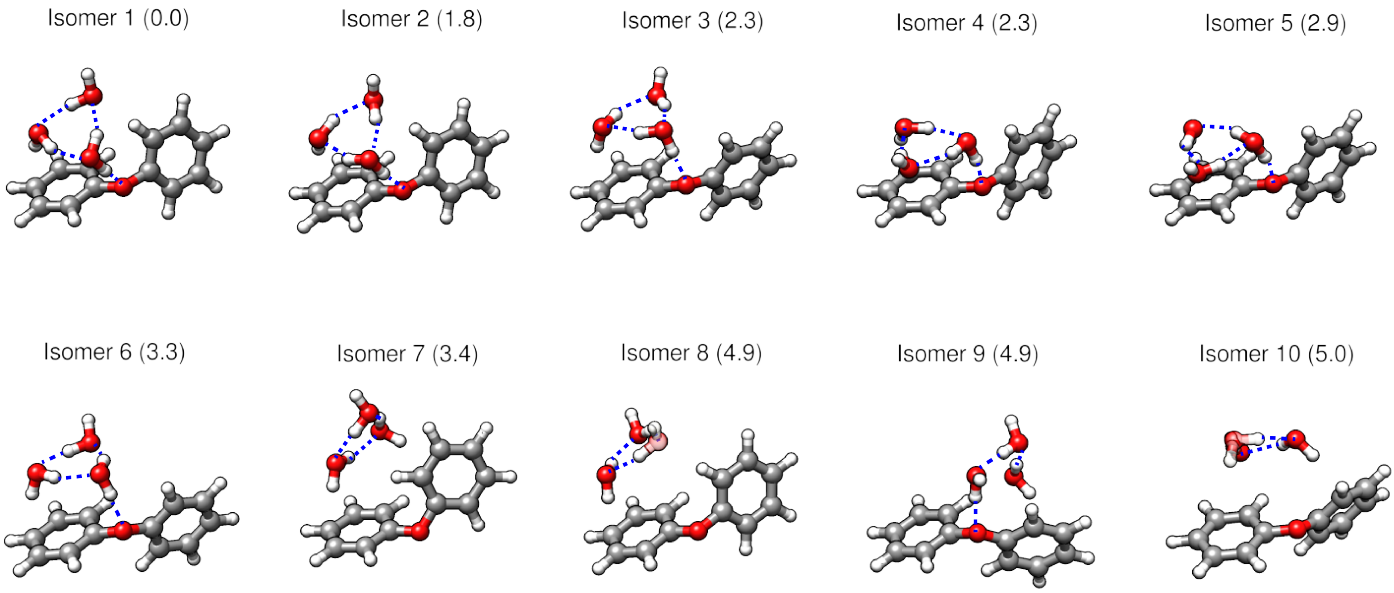


Fig. S11 Ten lowest energy conformers of DPE-3w calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory. The values in the parentheses are zero point and BSSE corrected relative energies with respect to the lowest energy structure, Isomer 1, in kJ mol^{-1}. Note that only in isomer 9 the water molecules form a chain structure. OH-O hydrogen bonds are represented by blue dotted lines.

S12 NCIPLOTS of DPE-2w and DPE-3w

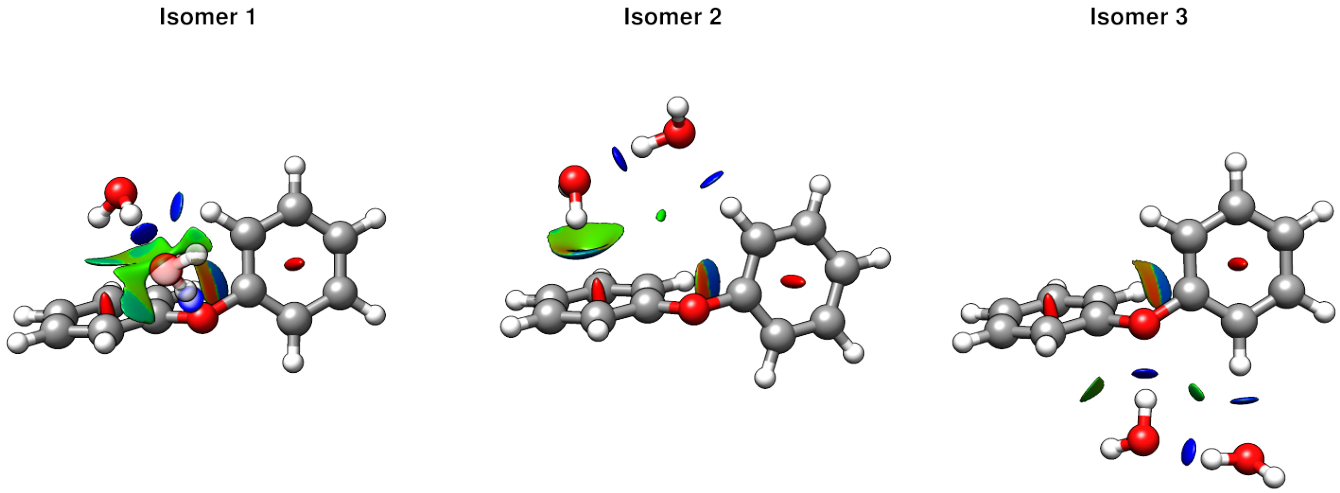


Fig. S12 Non-covalent interaction (NCI) analysis for the three lowest energy structures of DPE-2w (from Fig. S9). Blue and green colors identify the presence of hydrogen bonding (strong attraction, blue) and van der Waals interactions (weak attraction, green). Red indicates repulsive interactions.

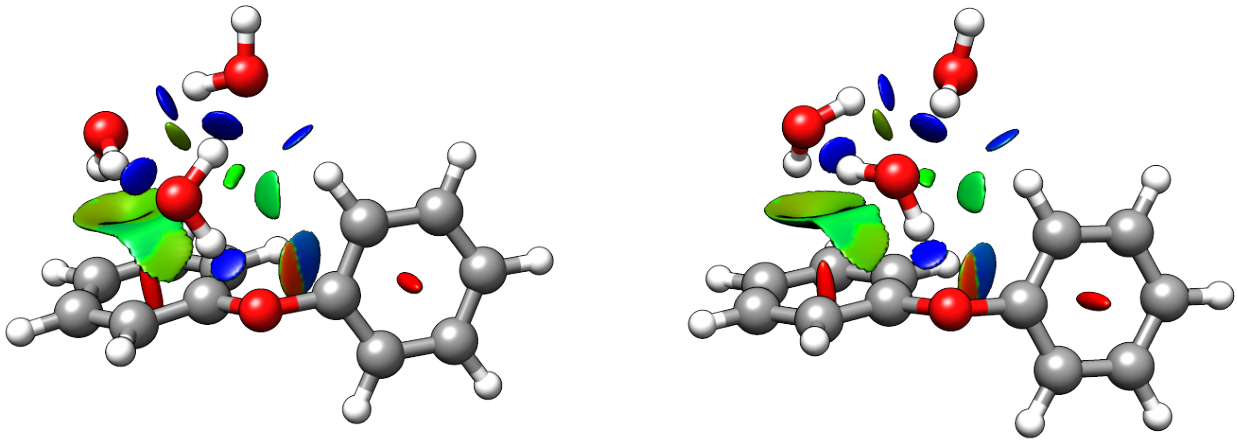


Fig. S13 Non-covalent interaction (NCI) analysis for the two lowest energy structures of DPE-3w (from Fig. S10). Blue and green colors identify the presence of hydrogen bonding (strong attraction, blue) and van der Waals interactions (weak attraction, green). Red indicates repulsive interactions.

S13 SAPT(2+3) of DPE-2w and DPE-3w

Table S15 Energy decompositions (kJ/mol) from an SAPT(2+3)/jun-cc-pVDZ analysis for the structures calculated at the B3LYP-D3(BJ)/def2-TZVP level.

species	Isomer	E_{tot}	E_{elec}	E_{exch}	E_{ind}	E_{disp}
DPE-H_2O	OH-O	-15.6	-29.4	37.3	-8.8	-14.6
	OH-π	-13.6	-23.9	33.0	-6.6	-16.1
DPE-$(H_2O)_2$		-29.5	-52.8	68.7	-17.4	-28.0

S14 Fitted rotational constants for the isotopologues of DPE-water complexes

Table S16 Experimental rotational constants of $H_2^{18}O$ for DPE-1w (OHO) complex. F_{bc} is a coriolis coupling constant and ΔE is the difference in vibrational energy between the tunnelling levels

States	00	11	22	33
A (MHz)	1007.19699(68)	1007.19496(66)	1007.2579(64)	1007.2478(65)
B (MHz)	433.3114(67)	433.3114(67)	433.378(56)	433.378(56)
C (MHz)	338.5745(67)	338.5723(67)	338.508(56)	338.506(56)
Δ_J (kHz)			0.0126(17)	0.0137(19)
Δ_{JK} (kHz)	1.366(13)	1.243(35)	1.367(13)	1.227(38)
F_{bc} (MHz)	9.315(34)		8.98(29)	
$\Delta E_{(11)}$ (MHz)	5.0858(24)			
$\Delta E_{(33-22)}$ (MHz)	5.1928(35)			
No. of lines	227			
σ (kHz)	8.0			

Table S17 Experimental rotational constants of ^{13}C and $H_2^{18}O$ for DPE-2w (OHO) complex. Quartic centrifugal distortion constants (Δ_J , Δ_{JK}, Δ_K, δ_J and δ_K) are kept fixed to the parent species for ^{13}C isotopologues. The atom numbers are given in Figure S8.

	Parent	^{13}C1'	^{13}C2'	^{13}C3'	^{13}C4'
A (MHz)	823.80379(24)	823.42918(34)	822.73802(26)	821.45225(28)	822.90370(25)
B (MHz)	390.51117(13)	389.95010(11)	389.526669(95)	387.48009(10)	386.026689(89)
C (MHz)	334.18534(13)	333.799712(74)	333.574738(65)	332.346553(75)	330.901354(69)
Δ_J (kHz)	0.02964(86)	[−0.0296]	[−0.0296]	[−0.0296]	[−0.0296]
Δ_{JK} (kHz)	0.1766(34)	[−0.1766]	[−0.1766]	[−0.1766]	[−0.1766]
Δ_K (kHz)	0.6324(47)	[−0.6324]	[−0.6324]	[−0.6324]	[−0.6324]
δ_J (kHz)	0.00787(31)	[−0.00787]	[−0.00787]	[−0.00787]	[−0.00787]
δ_K (kHz)	0.142(12)	[−0.142]	[−0.142]	[−0.142]	[−0.142]
No. of lines	292	82	83	81	80
σ (kHz)	9.9	8.1	7.7	8.7	7.6
	^{13}C5'	^{13}C6'	^{13}C1"	^{13}C2"	^{13}C3"
A (MHz)	821.76834(29)	820.99352(25)	823.33005(36)	820.80926(28)	817.55507(34)
B (MHz)	386.70198(13)	388.571276(91)	390.10948(13)	390.17214(11)	388.86279(10)
C (MHz)	331.25030(11)	332.936635(75)	333.929382(86)	333.505935(82)	332.250401(73)
Δ_J (kHz)	[−0.0296]	[−0.0296]	[−0.0296]	[−0.0296]	[−0.0296]
Δ_{JK} (kHz)	[−0.1766]	[−0.1766]	[−0.1766]	[−0.1766]	[−0.1766]
Δ_K (kHz)	[−0.6324]	[−0.6324]	[−0.6324]	[−0.6324]	[−0.6324]
δ_J (kHz)	[−0.00787]	[−0.00787]	[−0.00787]	[−0.00787]	[−0.00787]
δ_K (kHz)	[−0.142]	[−0.142]	[−0.142]	[−0.142]	[−0.142]
No. of lines	64	87	82	73	90
σ (kHz)	6.9	8.2	8.2	7.3	8.9

	^{13}C4"	^{13}C5"	^{13}C6"	$H_2^{18}O1$	$H_2^{18}O2$
A (MHz)	820.67291(25)	823.37461(30)	822.71725(30)	802.90231(24)	797.20568(18)
B (MHz)	386.96303(10)	386.91044(11)	388.722357(91)	387.971687(77)	389.872411(84)
C (MHz)	331.155092(73)	331.558730(85)	333.070389(81)	331.411123(93)	330.001284(91)
Δ_J (kHz)	[−0.0296]	[−0.0296]	[−0.0296]	0.02202(43)	0.02150(45)
Δ_{JK} (kHz)	[−0.1766]	[−0.1766]	[−0.1766]	0.2160(20)	0.2510(10)
Δ_K (kHz)	[−0.6324]	[−0.6324]	[−0.6324]	–	–
δ_J (kHz)	[−0.00787]	[−0.00787]	[−0.00787]	–	–
δ_K (kHz)	[−0.142]	[−0.142]	[−0.142]	–	–
No. of lines	86	84	87	181	189
σ (kHz)	7.6	7.5	9.4	7.4	7.8

S15 Linelist for DPE and its complexes with water

Table S18 Linelist for DPE monomer. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	OMC (MHz)	Center (MHz)	OMC (MHz)	Right (MHz)	OMC (MHz)
3	1	2	←	3	0	3	2014.3419	-0.1054	2014.5780	0.0045	2014.8104	0.0922
4	1	3	←	4	0	4	2067.4382	-0.0986	2067.6709	0.0039	2067.9029	0.0868
5	1	4	←	5	0	5	2135.2092	-0.0949	2135.4416	0.0023	2135.6731	0.0794
7	1	6	←	7	0	7	2318.6220	-0.0820	2318.8525	0.0015	2319.0830	0.0651
9	1	8	←	8	2	7	2404.6532	-0.2387	2404.9460	-0.0086	2405.2386	0.4407
5	0	5	←	4	1	4	2434.6491	-0.1167	2434.8485	-0.0072	2435.0490	0.1205
8	1	7	←	8	0	8	2436.5514	-0.0736	2436.7806	0.0020	2437.0091	0.0570
11	1	11	←	10	2	8	2554.8319	-0.3162	2555.1951	0.0132	2555.5570	0.5582
9	1	8	←	9	0	9	2573.6768	-0.0693	2573.9050	-0.0010	2574.1334	0.0472
10	1	9	←	10	0	10	2731.3802	-0.0617	2731.6076	-0.0002	2731.8339	0.0401
1	1	1	←	0	0	0	2774.2759	-0.0773	2774.5059	-0.0039	2774.7465	0.0618
11	1	10	←	11	0	11	2911.0356	-0.0556	2911.2637	0.0013	2911.4899	0.0369
12	1	11	←	12	0	12	3113.9724	-0.0381	3114.1994	0.0139	3114.4193	0.0403
6	0	6	←	5	1	5	3341.2305	-0.0563	3341.4175	-0.0034	3341.6036	0.0655
10	1	9	←	9	2	8	3376.6733	-0.1631	3376.9389	-0.0060	3377.2007	0.3673
2	1	2	←	1	0	1	3599.1639	-0.0385	3599.3947	0.0009	3599.6285	0.0253
15	1	14	←	15	0	15	3872.9863	-0.0684	3873.2198	-0.0070	3873.4554	0.0429
16	1	15	←	16	0	16	4178.2851	-0.0919	4178.5320	-0.0099	4178.7670	0.0496
7	0	7	←	6	1	6	4256.2181	0.0028	4256.3871	-0.0058	4256.5575	0.0033
11	1	10	←	10	2	9	4359.4611	-0.0955	4359.6906	-0.0171	4359.9272	0.2893
14	1	14	←	13	2	11	4372.3137	-0.0839	4372.5309	-0.0268	4372.7480	0.2360
3	1	3	←	2	0	2	4411.3694	-0.0051	4411.5964	-0.0017	4411.8250	-0.0149
15	2	13	←	15	1	14	4909.6266	-0.0240	4909.6911	0.0011	4909.7687	-0.1728
14	2	12	←	14	1	13	4957.2110	-0.0269	4957.3270	0.0077	4957.4329	-0.1831
13	2	11	←	13	1	12	5017.0226	-0.0192	5017.1662	0.0060	5017.3134	-0.1827
12	2	10	←	12	1	11	5086.4837	-0.0199	5086.6655	0.0105	5086.8494	-0.1760
11	2	9	←	11	1	10	5162.9760	-0.0203	5163.1910	0.0133	5163.4088	-0.1701
8	0	8	←	7	1	7	5178.2721	0.0668	5178.4250	-0.0004	5178.5777	-0.0522
4	1	4	←	3	0	3	5211.2207	0.0330	5211.4394	-0.0017	5211.6604	-0.0524
10	2	8	←	10	1	9	5243.8537	-0.0292	5244.1013	0.0097	5244.3507	-0.1699
9	2	7	←	9	1	8	5326.5403	-0.0353	5326.8217	0.0121	5327.1011	-0.1627
12	1	11	←	11	2	10	5352.5816	-0.0191	5352.7860	-0.0044	5352.9839	0.2258
8	2	6	←	8	1	7	5408.5529	-0.0421	5408.8636	0.0115	5409.1717	-0.1576
7	2	5	←	7	1	6	5487.5754	-0.0447	5487.9126	0.0141	5488.2460	-0.1507
6	2	4	←	6	1	5	5561.4798	-0.0512	5561.8417	0.0132	5562.1984	-0.1471
5	2	3	←	5	1	4	5628.3803	-0.0588	5628.7681	0.0145	5629.1404	-0.1468
5	1	5	←	4	0	4	5999.2234	0.0708	5999.4325	-0.0011	5999.6432	-0.0900
5	2	4	←	5	1	5	6002.6241	-0.0447	6003.0292	0.0009	6003.4512	-0.1579
6	2	5	←	6	1	6	6080.0654	-0.0397	6080.4689	0.0043	6080.8780	-0.1680
9	0	9	←	8	1	8	6105.8974	0.1274	6106.0320	0.0009	6106.1667	-0.1107
7	2	6	←	7	1	7	6170.6950	-0.0268	6171.0885	0.0078	6171.4887	-0.1743
8	2	7	←	8	1	8	6274.6011	-0.0231	6274.9878	0.0053	6275.3764	-0.1892
13	1	12	←	12	2	11	6355.4919	0.0501	6355.6567	-0.0083	6355.8311	0.1659
9	2	8	←	9	1	9	6391.9065	-0.0120	6392.2805	0.0044	6392.6582	-0.2017
11	2	10	←	11	1	11	6667.1001	0.0199	6667.4472	0.0121	6667.7997	-0.2202
6	1	6	←	5	0	5	6776.0848	0.1108	6776.2823	0.0016	6776.4816	-0.1243
13	2	12	←	13	1	13	6996.8961	0.0334	6997.2250	0.0110	6997.5493	-0.2500
10	0	10	←	9	1	9	7037.5013	0.1881	7037.6156	0.0024	7037.7315	-0.1679
14	2	13	←	14	1	14	7182.4078	0.0558	7182.7164	0.0154	7183.0566	-0.2297
14	1	13	←	13	2	12	7367.5921	0.1240	7367.7173	-0.0020	7367.8432	0.0971
7	1	7	←	6	0	6	7542.6903	0.1419	7542.8736	-0.0048	7543.0589	-0.1688
11	0	11	←	10	1	10	7971.4162	0.2439	7971.5108	0.0023	7971.6046	-0.2277
							RMS	91 kHz		6.1 kHz		92 kHz

Table S19 Linelist for DPE-1w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
3	1	3	2	←	2	1	2	3	2185.0003	0.0013
3	1	3	0	←	2	1	2	1	2185.1513	0.0077
3	1	3	1	←	2	1	2	0	2199.3284	0.0052
3	1	3	3	←	2	1	2	2	2199.4710	0.0008
3	0	3	2	←	2	0	2	3	2290.4124	0.0015
3	0	3	0	←	2	0	2	1	2290.5651	0.0089
3	0	3	1	←	2	0	2	0	2305.0283	0.0034
3	0	3	3	←	2	0	2	2	2305.1788	-0.0001
3	1	2	2	←	2	1	1	3	2456.4768	0.0007
3	1	2	0	←	2	1	1	1	2456.6232	0.0094
3	1	2	1	←	2	1	1	0	2470.8105	0.0011
3	1	2	3	←	2	1	1	2	2470.9611	-0.0040
5	1	4	0	←	4	2	3	0	2484.5959	0.0195
5	1	4	1	←	4	2	3	1	2485.0170	0.0213
4	0	4	0	←	3	1	3	0	2584.5747	0.0122
4	0	4	1	←	3	1	3	1	2584.6903	0.0141
4	1	4	2	←	3	1	3	3	2906.3619	0.0000
4	1	4	0	←	3	1	3	1	2906.5141	0.0067
4	1	4	1	←	3	1	3	0	2920.6694	0.0083
4	1	4	3	←	3	1	3	2	2920.8120	0.0052
4	0	4	2	←	3	0	3	3	3018.0222	-0.0084
4	0	4	0	←	3	0	3	1	3018.1854	0.0093
4	0	4	1	←	3	0	3	0	3032.6055	0.0042
4	0	4	3	←	3	0	3	2	3032.7516	-0.0033
4	2	3	2	←	3	2	2	3	3097.7134	0.0061
4	2	3	0	←	3	2	2	1	3097.8499	0.0082
4	2	3	1	←	3	2	2	0	3111.1440	0.0107
4	2	3	3	←	3	2	2	2	3111.2831	0.0074
4	3	2	0	←	3	3	1	1	3121.1160	0.0095
4	3	2	1	←	3	3	1	0	3136.0548	0.0110
4	3	1	3	←	3	3	0	2	3138.6975	0.0043
4	2	2	2	←	3	2	1	3	3183.8302	-0.0026
4	2	2	0	←	3	2	1	1	3183.9677	0.0066
4	2	2	1	←	3	2	1	0	3197.3009	0.0063
4	2	2	3	←	3	2	1	2	3197.4392	-0.0052
4	1	3	2	←	3	1	2	3	3265.6558	0.0007
4	1	3	0	←	3	1	2	1	3265.8020	0.0101
4	1	3	1	←	3	1	2	0	3279.9770	0.0047
4	1	3	3	←	3	1	2	2	3280.1261	-0.0037
4	1	4	1	←	3	0	3	1	3354.2773	0.0026
4	1	4	0	←	3	0	3	0	3354.4343	0.0019
5	0	5	0	←	4	1	4	0	3400.4690	-0.0044
6	1	5	0	←	5	2	4	0	3465.4008	0.0170
6	1	5	1	←	5	2	4	1	3465.8028	0.0192
2	2	1	1	←	1	1	0	1	3529.2444	-0.0190
2	2	1	0	←	1	1	0	0	3530.2184	-0.0085
5	1	5	2	←	4	1	4	3	3621.2227	0.0012
5	1	5	0	←	4	1	4	1	3621.3755	0.0068
2	2	0	1	←	1	1	1	1	3629.8727	-0.0027
2	2	0	0	←	1	1	1	0	3630.8225	-0.0123
2	2	0	2	←	1	1	1	2	3630.8879	-0.0204
5	1	5	1	←	4	1	4	0	3635.4931	0.0087
5	1	5	3	←	4	1	4	2	3635.6331	0.0056
5	0	5	2	←	4	0	4	3	3722.1491	-0.0086
5	0	5	0	←	4	0	4	1	3722.3043	-0.0002
5	0	5	1	←	4	0	4	0	3736.6645	0.0055
5	0	5	3	←	4	0	4	2	3736.8080	-0.0023
5	2	4	2	←	4	2	3	3	3862.4360	0.0028
5	2	4	0	←	4	2	3	1	3862.5764	0.0117
5	2	4	1	←	4	2	3	0	3875.8585	0.0126
5	2	4	3	←	4	2	3	2	3875.9988	0.0103
5	4	2	0	←	4	4	1	1	3902.3754	0.0135
5	4	2	2	←	4	4	1	3	3902.5310	-0.0182
5	4	1	0	←	4	4	0	1	3902.5310	0.0025

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
5	3	3	0	←	4	3	2	1	3907.7299	0.0120
5	4	2	1	←	4	4	1	0	3916.8831	0.0094
5	4	1	1	←	4	4	0	0	3917.0415	0.0010
5	3	2	2	←	4	3	1	3	3921.0042	0.0132
5	3	3	1	←	4	3	2	0	3921.1560	0.0273
5	1	5	1	←	4	0	4	1	3957.3056	-0.0099
5	1	5	0	←	4	0	4	0	3957.4550	-0.0122
5	2	3	2	←	4	2	2	3	4022.1741	0.0008
5	2	3	0	←	4	2	2	1	4022.3102	0.0069
5	2	3	3	←	4	2	2	2	4035.8216	-0.0036
5	1	4	2	←	4	1	3	3	4062.7501	-0.0030
5	1	4	0	←	4	1	3	1	4062.8958	0.0058
5	1	4	1	←	4	1	3	0	4077.0493	0.0077
5	1	4	3	←	4	1	3	2	4077.1981	-0.0017
6	0	6	0	←	5	1	5	0	4188.7178	0.0079
6	0	6	1	←	5	1	5	1	4188.7797	0.0145
3	2	2	1	←	2	1	1	1	4217.0510	-0.0068
3	2	2	0	←	2	1	1	0	4217.5119	-0.0018
6	1	6	2	←	5	1	5	3	4329.5839	-0.0026
6	1	6	0	←	5	1	5	1	4329.7388	0.0017
6	1	6	1	←	5	1	5	0	4343.8046	0.0034
6	1	6	3	←	5	1	5	2	4343.9464	0.0067
6	0	6	2	←	5	0	5	3	4409.3595	-0.0088
6	0	6	0	←	5	0	5	1	4409.5168	-0.0013
6	0	6	1	←	5	0	5	0	4423.7752	-0.0009
6	0	6	3	←	5	0	5	2	4423.9156	-0.0068
7	1	6	0	←	6	2	5	0	4446.4998	0.0141
7	1	6	1	←	6	2	5	1	4446.8662	0.0127
3	2	1	1	←	2	1	2	1	4534.2684	-0.0068
3	2	1	0	←	2	1	2	0	4534.6969	-0.0175
6	1	6	1	←	5	0	5	1	4564.6093	-0.0001
6	1	6	0	←	5	0	5	0	4564.7417	-0.0063
6	2	5	2	←	5	2	4	3	4619.8127	0.0023
6	2	5	0	←	5	2	4	1	4619.9522	0.0098
6	2	5	1	←	5	2	4	0	4633.2101	0.0201
6	2	5	3	←	5	2	4	2	4633.3511	0.0210
6	5	2	0	←	5	5	1	1	4682.6993	0.0094
6	5	1	0	←	5	5	0	1	4682.6993	0.0018
6	4	2	0	←	5	4	1	1	4691.5122	0.0028
6	5	2	1	←	5	5	1	0	4697.2104	-0.0071
6	3	4	0	←	5	3	3	1	4697.3245	0.0061
6	4	3	1	←	5	4	2	0	4705.3339	0.0067
6	4	2	1	←	5	4	1	0	4706.0687	0.0031
6	3	4	1	←	5	3	3	0	4708.9883	0.0113
6	3	3	2	←	5	3	2	3	4727.6320	-0.0130
6	3	3	0	←	5	3	2	1	4727.7564	0.0021
6	3	3	1	←	5	3	2	0	4739.4471	0.0054
6	1	5	2	←	5	1	4	3	4842.8189	0.0042
6	1	5	0	←	5	1	4	1	4842.9653	0.0125
6	1	5	1	←	5	1	4	0	4857.0627	0.0096
6	1	5	3	←	5	1	4	2	4857.2087	-0.0018
4	2	3	1	←	3	1	2	1	4857.8368	-0.0008
4	2	3	0	←	3	1	2	0	4858.2884	0.0025
6	2	4	2	←	5	2	3	3	4869.4268	0.0006
6	2	4	0	←	5	2	3	1	4869.5621	0.0040
6	2	4	3	←	5	2	3	2	4883.1130	-0.0046
9	2	7	0	←	8	3	6	0	4906.0028	-0.0230
9	2	7	1	←	8	3	6	1	4906.7695	-0.0371
7	0	7	2	←	6	1	6	2	4947.8818	-0.0054
7	1	7	2	←	6	1	6	3	5032.1076	0.0063
7	1	7	0	←	6	1	6	1	5032.2611	0.0043
7	1	7	1	←	6	1	6	0	5046.2562	0.0014
7	1	7	3	←	6	1	6	2	5046.3901	0.0035
7	0	7	2	←	6	0	6	3	5088.7413	0.0147
7	0	7	0	←	6	0	6	1	5088.8818	0.0005
7	0	7	1	←	6	0	6	0	5103.0205	-0.0043
7	0	7	3	←	6	0	6	2	5103.1575	-0.0059

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
7	1	7	1	←	6	0	6	1	5187.2155	-0.0111
7	1	7	0	←	6	0	6	0	5187.3374	-0.0107
7	2	6	2	←	6	2	5	3	5368.7189	0.0035
7	2	6	0	←	6	2	5	1	5368.8578	0.0080
7	2	6	1	←	6	2	5	0	5382.0564	0.0087
7	2	6	3	←	6	2	5	2	5382.1895	0.0066
8	1	7	0	←	7	2	6	0	5409.9424	0.0109
5	2	4	1	←	4	1	3	1	5454.1581	-0.0013
5	2	4	0	←	4	1	3	0	5454.6110	0.0005
7	5	2	0	←	6	5	1	1	5470.1960	-0.0102
7	4	4	0	←	6	4	3	1	5482.1501	0.0055
7	3	5	2	←	6	3	4	3	5483.6970	0.0165
7	3	5	0	←	6	3	4	1	5483.8175	0.0086
7	4	3	0	←	6	4	2	1	5484.2090	-0.0014
7	5	3	3	←	6	5	2	2	5484.3156	0.0047
7	3	5	1	←	6	3	4	0	5495.6797	0.0092
7	3	5	3	←	6	3	4	2	5495.8006	0.0020
7	4	4	1	←	6	4	3	0	5497.6391	-0.0033
7	4	3	3	←	6	4	2	2	5499.5851	0.0095
7	4	3	1	←	6	4	2	0	5499.7154	0.0027
4	2	2	1	←	3	1	3	1	5532.6811	-0.0047
7	3	4	2	←	6	3	3	3	5549.8673	-0.0076
7	3	4	0	←	6	3	3	1	5549.9927	-0.0002
7	3	4	1	←	6	3	3	0	5561.9242	-0.0017
7	3	4	3	←	6	3	3	2	5562.0539	-0.0127
7	1	6	2	←	6	1	5	3	5600.5102	0.0060
7	1	6	0	←	6	1	5	1	5600.6572	0.0128
7	1	6	1	←	6	1	5	0	5614.6664	0.0068
7	1	6	3	←	6	1	5	2	5614.8116	-0.0028
8	0	8	3	←	7	1	7	3	5682.6979	-0.0036
8	0	8	2	←	7	1	7	2	5682.6979	-0.0053
3	3	1	0	←	2	2	0	0	5695.1770	-0.0135
3	3	1	1	←	2	2	0	1	5696.2998	-0.0112
7	2	5	2	←	6	2	4	3	5714.4252	0.0059
7	2	5	0	←	6	2	4	1	5714.5606	0.0066
7	2	5	1	←	6	2	4	0	5728.0186	0.0186
8	1	8	2	←	7	1	7	3	5729.8097	0.0057
8	1	8	0	←	7	1	7	1	5729.9643	-0.0019
8	1	8	1	←	7	1	7	0	5743.8744	-0.0092
8	1	8	3	←	7	1	7	2	5744.0081	0.0018
8	0	8	2	←	7	0	7	3	5766.8731	-0.0182
8	0	8	0	←	7	0	7	1	5767.0294	-0.0236
8	0	8	1	←	7	0	7	0	5781.0574	-0.0153
8	0	8	3	←	7	0	7	2	5781.1904	-0.0103
8	1	8	1	←	7	0	7	1	5828.2133	0.0063
8	1	8	0	←	7	0	7	0	5828.2983	-0.0132
6	2	5	1	←	5	1	4	1	6010.7567	-0.0021
6	2	5	0	←	5	1	4	0	6011.2106	-0.0012
8	2	7	2	←	7	2	6	3	6108.4033	0.0036
8	2	7	0	←	7	2	6	1	6108.5442	0.0059
8	2	7	1	←	7	2	6	0	6121.6852	0.0167
8	2	7	3	←	7	2	6	2	6121.8157	0.0194
8	5	4	0	←	7	5	3	1	6260.3199	0.0010
8	5	3	0	←	7	5	2	1	6260.4796	-0.0048
8	3	6	2	←	7	3	5	3	6267.2232	0.0093
8	3	6	0	←	7	3	5	1	6267.3425	0.0030
8	5	3	3	←	7	5	2	2	6274.5910	-0.0173
8	5	4	1	←	7	5	3	0	6274.7864	-0.0167
8	5	3	1	←	7	5	2	0	6274.9770	0.0077
8	3	6	1	←	7	3	5	0	6279.2166	0.0079
8	3	6	3	←	7	3	5	2	6279.3379	0.0055
8	1	7	2	←	7	1	6	3	6331.7883	0.0039
8	1	7	0	←	7	1	6	1	6331.9363	0.0084
9	1	8	0	←	8	2	7	0	6338.4389	0.0115
8	1	7	1	←	7	1	6	0	6345.8230	0.0102
8	1	7	3	←	7	1	6	2	6345.9640	0.0018
8	3	5	2	←	7	3	4	3	6390.3242	-0.0088

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
8	3	5	0	←	7	3	4	1	6390.4447	-0.0141
9	0	9	3	←	8	1	8	3	6399.6370	-0.0276
9	0	9	2	←	8	1	8	2	6399.6748	-0.0134
8	3	5	1	←	7	3	4	0	6402.4615	-0.0144
8	3	5	3	←	7	3	4	2	6402.5902	-0.0142
9	1	9	2	←	8	1	8	3	6423.8496	-0.0062
9	1	9	0	←	8	1	8	1	6424.0067	-0.0203
9	1	9	1	←	8	1	8	0	6437.8306	-0.0200
9	1	9	3	←	8	1	8	2	6437.9675	0.0060
9	0	9	2	←	8	0	8	3	6446.7972	0.0065
9	0	9	0	←	8	0	8	1	6446.9506	-0.0109
4	3	2	0	←	3	2	1	0	6454.5565	0.0033
4	3	2	1	←	3	2	1	1	6455.5780	0.0042
9	0	9	1	←	8	0	8	0	6460.8145	-0.0385
9	0	9	3	←	8	0	8	2	6460.9412	-0.0265
9	1	9	1	←	8	0	8	1	6485.0772	-0.0122
9	1	9	0	←	8	0	8	0	6485.1730	-0.0079
7	2	6	1	←	6	1	5	1	6536.2215	0.0149
7	2	6	0	←	6	1	5	0	6536.6654	0.0095
8	2	6	2	←	7	2	5	3	6547.8306	-0.0046
8	2	6	0	←	7	2	5	1	6547.9612	-0.0132
8	2	6	1	←	7	2	5	0	6561.4333	-0.0021
8	2	6	3	←	7	2	5	2	6561.5800	0.0005
9	2	8	0	←	8	2	7	1	6838.7390	-0.0044
9	2	8	1	←	8	2	7	0	6851.8198	0.0345
9	2	8	3	←	8	2	7	2	6851.9367	0.0339
9	1	8	0	←	8	1	7	1	7036.7249	0.0100
8	2	7	1	←	7	1	6	1	7043.6782	0.0134
8	2	7	0	←	7	1	6	0	7044.1029	0.0025
9	3	7	2	←	8	3	6	3	7045.3801	0.0091
9	3	7	0	←	8	3	6	1	7045.5040	0.0046
9	1	8	1	←	8	1	7	0	7050.4316	0.0129
9	1	8	3	←	8	1	7	2	7050.5666	0.0074
9	5	5	0	←	8	5	4	1	7053.4863	0.0055
9	5	4	0	←	8	5	3	1	7054.0140	0.0075
9	3	7	1	←	8	3	6	0	7057.3562	0.0088
9	3	7	3	←	8	3	6	2	7057.4789	0.0162
9	5	5	1	←	8	5	4	0	7068.0216	-0.0040
9	5	4	1	←	8	5	3	0	7068.5438	-0.0090
9	4	6	0	←	8	4	5	1	7074.9207	0.0041
9	4	6	1	←	8	4	5	0	7084.5559	-0.0109
9	4	6	3	←	8	4	5	2	7084.6611	-0.0102
9	4	5	2	←	8	4	4	3	7096.4282	-0.0128
9	4	5	0	←	8	4	4	1	7096.5329	-0.0113
10	0	10	3	←	9	1	9	3	7104.6760	-0.0343
9	4	5	1	←	8	4	4	0	7106.2154	-0.0126
9	4	5	3	←	8	4	4	2	7106.3943	-0.0209
10	1	10	2	←	9	1	9	3	7115.3339	0.0057
10	1	10	0	←	9	1	9	1	7115.4885	-0.0223
10	1	10	1	←	9	1	9	0	7129.1913	-0.0371
10	1	10	3	←	9	1	9	2	7129.3140	-0.0101
5	3	3	1	←	4	2	2	1	7178.3974	0.0100
5	3	3	0	←	4	2	2	0	7179.3355	0.0049
10	1	9	0	←	9	2	8	0	7220.4512	0.0024
9	3	6	2	←	8	3	5	3	7247.7622	-0.0007
9	3	6	0	←	8	3	5	1	7247.8836	-0.0144
9	3	6	1	←	8	3	5	0	7259.9779	-0.0328
9	3	6	3	←	8	3	5	2	7260.1111	-0.0183
9	2	7	2	←	8	2	6	3	7363.3502	0.0171
9	2	7	0	←	8	2	6	1	7363.4873	0.0090
9	2	7	1	←	8	2	6	0	7376.9125	-0.0092
9	2	7	3	←	8	2	6	2	7377.0557	-0.0056
9	2	8	1	←	8	1	7	1	7550.0858	0.0130
9	2	8	0	←	8	1	7	0	7550.4840	0.0036
10	2	9	2	←	9	2	8	3	7559.6066	0.0075
10	2	9	0	←	9	2	8	1	7559.7475	-0.0044
10	2	9	1	←	9	2	8	0	7572.6902	0.0071

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
10	2	9	3	←	9	2	8	2	7572.8162	0.0290
10	1	9	2	←	9	1	8	3	7720.3543	-0.0016
10	1	9	0	←	9	1	8	1	7720.5063	-0.0042
10	1	9	1	←	9	1	8	0	7733.9950	0.0075
10	1	9	3	←	9	1	8	2	7734.1233	0.0090
10	3	8	2	←	9	3	7	3	7816.1196	0.0192
10	3	8	0	←	9	3	7	1	7816.2461	0.0112
10	3	8	1	←	9	3	7	0	7828.0557	0.0121
10	3	8	3	←	9	3	7	2	7828.1699	0.0228
10	5	6	0	←	9	5	5	1	7849.7239	-0.0115
10	5	5	0	←	9	5	4	1	7850.9766	-0.0124
6	3	4	1	←	5	2	3	1	7852.6398	0.0097
6	3	4	0	←	5	2	3	0	7853.4147	0.0123
10	4	7	1	←	9	4	6	0	7881.6233	-0.0063
10	4	7	3	←	9	4	6	2	7881.7293	0.0000
10	4	6	2	←	9	4	5	3	7917.4349	-0.0164
10	4	6	0	←	9	4	5	1	7917.5412	-0.0295
10	4	6	1	←	9	4	5	0	7927.5895	-0.0332
									RMS	11.8 kHz

Table S20 Linelist for DPE-2w. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
6	2	5	←	6	1	6	2003.1232	-0.0078
3	1	3	←	2	1	2	2086.5230	0.0037
6	3	3	←	6	2	4	2105.6892	0.0112
3	0	3	←	2	0	2	2153.7929	-0.0048
19	5	15	←	19	4	15	2172.3953	0.0254
3	2	2	←	2	2	1	2174.0803	-0.0018
5	3	3	←	5	2	3	2183.6128	0.0056
5	3	2	←	5	2	3	2191.7553	0.0077
3	2	1	←	2	2	0	2194.3666	-0.0041
4	0	4	←	3	1	2	2197.2740	0.0077
7	2	6	←	7	1	7	2212.1208	0.0001
4	3	2	←	4	2	2	2249.3259	0.0094
4	3	1	←	4	2	2	2251.3796	0.0089
3	1	2	←	2	1	1	2255.1984	-0.0001
3	3	0	←	3	2	1	2285.1823	0.0130
6	2	4	←	5	3	3	2287.2313	-0.0073
3	3	1	←	3	2	2	2310.3094	0.0045
3	3	0	←	3	2	2	2310.6069	0.0072
6	2	4	←	6	1	6	2315.1662	-0.0122
4	3	2	←	4	2	3	2323.7675	0.0064
4	3	1	←	4	2	3	2325.8178	0.0025
5	3	3	←	5	2	4	2349.9590	0.0049
5	3	2	←	5	2	4	2358.0941	-0.0003
6	3	4	←	6	2	5	2393.7088	0.0039
6	3	3	←	6	2	5	2417.7279	0.0025
8	2	7	←	8	1	8	2448.2122	0.0028
7	3	5	←	7	2	6	2459.5772	0.0028
3	1	3	←	2	0	2	2468.6366	0.0091
7	3	4	←	7	2	6	2518.0152	-0.0004
4	0	4	←	3	1	3	2534.9188	-0.0018
5	1	4	←	4	2	2	2550.8140	-0.0013
8	3	6	←	8	2	7	2551.4470	0.0010
7	2	6	←	6	3	3	2615.6789	-0.0011
5	1	4	←	4	2	3	2625.2499	-0.0099
7	2	6	←	6	3	4	2639.6972	-0.0033
9	3	7	←	9	2	8	2672.2041	0.0084
8	3	5	←	8	2	7	2674.7397	0.0046
5	0	5	←	4	1	3	2728.5270	0.0168
8	3	5	←	7	4	3	2736.0397	0.0033
4	1	4	←	3	1	3	2776.6732	0.0010
2	2	1	←	1	1	0	2805.5855	0.0028
3	1	2	←	2	0	2	2806.2797	-0.0022
2	2	0	←	1	1	0	2810.7267	0.0020

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
10	3	8	←	10	2	9	2823.4805	0.0180
4	0	4	←	3	0	3	2849.7491	-0.0012
2	2	1	←	1	1	1	2861.9111	0.0032
2	2	0	←	1	1	1	2867.0502	0.0004
4	2	3	←	3	2	2	2894.7669	0.0009
10	4	6	←	10	3	7	2898.8785	-0.0135
9	3	6	←	9	2	8	2904.2138	0.0206
4	3	2	←	3	3	1	2908.2185	-0.0036
4	3	1	←	3	3	0	2909.9791	-0.0024
4	2	2	←	3	2	1	2943.7820	0.0019
9	4	6	←	9	3	6	2997.6087	-0.0069
4	1	3	←	3	1	2	3000.2101	0.0001
9	4	5	←	9	3	6	3014.7754	-0.0015
4	1	4	←	3	0	3	3091.5062	0.0043
8	4	5	←	8	3	5	3093.4920	0.0008
8	4	4	←	8	3	5	3100.2192	-0.0003
7	4	4	←	7	3	4	3154.7484	0.0031
7	2	5	←	6	3	4	3156.5977	-0.0013
7	4	3	←	7	3	4	3157.0235	0.0058
6	4	3	←	6	3	3	3190.6754	0.0038
6	4	2	←	6	3	3	3191.3018	0.0051
6	0	6	←	5	1	4	3191.9140	0.0162
5	4	2	←	5	3	2	3210.0108	0.0078
5	4	1	←	5	3	2	3210.1375	0.0088
7	4	4	←	7	3	5	3213.1908	0.0042
6	4	3	←	6	3	4	3214.6955	0.0035
6	4	2	←	6	3	4	3215.3225	0.0054
7	4	3	←	7	3	5	3215.4628	0.0037
8	4	5	←	8	3	6	3216.7843	0.0040
5	4	2	←	5	3	3	3218.1544	0.0110
5	4	1	←	5	3	3	3218.2856	0.0164
4	4	1	←	4	3	2	3221.5136	-0.0112
8	4	4	←	8	3	6	3223.5108	0.0022
9	4	6	←	9	3	7	3229.6156	0.0025
9	4	5	←	9	3	7	3246.7754	0.0009
10	4	7	←	10	3	8	3256.4731	0.0057
8	2	7	←	7	3	5	3276.7569	-0.0035
5	0	5	←	4	1	4	3289.7007	-0.0015
10	4	6	←	10	3	8	3295.4444	0.0088
11	4	8	←	11	3	9	3302.3167	0.0166
6	1	5	←	5	2	3	3314.4412	-0.0017
12	4	9	←	12	3	10	3371.7639	0.0214
11	4	7	←	11	3	9	3382.7195	0.0172
5	1	5	←	4	1	4	3463.0271	-0.0072
13	4	10	←	13	3	11	3468.6798	0.0324
3	2	2	←	2	1	1	3473.9611	0.0126
3	2	1	←	2	1	1	3499.3838	0.0048
5	0	5	←	4	0	4	3531.4516	-0.0023
9	3	6	←	8	4	5	3569.6623	0.0130
7	0	7	←	6	1	5	3590.6711	0.0113
5	2	4	←	4	2	3	3612.0427	-0.0016
5	4	2	←	4	4	1	3634.8551	-0.0007
5	4	1	←	4	4	0	3634.9639	-0.0036
5	3	3	←	4	3	2	3638.2333	-0.0040
14	5	10	←	14	4	10	3642.9228	0.0007
5	3	2	←	4	3	1	3644.3211	-0.0025
4	1	3	←	3	0	3	3652.6867	-0.0073
3	2	1	←	2	1	2	3668.3507	-0.0034
5	2	3	←	4	2	2	3703.9434	-0.0032
5	1	5	←	4	0	4	3704.7877	0.0018
9	1	9	←	8	2	7	3725.5269	0.0788
5	1	4	←	4	1	3	3738.5669	0.0009
4	4	0	←	5	1	5	3756.7546	-0.0090
8	2	6	←	7	3	4	3999.3025	0.0056
11	5	7	←	11	4	7	4005.3320	-0.0148
11	5	6	←	11	4	7	4009.9263	-0.0147
7	1	6	←	6	2	4	4027.8130	-0.0014

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
6	0	6	←	5	1	5	4028.6178	-0.0036
10	3	8	←	9	4	5	4029.9819	0.0066
8	2	6	←	7	3	5	4057.7484	0.0101
10	5	6	←	10	4	6	4058.9277	-0.0018
10	5	5	←	10	4	6	4060.6701	-0.0094
13	5	9	←	13	4	10	4075.3859	-0.0028
12	5	7	←	12	4	9	4087.8913	-0.0093
11	5	6	←	11	4	8	4090.3436	0.0003
9	5	5	←	9	4	5	4093.4144	0.0015
9	5	4	←	9	4	5	4094.0053	0.0023
10	5	6	←	10	4	7	4097.9007	0.0030
9	5	5	←	9	4	6	4110.5675	-0.0067
9	5	4	←	9	4	6	4111.1586	-0.0057
4	2	3	←	3	1	2	4113.5264	0.0105
8	5	4	←	8	4	4	4115.2291	0.0075
8	5	3	←	8	4	4	4115.3967	0.0050
8	5	4	←	8	4	5	4121.9538	0.0038
8	5	3	←	8	4	5	4122.1237	0.0036
7	5	2	←	7	4	3	4128.8556	-0.0100
7	5	3	←	7	4	4	4131.1119	0.0130
6	5	1	←	6	4	2	4137.1713	0.0030
6	5	1	←	6	4	3	4137.7918	-0.0015
5	5	1	←	5	4	1	4142.1211	0.0143
5	5	0	←	5	4	2	4142.2441	0.0109
6	1	6	←	5	1	5	4145.5279	0.0054
4	2	2	←	3	1	2	4187.9695	0.0090
6	0	6	←	5	0	5	4201.9591	0.0055
6	1	6	←	5	0	5	4318.8492	-0.0052
6	2	5	←	5	2	4	4325.1466	0.0013
7	1	6	←	6	2	5	4339.8588	-0.0030
6	5	2	←	5	5	1	4361.0000	0.0010
6	4	3	←	5	4	2	4365.4426	-0.0020
6	4	2	←	5	4	1	4365.9421	-0.0020
6	3	4	←	5	3	3	4368.8995	0.0034
6	3	3	←	5	3	2	4384.7626	-0.0135
10	3	7	←	9	4	6	4443.7089	0.0287
4	2	3	←	3	1	3	4451.1608	-0.0094
6	1	5	←	5	1	4	4467.5787	0.0043
6	2	4	←	5	2	3	4470.8327	-0.0131
3	3	1	←	2	2	0	4479.2447	-0.0004
3	3	0	←	2	2	0	4479.5398	-0.0002
3	3	1	←	2	2	1	4484.3892	0.0021
3	3	0	←	2	2	1	4484.6839	0.0020
4	2	2	←	3	1	3	4525.5961	-0.0188
5	1	4	←	4	0	4	4541.4946	-0.0149
8	1	7	←	7	2	5	4675.3951	-0.0003
5	2	4	←	4	1	3	4725.3587	0.0082
7	3	5	←	7	0	7	4746.6785	0.0030
7	0	7	←	6	1	6	4749.4333	-0.0020
7	1	7	←	6	1	6	4824.4120	-0.0037
9	2	7	←	8	3	5	4859.4589	0.0082
7	0	7	←	6	0	6	4866.3306	-0.0056
5	2	3	←	4	1	3	4891.6992	0.0019
7	1	7	←	6	0	6	4941.3213	0.0045
9	2	7	←	8	3	6	4982.7556	0.0158
11	6	6	←	11	5	6	5015.8667	-0.0115
11	6	5	←	11	5	6	5016.0104	-0.0143
11	6	6	←	11	5	7	5020.4625	-0.0098
11	6	5	←	11	5	7	5020.6129	-0.0060
10	6	4	←	10	5	5	5032.9295	-0.0129
7	2	6	←	6	2	5	5033.4026	-0.0027
9	6	3	←	9	5	4	5045.0477	-0.0043
9	6	4	←	9	5	5	5045.6311	-0.0001
8	6	3	←	8	5	3	5053.6139	0.0055
8	6	2	←	8	5	4	5053.7849	0.0043
7	6	1	←	7	5	3	5059.5468	-0.0080
7	6	2	←	6	6	1	5087.1838	-0.0078

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
7	5	3	←	6	5	2	5091.0868	0.0054
7	4	4	←	6	4	3	5097.7691	-0.0003
7	3	5	←	6	3	4	5099.2731	-0.0017
7	4	3	←	6	4	2	5099.4124	-0.0043
7	3	4	←	6	3	3	5133.6906	-0.0051
7	1	6	←	6	1	5	5184.2232	0.0059
8	1	7	←	7	2	6	5192.3021	0.0081
4	3	2	←	3	2	1	5193.0984	0.0018
4	3	1	←	3	2	1	5195.1619	0.0111
4	3	2	←	3	2	2	5218.5279	0.0008
4	3	1	←	3	2	2	5220.5833	0.0020
7	2	5	←	6	2	4	5238.2558	-0.0007
9	1	8	←	8	2	6	5246.3862	-0.0054
5	2	4	←	4	1	4	5286.5408	-0.0017
5	2	3	←	4	1	4	5452.8733	-0.0160
8	0	8	←	7	1	7	5453.9900	-0.0039
6	1	5	←	5	0	5	5477.6209	-0.0091
8	1	8	←	7	1	7	5500.2469	0.0008
8	0	8	←	7	0	7	5528.9673	-0.0071
8	1	8	←	7	0	7	5575.2200	-0.0064
6	2	4	←	5	1	4	5623.9769	-0.0003
8	2	7	←	7	2	6	5736.3326	-0.0020
8	6	3	←	7	6	2	5816.8699	-0.0051
8	5	4	←	7	5	3	5822.6488	-0.0024
8	5	3	←	7	5	2	5822.7793	-0.0024
8	4	5	←	7	4	4	5831.8032	0.0032
8	4	4	←	7	4	3	5836.2490	-0.0069
7	2	6	←	6	1	5	5877.7604	-0.0004
8	1	7	←	7	1	6	5885.8379	0.0003
5	3	3	←	4	2	2	5887.5534	-0.0003
8	3	5	←	7	3	4	5893.0906	0.0365
5	3	2	←	4	2	2	5895.6927	-0.0016
10	2	8	←	9	3	7	5922.0517	0.0238
11	7	4	←	11	6	5	5960.2473	-0.0126
11	7	5	←	11	6	6	5960.3804	-0.0232
5	3	3	←	4	2	3	5962.0019	0.0034
5	3	2	←	4	2	3	5970.1386	-0.0003
9	7	2	←	9	6	4	5976.1204	-0.0027
8	7	1	←	8	6	2	5981.0469	0.0112
7	7	0	←	7	6	1	5984.5027	0.0100
8	2	6	←	7	2	5	6000.4186	0.0045
9	1	8	←	8	2	7	6027.3844	0.0148
4	4	1	←	3	3	0	6129.4567	0.0044
4	4	1	←	3	3	1	6129.7621	0.0150
4	4	0	←	3	3	1	6129.7621	0.0010
9	0	9	←	8	1	8	6145.9529	-0.0100
6	2	5	←	5	1	5	6148.6498	-0.0036
9	1	9	←	8	1	8	6173.6487	-0.0086
9	0	9	←	8	0	8	6192.2153	0.0002
9	1	9	←	8	0	8	6219.8968	-0.0126
7	2	5	←	6	1	5	6394.6617	0.0023
8	2	7	←	7	1	6	6429.8913	0.0130
9	2	8	←	8	2	7	6433.6677	-0.0145
7	1	6	←	6	0	6	6459.8945	0.0007
6	2	4	←	5	1	5	6460.6958	-0.0050
9	7	3	←	8	7	2	6542.8235	-0.0035
6	3	4	←	5	2	3	6552.5019	-0.0013
9	3	7	←	8	3	6	6554.4373	0.0052
9	5	5	←	8	5	4	6555.8944	0.0053
9	5	4	←	8	5	3	6556.3164	0.0071
9	4	6	←	8	4	5	6567.2664	0.0014
9	1	8	←	8	1	7	6571.4044	-0.0057
6	3	3	←	5	2	3	6576.5267	0.0029
9	4	5	←	8	4	4	6577.6996	0.0018
9	3	6	←	8	3	5	6663.1457	0.0053
6	3	4	←	5	2	4	6718.8513	0.0011
6	3	3	←	5	2	4	6742.8626	-0.0080

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
9	2	7	←	8	2	6	6753.2158	0.0080
10	0	10	←	9	1	9	6829.0562	-0.0195
10	1	9	←	9	2	8	6836.4604	0.0065
10	1	10	←	9	1	9	6845.2664	-0.0169
5	4	2	←	4	3	1	6854.3242	-0.0023
5	4	1	←	4	3	1	6854.4475	-0.0047
5	4	2	←	4	3	2	6856.3794	-0.0013
5	4	1	←	4	3	2	6856.5051	-0.0013
10	0	10	←	9	0	9	6856.7535	-0.0166
10	1	10	←	9	0	9	6872.9575	-0.0202
9	8	1	←	9	7	2	6902.2072	0.0047
8	8	1	←	8	7	2	6905.3850	0.0140
9	2	8	←	8	1	7	6977.7221	-0.0008
7	2	6	←	6	1	6	7036.5314	-0.0050
10	2	9	←	9	2	8	7125.4776	-0.0054
13	3	10	←	12	4	8	7158.2583	0.0026
12	2	10	←	11	3	8	7174.5608	0.0181
7	3	5	←	6	2	4	7180.9285	-0.0038
8	2	6	←	7	1	6	7210.8548	-0.0013
7	3	4	←	6	2	4	7239.3837	0.0100
10	1	9	←	9	1	8	7242.7683	0.0017
10	3	8	←	9	3	7	7276.7453	-0.0044
10	5	6	←	9	5	5	7290.9227	-0.0048
10	5	5	←	9	5	4	7292.0843	-0.0030
10	4	7	←	9	4	6	7303.6170	0.0129
10	4	6	←	9	4	5	7325.4131	0.0022
10	3	7	←	9	3	6	7441.3074	0.0117
8	1	7	←	7	0	7	7479.3920	-0.0031
7	3	5	←	6	2	5	7492.9783	-0.0014
10	2	8	←	9	2	7	7493.7357	0.0154
11	0	11	←	10	1	10	7506.3358	-0.0148
11	1	11	←	10	1	10	7515.6517	-0.0151
10	2	9	←	9	1	8	7531.7779	-0.0178
11	1	11	←	10	0	10	7531.8516	-0.0229
7	3	4	←	6	2	5	7551.4187	-0.0023
7	2	5	←	6	1	6	7553.4135	-0.0215
6	4	3	←	5	3	2	7575.4437	-0.0038
6	4	2	←	5	3	2	7576.0707	-0.0020
6	4	3	←	5	3	3	7583.5892	0.0011
6	4	2	←	5	3	3	7584.2143	0.0010
11	1	10	←	10	2	9	7615.4318	-0.0005
8	3	6	←	7	2	5	7770.8819	-0.0002
5	5	1	←	4	4	0	7777.0804	0.0060
5	5	1	←	4	4	1	7777.0804	-0.0079
11	2	10	←	10	2	9	7812.0559	-0.0103
5	3	3	←	4	0	4	7878.2444	-0.0036
5	3	2	←	4	0	4	7886.3826	-0.0059
8	3	5	←	7	2	5	7894.1674	-0.0038
11	1	10	←	10	1	9	7904.4516	-0.0098
11	3	9	←	10	3	8	7994.1239	-0.0062
							RMS	9.9 kHz

Table S21 Linelist for DPE-3w. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
2	2	0	←	1	1	0	2159.5388	0.0051
2	2	1	←	1	1	1	2222.9370	0.0079
2	2	0	←	1	1	1	2237.9954	-0.0031
4	0	4	←	3	1	3	2295.0126	0.0006
4	1	4	←	3	1	3	2369.1878	0.0010
4	0	4	←	3	0	3	2425.6105	0.0033
3	1	2	←	2	0	2	2456.2294	-0.0010
4	1	4	←	3	0	3	2499.7826	0.0007
4	2	3	←	3	2	2	2539.6675	-0.0091
4	1	3	←	3	1	2	2672.2346	0.0082
3	2	2	←	2	1	1	2703.8863	0.0109

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	2	1	←	2	1	1	2775.8833	0.0051
5	0	5	←	4	1	4	2905.6160	0.0001
3	2	2	←	2	1	2	2939.2776	0.0079
5	1	5	←	4	1	4	2943.4535	0.0065
5	0	5	←	4	0	4	2979.7916	0.0009
5	1	5	←	4	0	4	3017.6237	0.0019
6	1	5	←	5	2	3	3084.3062	-0.0096
5	2	4	←	4	2	3	3155.9991	0.0025
4	2	3	←	3	1	2	3222.7447	0.0077
5	4	2	←	4	4	1	3222.7447	-0.0125
5	3	3	←	4	3	2	3224.7849	-0.0049
5	3	2	←	4	3	1	3260.5531	-0.0081
4	1	3	←	3	0	3	3271.7582	-0.0011
5	1	4	←	4	1	3	3299.9735	-0.0014
5	2	3	←	4	2	2	3364.1059	0.0000
4	2	2	←	3	1	2	3420.4516	0.0016
3	3	1	←	2	2	0	3420.4516	0.0048
3	3	1	←	2	2	1	3435.5175	0.0012
3	3	0	←	2	2	1	3437.3723	0.0064
6	1	5	←	5	2	4	3490.1422	0.0038
6	0	6	←	5	1	5	3493.7529	0.0020
6	1	6	←	5	1	5	3511.6543	-0.0128
6	0	6	←	5	0	5	3531.5821	0.0001
7	2	5	←	6	3	3	3538.7483	0.0049
6	1	6	←	5	0	5	3549.4990	0.0007
4	2	3	←	3	1	3	3691.6744	-0.0003
5	2	4	←	4	1	3	3706.5115	0.0044
6	2	5	←	5	2	4	3761.1247	0.0023
6	4	3	←	5	4	2	3876.5019	-0.0119
6	1	5	←	5	1	4	3896.6731	0.0026
6	3	3	←	5	3	2	3954.7809	-0.0026
4	3	2	←	3	2	1	4026.7831	0.0050
4	3	1	←	3	2	1	4039.4472	0.0035
6	2	4	←	5	2	3	4050.3435	0.0070
7	0	7	←	6	1	6	4067.7457	-0.0003
7	1	7	←	6	1	6	4075.8136	-0.0013
7	0	7	←	6	0	6	4085.6641	0.0017
7	1	7	←	6	0	6	4093.7286	-0.0026
4	3	2	←	3	2	2	4098.7814	0.0004
4	3	1	←	3	2	2	4111.4465	0.0000
5	2	3	←	4	1	3	4112.3293	-0.0002
5	1	4	←	4	0	4	4146.1276	0.0003
6	2	5	←	5	1	4	4167.6617	0.0073
7	1	6	←	6	2	5	4192.0718	0.0071
7	2	6	←	6	2	5	4354.6800	0.0041
7	1	6	←	6	1	5	4463.0502	0.0016
5	2	4	←	4	1	4	4478.4856	0.0010
7	3	5	←	6	3	4	4506.3272	0.0031
8	2	6	←	7	3	5	4513.2920	0.0064
7	4	4	←	6	4	3	4532.6248	-0.0065
5	3	3	←	4	2	2	4586.1918	0.0108
7	2	6	←	6	1	5	4625.6616	0.0018
8	0	8	←	7	1	7	4634.0489	0.0001
5	3	2	←	4	2	2	4634.6277	0.0097
8	1	8	←	7	1	7	4637.5581	0.0020
8	0	8	←	7	0	7	4642.1177	-0.0001
8	1	8	←	7	0	7	4645.6271	0.0019
7	3	4	←	6	3	3	4667.4041	-0.0039
4	4	1	←	3	3	0	4671.3164	0.0109
4	4	0	←	3	3	0	4671.5081	0.0150
4	4	1	←	3	3	1	4673.1634	0.0084
4	4	0	←	3	3	1	4673.3529	0.0102
7	2	5	←	6	2	4	4713.7070	0.0047
5	3	3	←	4	2	3	4783.8929	-0.0010
5	3	2	←	4	2	3	4832.3345	0.0034
8	1	7	←	7	2	6	4848.5295	0.0039
6	2	4	←	5	1	4	4862.6963	0.0052

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
8	1	7	←	7	1	6	5011.1372	0.0004
6	1	5	←	5	0	5	5063.0073	0.0003
6	3	4	←	5	2	3	5091.2565	0.0008
8	2	7	←	7	1	6	5100.1720	0.0022
8	3	6	←	7	3	5	5133.0682	0.0005
8	4	5	←	7	4	4	5188.6496	-0.0088
9	0	9	←	8	1	8	5196.5274	-0.0076
9	1	9	←	8	1	8	5198.0195	-0.0004
9	0	9	←	8	0	8	5200.0388	-0.0035
9	1	9	←	8	0	8	5201.5263	-0.0009
6	3	3	←	5	2	3	5225.2939	-0.0015
8	4	4	←	7	4	3	5240.1269	-0.0066
6	2	5	←	5	1	5	5296.1598	0.0000
5	4	2	←	4	3	1	5306.3546	0.0033
5	4	1	←	4	3	1	5308.0322	0.0166
5	4	2	←	4	3	2	5319.0195	0.0027
5	4	1	←	4	3	2	5320.6901	0.0089
9	2	7	←	8	3	6	5324.5976	0.0155
8	2	6	←	7	2	5	5346.8165	-0.0099
8	3	5	←	7	3	4	5383.6304	0.0009
9	1	8	←	8	2	7	5466.3001	0.0075
6	3	4	←	5	2	4	5497.0770	-0.0012
9	2	8	←	8	2	7	5511.7232	0.0022
7	3	5	←	6	2	4	5547.2430	-0.0002
9	1	8	←	8	1	7	5555.3260	0.0004
6	3	3	←	5	2	4	5631.1137	-0.0042
7	2	5	←	6	1	5	5679.7203	-0.0027
9	3	7	←	8	3	6	5747.3870	0.0060
10	0	10	←	9	1	9	5757.2364	-0.0093
10	1	10	←	9	1	9	5757.8592	-0.0025
10	0	10	←	9	0	9	5758.7268	-0.0038
10	1	10	←	9	0	9	5759.3606	0.0139
9	5	5	←	8	5	4	5837.7473	-0.0178
9	4	6	←	8	4	5	5841.1109	-0.0071
7	3	4	←	6	2	4	5842.3633	-0.0037
6	4	3	←	5	3	2	5922.3049	0.0010
6	4	2	←	5	3	2	5930.4166	0.0002
9	2	7	←	8	2	6	5944.3690	0.0049
9	4	5	←	8	4	4	5948.7424	-0.0081
8	3	6	←	7	2	5	5966.6051	-0.0034
6	4	3	←	5	3	3	5970.7422	0.0012
6	4	2	←	5	3	3	5978.8534	0.0000
10	1	9	←	9	2	8	6057.5658	0.0037
10	2	9	←	9	2	8	6079.5755	0.0024
10	1	9	←	9	1	8	6103.0081	0.0176
10	2	9	←	9	1	8	6125.0067	0.0052
7	2	6	←	6	1	6	6139.1746	0.0061
7	3	5	←	6	2	5	6242.2758	-0.0040
11	0	11	←	10	1	10	6317.1550	-0.0151
11	1	11	←	10	1	10	6317.4182	-0.0033
11	0	11	←	10	0	10	6317.7762	-0.0099
11	1	11	←	10	0	10	6318.0375	0.0000
10	3	8	←	9	3	7	6348.6269	0.0090
9	3	7	←	8	2	6	6367.1548	-0.0082
10	4	7	←	9	4	6	6486.1794	-0.0006
7	4	4	←	6	3	3	6500.1506	-0.0012
10	5	6	←	9	5	5	6500.8553	-0.0152
10	2	8	←	9	2	7	6507.9779	0.0057
8	3	5	←	7	2	5	6512.2844	-0.0097
7	4	3	←	6	3	3	6528.6704	0.0009
10	5	5	←	9	5	4	6529.4191	-0.0142
7	3	4	←	6	2	5	6537.3988	-0.0050
6	5	2	←	5	4	1	6556.7131	0.0076
6	5	1	←	5	4	1	6556.9029	0.0105
6	5	2	←	5	4	2	6558.3781	0.0083
6	5	1	←	5	4	2	6558.5688	0.0121
8	2	6	←	7	1	6	6563.5004	-0.0005

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
11	1	10	←	10	2	9	6633.1009	0.0044
7	4	4	←	6	3	4	6634.1872	-0.0043
11	2	10	←	10	2	9	6643.3635	0.0049
11	1	10	←	10	1	9	6655.1110	0.0037
7	4	3	←	6	3	4	6662.7051	-0.0041
11	2	10	←	10	1	9	6665.3709	0.0014
10	4	6	←	9	4	5	6675.8808	0.0055
10	3	7	←	9	3	6	6759.4561	0.0106
10	3	8	←	9	2	7	6771.4059	-0.0109
11	2	9	←	10	3	8	6786.4701	0.0125
8	1	7	←	7	0	7	6919.9580	0.0100
8	2	7	←	7	1	7	7000.9130	0.0009
8	3	6	←	7	2	6	7020.6657	-0.0060
8	4	5	←	7	3	4	7021.3940	-0.0082
11	2	9	←	10	2	8	7049.9099	0.0076
8	4	4	←	7	3	4	7101.3803	-0.0145
7	5	2	←	6	4	2	7194.0593	0.0025
12	1	11	←	11	2	10	7200.1449	0.0024
7	5	2	←	6	4	3	7202.1684	-0.0009
7	5	3	←	6	4	3	7201.0679	0.0000
12	2	11	←	11	2	10	7204.7807	-0.0065
12	1	11	←	11	1	10	7210.4049	0.0002
12	2	11	←	11	1	10	7215.0495	0.0001
11	5	6	←	10	5	5	7227.8095	-0.0092
9	3	6	←	8	2	6	7250.6950	-0.0076
8	4	5	←	7	3	5	7316.5154	-0.0106
8	4	4	←	7	3	5	7396.5047	-0.0140
11	3	8	←	10	3	7	7398.4431	0.0049
11	4	7	←	10	4	6	7406.9841	0.0050
12	2	10	←	11	3	9	7435.0881	0.0147
9	4	6	←	8	3	5	7478.8732	-0.0175
9	2	7	←	8	1	7	7496.7312	0.0029
12	3	10	←	11	3	9	7516.0980	0.0083
8	3	5	←	7	2	6	7566.3462	-0.0112
12	2	10	←	11	2	9	7586.1664	0.0032
9	4	5	←	8	3	5	7666.5006	-0.0153
12	3	10	←	11	2	9	7667.1738	-0.0057
12	4	9	←	11	4	8	7741.6336	0.0095
13	1	12	←	12	2	11	7762.9244	0.0022
13	2	12	←	12	1	11	7769.6225	0.0025
8	5	4	←	7	4	3	7816.6774	-0.0089
8	5	3	←	7	4	3	7821.3216	-0.0084
9	3	7	←	8	2	7	7830.4823	-0.0119
9	1	8	←	8	0	8	7833.1581	0.0022
8	5	4	←	7	4	4	7845.1920	-0.0120
8	5	3	←	7	4	4	7849.8384	-0.0093
9	2	8	←	8	1	8	7875.0845	0.0076
							RMS	7.0 kHz

S16 Linelist for isotopologues of DPE and its complexes with water

S16.1 Isotopologues of DPE

The spectrum of the ^{13}C isotopologues of DPE splits into triplet for 1, 1", 4, and 4", and into doublet for 2, 2", 3, 3", 5, 5", 6, and 6". To obtain the fits in the case of doublet splitting only the center frequencies of the doublet were considered. The center frequency were calculated by taking the average of left and right frequencies of the doublet, as given in the following tables. For the 1, 1", 4, and 4" isotopologues, only the center transition was considered to obtain the fit.

Table S22 Linelist for ^{13}C1,1" isotopologue of DPE. AOMC is the difference between the observed average and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
5	1	4	←	5	0	5	2133.3199	0.0134
6	1	5	←	6	0	6	2216.7709	0.0068
1	1	1	←	0	0	0	2771.1144	-0.0047
2	1	2	←	1	0	1	3594.9140	-0.0117
3	1	3	←	2	0	2	4406.0463	0.0045
4	1	4	←	3	0	3	5204.7774	-0.0088
8	2	6	←	8	1	7	5401.6459	0.0042
7	2	5	←	7	1	6	5480.7155	0.0053
5	2	3	←	5	1	4	5621.6297	-0.0080
4	2	2	←	4	1	3	5679.9669	0.0050
4	2	3	←	4	1	4	5931.8088	-0.0042
5	1	5	←	4	0	4	5991.6789	0.0072
6	2	5	←	6	1	6	6073.7295	-0.0056
6	1	6	←	5	0	5	6767.4141	0.0090
7	1	7	←	6	0	6	7532.8796	-0.0058
							RMS	7.5 kHz

Table S23 Linelist for ^{13}C2,2" isotopologue of DPE. AOMC is the difference between the observed average and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	Right (MHz)	Average (MHz)	AOMC (MHz)
6	1	5	←	6	0	6	2205.5589	2205.7738	2205.6664	0.0019
7	1	6	←	7	0	7	2304.8220	2305.0299	2304.9259	0.0053
8	1	7	←	8	0	8	2421.8089	2422.0244	2421.9167	0.0011
1	1	1	←	0	0	0	2761.8511	2762.0852	2761.9682	0.0001
6	0	6	←	5	1	5	3340.8973	3341.0749	3340.9861	0.0013
2	1	2	←	1	0	1	3585.2548	3585.4758	3585.3653	-0.0017
7	0	7	←	6	1	6	4253.7307	4253.8866	4253.8086	0.0024
3	1	3	←	2	0	2	4396.0801	4396.2910	4396.1855	0.0022
4	1	4	←	3	0	3	5194.6294	5194.8346	5194.7320	0.0001
7	2	5	←	7	1	6	5457.2671	5457.5811	5457.4241	0.0045
6	2	4	←	6	1	5	5530.6513	5530.9852	5530.8182	0.0034
5	2	3	←	5	1	4	5597.0738	5597.4291	5597.2515	0.0042
4	2	2	←	4	1	3	5654.9158	5655.2889	5655.1024	0.0057
3	2	2	←	3	1	3	5853.6335	5854.0285	5853.8310	-0.0092
4	2	3	←	4	1	4	5904.6120	5905.0022	5904.8071	-0.0059
5	2	4	←	5	1	5	5968.4748	5968.8694	5968.6721	-0.0036
5	1	5	←	4	0	4	5981.4240	5981.6192	5981.5216	0.0027
6	1	6	←	5	0	5	6757.1559	6757.3399	6757.2479	0.0056
7	1	7	←	6	0	6	7522.6909	7522.8669	7522.7789	-0.0108
									RMS	4.7 kHz

Table S24 Linelist for ^{13}C3,3" isotopologue of DPE. AOMC is the difference between the observed average and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	Right (MHz)	Average (MHz)	AOMC (MHz)
4	1	3	←	4	0	4	2045.1248	2045.3453	2045.2350	0.0007
5	1	4	←	5	0	5	2112.8456	2113.0724	2112.9590	0.0087
7	1	6	←	7	0	7	2296.1627	2296.3881	2296.2754	-0.0006
8	1	7	←	8	0	8	2414.0846	2414.3049	2414.1948	0.0037
5	0	5	←	4	1	4	2428.8300	2429.0090	2428.9195	0.0084
1	1	1	←	0	0	0	2746.5404	2746.7658	2746.6531	-0.0012
2	1	2	←	1	0	1	3565.8644	3566.0865	3565.9754	-0.0046
3	1	3	←	2	0	2	4372.5309	4372.7480	4372.6395	-0.0058
8	0	8	←	7	1	7	5154.9671	5155.1171	5155.0421	-0.0048

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	Right (MHz)	Average (MHz)	AOMC (MHz)
4	1	4	←	3	0	3	5166.8666	5167.0718	5166.9692	-0.0016
7	2	5	←	7	1	6	5421.7146	5422.0432	5421.8789	0.0039
6	2	4	←	6	1	5	5495.3743	5495.7229	5495.5486	0.0057
4	2	2	←	4	1	3	5620.2263	5620.6179	5620.4221	0.0039
3	2	2	←	3	1	3	5820.1380	5820.5488	5820.3434	-0.0172
4	2	3	←	4	1	4	5871.4484	5871.8617	5871.6551	-0.0025
5	2	4	←	5	1	5	5935.7241	5936.1259	5935.9250	-0.0030
5	1	5	←	4	0	4	5949.3621	5949.5618	5949.4620	-0.0103
6	2	5	←	6	1	6	6013.0656	6013.4794	6013.2725	0.0096
6	1	6	←	5	0	5	6720.7837	6720.9651	6720.8744	0.0137
7	1	7	←	6	0	6	7481.9528	7482.1282	7482.0405	0.0001
									RMS	7.1 kHz

Table S25 Linelist for ^{13}C4,4" isotopologue of DPE. OMC is the difference between the observed average and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
4	1	3	←	4	0	4	2064.3480	0.0048
6	1	5	←	6	0	6	2212.9687	-0.0048
7	1	6	←	7	0	7	2311.3068	0.0032
5	0	5	←	4	1	4	2385.7922	-0.0004
8	1	7	←	8	0	8	2427.1666	-0.0028
1	1	1	←	0	0	0	2763.7593	0.0010
6	0	6	←	5	1	5	3281.8807	-0.0035
2	1	2	←	1	0	1	3579.3244	-0.0039
7	0	7	←	6	1	6	4186.3023	-0.0125
3	1	3	←	2	0	2	4382.4033	-0.0120
8	0	8	←	7	1	7	5097.7747	-0.0024
4	1	4	←	3	0	3	5173.3235	-0.0036
6	2	4	←	6	1	5	5561.6969	-0.0012
5	2	3	←	5	1	4	5627.7239	0.0000
5	1	5	←	4	0	4	5952.5634	0.0038
9	0	9	←	8	1	8	6014.8284	0.0026
7	2	6	←	7	1	7	6161.7027	0.0029
6	1	6	←	5	0	5	6720.7835	-0.0121
10	0	10	←	9	1	9	6935.9180	0.0110
7	1	7	←	6	0	6	7478.9206	0.0156
							RMS	6.9 kHz

Table S26 Linelist for ^{13}C5,5" isotopologue of DPE. AOMC is the difference between the observed average and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	Right (MHz)	Average (MHz)	AOMC (MHz)
3	1	2	←	3	0	3	2010.9209	2011.1216	2011.0212	0.0131
6	1	5	←	6	0	6	2210.0104	2210.2308	2210.1206	0.0015
5	0	5	←	4	1	4	2389.6326	2389.8305	2389.7316	-0.0037
8	1	7	←	8	0	8	2422.2390	2422.4561	2422.3476	-0.0010
1	1	1	←	0	0	0	2764.1645	2764.3962	2764.2803	-0.0020
6	0	6	←	5	1	5	3286.2226	3286.3972	3286.3099	0.0020
2	1	2	←	1	0	1	3580.8259	3581.0482	3580.9370	-0.0019
7	0	7	←	6	1	6	4191.1028	4191.2706	4191.1867	0.0032
3	1	3	←	2	0	2	4385.0972	4385.3197	4385.2084	-0.0061
8	0	8	←	7	1	7	5103.0097	5103.1592	5103.0844	0.0088
4	1	4	←	3	0	3	5177.3016	5177.5152	5177.4084	-0.0041
9	2	7	←	9	1	8	5331.0240	5331.3294	5331.1767	0.0123
8	2	6	←	8	1	7	5411.8364	5412.1351	5411.9858	-0.0005
7	2	5	←	7	1	6	5489.5113	5489.8376	5489.6744	0.0023
5	2	3	←	5	1	4	5627.5617	5627.9309	5627.7463	-0.0043
3	2	1	←	3	1	2	5731.7848	5732.1762	5731.9805	0.0100
4	2	3	←	4	1	4	5930.3159	5930.7197	5930.5178	-0.0125
5	1	5	←	4	0	4	5957.9146	5958.1179	5958.0163	-0.0038
5	2	4	←	5	1	5	5993.1455	5993.5405	5993.3430	-0.0053
6	2	5	←	6	1	6	6068.7409	6069.1289	6068.9349	0.0052
7	2	6	←	7	1	7	6157.1765	6157.5628	6157.3696	-0.0006
6	1	6	←	5	0	5	6727.6105	6727.8007	6727.7056	-0.0038
7	1	7	←	6	0	6	7487.2462	7487.4247	7487.3355	-0.0004

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	Right (MHz)	Average (MHz)	AOMC (MHz)
									RMS	6.1 kHz

Table S27 Linelist for ^{13}C6,6" isotopologue of DPE. AOMC is the difference between the observed average and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Left (MHz)	Right (MHz)	Average (MHz)	AOMC (MHz)
5	1	4	←	5	0	5	2120.4213	2120.6443	2120.5328	0.0020
6	1	5	←	6	0	6	2203.7319	2203.9599	2203.8459	0.0043
7	1	6	←	7	0	7	2303.7170	2303.9458	2303.8314	0.0020
8	1	7	←	8	0	8	2421.5998	2421.8089	2421.7044	-0.0068
5	0	5	←	4	1	4	2428.6500	2428.8300	2428.7400	-0.0115
1	1	1	←	0	0	0	2755.5715	2755.8023	2755.6869	-0.0021
2	1	2	←	1	0	1	3576.3631	3576.5906	3576.4768	-0.0032
3	1	3	←	2	0	2	4384.4927	4384.7125	4384.6026	-0.0050
8	0	8	←	7	1	7	5159.4059	5159.5571	5159.4815	0.0040
4	1	4	←	3	0	3	5180.2824	5180.4926	5180.3875	-0.0040
5	2	3	←	5	1	4	5584.7133	5585.0940	5584.9036	0.0034
4	2	2	←	4	1	3	5642.8891	5643.2810	5643.0851	0.0075
3	2	2	←	3	1	3	5842.8503	5843.2644	5843.0573	-0.0185
4	2	3	←	4	1	4	5894.1704	5894.5912	5894.3808	-0.0013
5	2	4	←	5	1	5	5958.4561	5958.8699	5958.6630	-0.0006
5	1	5	←	4	0	4	5964.2394	5964.4456	5964.3425	-0.0028
6	2	5	←	6	1	6	6035.8142	6036.2183	6036.0162	0.0051
9	0	9	←	8	1	8	6082.6518	6082.7798	6082.7158	0.0061
7	2	6	←	7	1	7	6126.3361	6126.7261	6126.5311	0.0062
6	1	6	←	5	0	5	6737.0907	6737.2712	6737.1809	0.0033
10	0	10	←	9	1	9	7009.8068	7009.9134	7009.8601	-0.0018
7	1	7	←	6	0	6	7499.7055	7499.8801	7499.7928	0.0031
									RMS	6.1 kHz

S16.2 Isotopologues of DPE-1w OHO complex

Table S28 Linelist for $H_2^{18}O$ isotopologue of DPE-1w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
2	1	2	1	←	1	0	1	1	2020.1313	-0.0025
2	1	2	0	←	1	0	1	0	2020.2363	-0.0016
3	1	3	2	←	2	1	2	3	2159.1077	0.0099
3	1	3	0	←	2	1	2	1	2159.2098	0.0037
3	2	2	1	←	3	1	3	1	2159.8426	-0.0076
3	2	2	0	←	3	1	3	0	2160.1259	-0.0043
3	1	3	1	←	2	1	2	0	2169.1616	0.0074
3	1	3	3	←	2	1	2	2	2169.2603	0.0059
3	0	3	2	←	2	0	2	3	2266.6325	0.0023
3	0	3	0	←	2	0	2	1	2266.7404	0.0044
3	0	3	1	←	2	0	2	0	2276.8788	0.0041
3	0	3	3	←	2	0	2	2	2276.9856	0.0031
3	1	2	2	←	2	1	1	3	2447.9373	0.0015
3	1	2	0	←	2	1	1	1	2448.0370	0.0038
3	1	2	1	←	2	1	1	0	2458.0038	0.0038
3	1	2	3	←	2	1	1	2	2458.1097	0.0000
4	0	4	0	←	3	1	3	0	2603.5139	0.0039
4	0	4	1	←	3	1	3	1	2603.5840	0.0073
5	1	4	0	←	4	2	3	0	2638.0430	0.0091
5	1	4	1	←	4	2	3	1	2638.3134	0.0077
3	1	3	1	←	2	0	2	1	2651.7391	-0.0069
3	1	3	0	←	2	0	2	0	2651.8583	0.0039
4	1	4	2	←	3	1	3	3	2869.2033	0.0083
4	1	4	0	←	3	1	3	1	2869.3088	0.0028
4	1	4	1	←	3	1	3	0	2879.2328	0.0062
4	1	4	3	←	3	1	3	2	2879.3316	0.0072
4	0	4	2	←	3	0	3	3	2978.3850	0.0011
4	0	4	0	←	3	0	3	1	2978.4956	0.0058
4	0	4	1	←	3	0	3	0	2988.5908	0.0040
4	0	4	3	←	3	0	3	2	2988.6926	-0.0012

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
4	2	3	2	←	3	2	2	3	3073.9852	0.0008
4	2	3	0	←	3	2	2	1	3074.0808	0.0024
4	2	3	1	←	3	2	2	0	3083.4342	-0.0136
4	2	2	0	←	3	2	1	1	3177.9884	0.0000
4	2	2	1	←	3	2	1	0	3187.3976	0.0012
4	2	2	3	←	3	2	1	2	3187.4917	-0.0032
4	1	3	2	←	3	1	2	3	3250.5266	-0.0044
4	1	3	0	←	3	1	2	1	3250.6290	0.0020
4	1	4	1	←	3	0	3	1	3254.2036	-0.0026
4	1	4	0	←	3	0	3	0	3254.3126	-0.0035
4	1	3	1	←	3	1	2	0	3260.5817	0.0027
4	1	3	3	←	3	1	2	2	3260.6843	-0.0050
2	2	1	1	←	1	1	0	1	3358.9239	-0.0142
2	2	1	0	←	1	1	0	0	3359.3018	-0.0075
5	0	5	0	←	4	1	4	0	3399.2512	0.0015
5	0	5	1	←	4	1	4	1	3399.3002	0.0062
2	2	0	1	←	1	1	1	1	3466.8901	-0.0071
2	2	0	0	←	1	1	1	0	3467.2624	-0.0017
5	1	5	2	←	4	1	4	3	3571.7495	0.0106
5	1	5	0	←	4	1	4	1	3571.8564	0.0026
5	1	5	1	←	4	1	4	0	3581.7388	0.0039
5	1	5	3	←	4	1	4	2	3581.8362	0.0072
6	1	5	1	←	5	2	4	1	3612.1333	0.0102
5	0	5	2	←	4	0	4	3	3664.8698	-0.0012
5	0	5	0	←	4	0	4	1	3664.9798	0.0008
5	0	5	1	←	4	0	4	0	3675.0142	0.0037
5	0	5	3	←	4	0	4	2	3675.1111	-0.0035
5	2	4	2	←	4	2	3	3	3829.7288	-0.0051
5	2	4	0	←	4	2	3	1	3829.8302	0.0013
5	2	4	1	←	4	2	3	0	3839.1849	0.0086
5	2	4	3	←	4	2	3	2	3839.2776	0.0027
5	1	5	1	←	4	0	4	1	3847.4633	-0.0008
5	1	5	0	←	4	0	4	0	3847.5673	-0.0029
5	3	3	1	←	4	3	2	0	3894.2872	0.0069
5	3	2	0	←	4	3	1	1	3902.3750	-0.0061
5	2	3	2	←	4	2	2	3	4018.7198	0.0011
5	2	3	0	←	4	2	2	1	4018.8130	-0.0025
5	2	3	1	←	4	2	2	0	4028.2442	-0.0022
5	2	3	3	←	4	2	2	2	4028.3469	0.0037
3	2	2	1	←	2	1	1	1	4034.3569	-0.0065
3	2	2	0	←	2	1	1	0	4034.6552	-0.0057
5	1	4	2	←	4	1	3	3	4037.7599	-0.0091
5	1	4	0	←	4	1	3	1	4037.8660	0.0024
5	1	4	1	←	4	1	3	0	4047.7873	-0.0002
5	1	4	3	←	4	1	3	2	4047.8886	-0.0093
6	0	6	1	←	5	1	5	1	4163.3872	0.0064
6	1	6	0	←	5	1	5	1	4267.1355	-0.0089
6	1	6	1	←	5	1	5	0	4276.9751	0.0022
6	1	6	3	←	5	1	5	2	4277.0695	0.0079
6	0	6	2	←	5	0	5	3	4335.8052	-0.0030
6	0	6	0	←	5	0	5	1	4335.9176	-0.0032
6	0	6	1	←	5	0	5	0	4345.8639	-0.0021
6	0	6	3	←	5	0	5	2	4345.9562	-0.0081
3	2	1	1	←	2	1	2	1	4379.1121	-0.0039
3	2	1	0	←	2	1	2	0	4379.3940	-0.0026
6	1	6	1	←	5	0	5	1	4449.5315	-0.0011
6	1	6	0	←	5	0	5	0	4449.6251	-0.0046
7	1	6	0	←	6	2	5	0	4576.4902	0.0051
6	2	5	0	←	5	2	4	1	4576.6477	0.0098
6	2	5	3	←	5	2	4	2	4586.0579	0.0123
4	2	3	1	←	3	1	2	1	4660.1043	-0.0045
4	2	3	0	←	3	1	2	0	4660.4063	-0.0024
6	3	4	0	←	5	3	3	1	4668.4211	0.0011
6	3	4	2	←	5	3	3	3	4668.3378	0.0052
6	3	4	1	←	5	3	3	0	4676.8227	0.0018
6	3	4	3	←	5	3	3	2	4676.9015	-0.0125
6	3	3	2	←	5	3	2	3	4711.2093	-0.0084

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
6	3	3	0	←	5	3	2	1	4711.2956	-0.0077
6	3	3	1	←	5	3	2	0	4719.7277	-0.0069
6	1	5	2	←	5	1	4	3	4803.2987	0.0004
6	1	5	0	←	5	1	4	1	4803.4033	0.0119
6	1	5	1	←	5	1	4	0	4813.2698	0.0043
6	1	5	3	←	5	1	4	2	4813.3724	-0.0028
6	2	4	2	←	5	2	3	3	4865.1199	-0.0030
6	2	4	0	←	5	2	3	1	4865.2185	-0.0022
6	2	4	1	←	5	2	3	0	4874.6693	-0.0069
6	2	4	3	←	5	2	3	2	4874.7687	-0.0028
7	0	7	1	←	6	1	6	1	4897.9227	-0.0103
7	0	7	0	←	6	1	6	0	4897.9227	-0.0133
7	1	7	0	←	6	1	6	1	4956.2002	-0.0072
7	1	7	1	←	6	1	6	0	4965.9688	-0.0006
7	1	7	3	←	6	1	6	2	4966.0629	0.0123
7	0	7	0	←	6	0	6	1	5001.6930	-0.0068
7	0	7	1	←	6	0	6	0	5011.5349	-0.0099
7	0	7	3	←	6	0	6	2	5011.6256	-0.0082
7	1	7	1	←	6	0	6	1	5069.7257	-0.0074
7	1	7	0	←	6	0	6	0	5069.8097	-0.0095
5	2	4	1	←	4	1	3	1	5239.0055	-0.0005
5	2	4	0	←	4	1	3	0	5239.3098	-0.0009
7	2	6	2	←	6	2	5	3	5313.2003	0.0058
7	2	6	0	←	6	2	5	1	5313.3010	0.0059
7	2	6	1	←	6	2	5	0	5322.5696	0.0135
7	2	6	3	←	6	2	5	2	5322.6628	0.0147
4	2	2	1	←	3	1	3	1	5397.6291	-0.0098
4	2	2	0	←	3	1	3	0	5397.8888	-0.0095
3	3	1	1	←	2	2	0	1	5417.4460	0.0007
3	3	0	0	←	2	2	1	0	5429.0794	0.0190
7	3	5	2	←	6	3	4	3	5448.6677	-0.0008
7	3	5	0	←	6	3	4	1	5448.7564	-0.0005
7	3	5	1	←	6	3	4	0	5457.1803	0.0050
7	3	5	3	←	6	3	4	2	5457.2638	-0.0035
8	1	7	0	←	7	2	6	0	5511.0885	0.0085
8	1	7	1	←	7	2	6	1	5511.2703	0.0076
7	3	4	2	←	6	3	3	3	5539.4913	-0.0103
7	3	4	0	←	6	3	3	1	5539.5800	-0.0163
7	1	6	2	←	6	1	5	3	5540.8976	-0.0108
7	1	6	0	←	6	1	5	1	5541.0024	0.0025
7	3	4	1	←	6	3	3	0	5548.0797	-0.0083
7	3	4	3	←	6	3	3	2	5548.1648	-0.0089
7	1	6	1	←	6	1	5	0	5550.8026	0.0105
7	1	6	3	←	6	1	5	2	5550.9010	0.0004
8	0	8	0	←	7	1	7	0	5609.9666	-0.0112
8	1	8	2	←	7	1	7	3	5640.3044	0.0066
8	1	8	0	←	7	1	7	1	5640.4182	-0.0152
8	1	8	1	←	7	1	7	0	5650.1049	-0.0105
8	1	8	3	←	7	1	7	2	5650.1923	0.0060
8	0	8	2	←	7	0	7	3	5668.1039	-0.0177
8	0	8	1	←	7	0	7	0	5677.9659	-0.0236
8	0	8	3	←	7	0	7	2	5678.0553	-0.0108
7	2	5	2	←	6	2	4	3	5703.9006	-0.0001
7	2	5	0	←	6	2	4	1	5704.0006	0.0019
8	1	8	1	←	7	0	7	1	5708.3874	-0.0024
8	1	8	0	←	7	0	7	0	5708.4652	-0.0015
7	2	5	1	←	6	2	4	0	5713.4699	-0.0008
7	2	5	3	←	6	2	4	2	5713.5717	0.0072
6	2	5	1	←	5	1	4	1	5777.4773	0.0048
6	2	5	0	←	5	1	4	0	5777.7822	0.0019
8	2	7	2	←	7	2	6	3	6039.0556	0.0154
8	2	7	0	←	7	2	6	1	6039.1594	0.0137
8	2	7	1	←	7	2	6	0	6048.3512	0.0121
4	3	2	0	←	3	2	1	0	6165.3987	-0.0012
4	3	2	1	←	3	2	1	1	6167.4236	0.0081
8	3	6	0	←	7	3	5	1	6224.2046	0.0105
4	3	1	1	←	3	2	2	1	6226.0963	0.0063

J'	$K_{a'}$	$K_{c'}$	v'		J	K_a	K_c	v	Observed (MHz)	OMC (MHz)
8	3	6	1	←	7	3	5	0	6232.6065	0.0123
8	1	7	2	←	7	1	6	3	6247.5629	-0.0107
8	1	7	0	←	7	1	6	1	6247.6677	0.0035
8	4	5	1	←	7	4	4	0	6251.0236	-0.0105
8	1	7	1	←	7	1	6	0	6257.3377	0.0041
8	1	7	3	←	7	1	6	2	6257.4327	-0.0068
7	2	6	1	←	6	1	5	1	6287.0864	0.0156
7	2	6	0	←	6	1	5	0	6287.3826	0.0063
9	1	9	0	←	8	1	8	1	6321.2086	-0.0090
9	1	9	1	←	8	1	8	0	6330.7899	-0.0177
9	1	9	3	←	8	1	8	2	6330.8651	0.0003
9	0	9	3	←	8	0	8	2	6346.9925	-0.0201
9	1	9	1	←	8	0	8	1	6361.2741	-0.0106
9	1	9	0	←	8	0	8	0	6361.3528	-0.0024
8	3	5	2	←	7	3	4	3	6388.6087	-0.0030
8	3	5	0	←	7	3	4	1	6388.6978	-0.0187
8	3	5	1	←	7	3	4	0	6397.2442	-0.0199
8	3	5	3	←	7	3	4	2	6397.3386	-0.0007
8	2	6	0	←	7	2	5	1	6525.5444	0.0003
8	2	6	2	←	7	2	5	3	6525.4628	0.0160
8	2	6	1	←	7	2	5	0	6535.0077	-0.0044
8	2	6	3	←	7	2	5	2	6535.1101	0.0065
5	2	3	1	←	4	1	4	1	6546.9279	0.0095
9	2	8	0	←	8	2	7	1	6754.2387	0.0083
8	2	7	0	←	7	1	6	0	6785.2210	0.0044
5	3	3	1	←	4	2	2	1	6872.2860	0.0020
5	3	3	0	←	4	2	2	0	6872.8085	0.0043
9	1	8	2	←	8	1	7	3	6926.8998	-0.0053
9	1	8	0	←	8	1	7	1	6927.0068	0.0095
9	1	8	3	←	8	1	7	2	6936.6078	0.0049
9	3	7	2	←	8	3	6	3	6991.9526	0.0010
9	3	7	0	←	8	3	6	1	6992.0405	-0.0091
10	1	10	0	←	9	1	9	1	6999.7238	-0.0078
9	3	7	1	←	8	3	6	0	7000.4235	0.0064
9	3	7	3	←	8	3	6	2	7000.5053	0.0064
10	1	10	3	←	9	1	9	2	7009.2585	0.0003
10	1	10	1	←	9	0	9	1	7023.6290	0.0070
9	4	6	0	←	8	4	5	1	7036.3780	-0.0077
9	4	6	1	←	8	4	5	0	7043.5233	-0.0059
5	3	2	1	←	4	2	3	1	7053.9064	-0.0020
5	3	2	0	←	4	2	3	0	7054.3852	-0.0074
9	3	6	2	←	8	3	5	3	7253.1710	0.0055
9	3	6	3	←	8	3	5	2	7261.9628	-0.0019
9	2	8	0	←	8	1	7	0	7291.5017	0.0122
9	2	7	2	←	8	2	6	3	7323.2752	0.0016
9	2	7	0	←	8	2	6	1	7323.3707	0.0011
9	2	7	1	←	8	2	6	0	7332.7992	-0.0020
9	2	7	3	←	8	2	6	2	7332.8848	-0.0047
10	2	9	2	←	9	2	8	3	7459.2091	0.0155
10	2	9	0	←	9	2	8	1	7459.3210	0.0072
10	2	9	1	←	9	2	8	0	7468.3254	0.0109
6	3	4	1	←	5	2	3	1	7521.3843	0.0057
6	3	4	0	←	5	2	3	0	7521.8950	0.0066
10	1	9	2	←	9	1	8	3	7588.9633	-0.0061
10	1	9	0	←	9	1	8	1	7589.0722	0.0040
10	1	9	1	←	9	1	8	0	7598.3907	0.0117
10	1	9	3	←	9	1	8	2	7598.4768	0.0099
11	0	11	2	←	10	0	10	3	7681.5226	-0.0084
10	3	8	2	←	9	3	7	3	7750.0123	0.0192
10	3	8	0	←	9	3	7	1	7750.1051	0.0072
10	3	8	1	←	9	3	7	0	7758.4299	0.0136
10	4	7	0	←	9	4	6	1	7828.6631	-0.0090
10	4	7	1	←	9	4	6	0	7835.8350	-0.0185
10	4	6	2	←	9	4	5	3	7900.6696	-0.0157
									RMS	8.0 kHz

S16.3 Isotopologues of DPE-2w

Table S29 Linelist for ^{13}C1' isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	1	2	←	2	1	1	2252.1228	0.0052
4	1	4	←	3	1	3	2773.2940	-0.0004
4	0	4	←	3	0	3	2846.2652	0.0016
9	0	9	←	8	2	6	2916.2222	0.0075
4	2	2	←	3	2	1	2939.7189	-0.0003
4	1	3	←	3	1	2	2996.1389	-0.0084
4	1	4	←	3	0	3	3088.6044	-0.0027
5	1	5	←	4	1	4	3458.8579	0.0013
3	2	2	←	2	1	1	3471.6660	-0.0016
3	2	1	←	2	1	1	3496.9542	0.0173
5	2	4	←	4	2	3	3607.3896	0.0055
5	3	3	←	4	3	2	3633.4177	-0.0001
3	2	2	←	2	1	2	3640.1136	-0.0030
3	2	1	←	2	1	2	3665.3794	-0.0063
5	2	3	←	4	2	2	3698.7503	-0.0067
5	1	5	←	4	0	4	3701.2101	0.0099
6	0	6	←	5	1	5	4023.1020	0.0004
4	2	3	←	3	1	2	4110.5643	0.0092
10	1	10	←	9	2	8	4132.8062	-0.0069
6	1	6	←	5	1	5	4140.5616	-0.0009
4	2	2	←	3	1	2	4184.5294	-0.0092
6	0	6	←	5	0	5	4197.0523	0.0016
9	0	9	←	8	1	7	4239.5183	0.0128
6	1	6	←	5	0	5	4314.5115	-0.0002
6	2	5	←	5	2	4	4319.6208	0.0090
6	4	2	←	5	4	1	4360.1621	0.0147
6	3	4	←	5	3	3	4363.0868	-0.0180
4	2	3	←	3	1	3	4447.1518	-0.0080
6	1	5	←	5	1	4	4461.7082	-0.0041
3	3	1	←	2	2	0	4476.9042	-0.0081
3	3	0	←	2	2	0	4477.2013	-0.0030
5	1	4	←	4	0	4	4535.3728	0.0019
5	2	4	←	4	1	3	4721.7867	-0.0051
7	0	7	←	6	1	6	4743.2427	-0.0088
5	2	3	←	4	1	3	4887.1460	-0.0023
7	1	7	←	6	0	6	4936.1589	0.0106
7	2	6	←	6	2	5	5027.0287	0.0009
7	3	5	←	6	3	4	5092.5271	0.0036
7	4	3	←	6	4	2	5092.6182	0.0057
7	3	4	←	6	3	3	5126.6356	0.0081
4	3	2	←	3	2	1	5189.8995	0.0121
4	3	1	←	3	2	1	5191.9257	0.0040
7	2	5	←	6	2	4	5230.8979	0.0010
5	2	4	←	4	1	4	5281.2552	0.0056
8	0	8	←	7	1	7	5447.1614	-0.0028
6	1	5	←	5	0	5	5469.8410	0.0088
8	1	8	←	7	1	7	5493.7544	-0.0020
8	0	8	←	7	0	7	5522.5958	-0.0040
8	1	8	←	7	0	7	5569.1827	-0.0092
6	2	4	←	5	1	4	5618.1217	0.0014
7	2	6	←	6	1	5	5873.1460	-0.0033
8	1	7	←	7	1	6	5878.5213	0.0050
5	3	3	←	4	2	2	5883.5774	-0.0084
5	3	2	←	4	2	2	5891.6587	0.0107
5	3	3	←	4	2	3	5957.5624	-0.0070
8	2	6	←	7	2	5	5992.0979	0.0174
9	1	8	←	8	2	7	6017.2719	-0.0094
9	0	9	←	8	1	8	6138.4770	0.0004
9	1	9	←	8	1	8	6166.4014	-0.0084
9	0	9	←	8	0	8	6185.0787	0.0100
9	1	9	←	8	0	8	6212.9945	-0.0075
7	2	5	←	6	1	5	6387.3219	0.0173

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
8	2	7	←	7	1	6	6424.7248	0.0103
7	1	6	←	6	0	6	6450.3742	0.0147
6	3	3	←	5	2	3	6571.7335	0.0082
10	0	10	←	9	1	9	6820.9171	0.0072
10	1	9	←	9	2	8	6825.8181	-0.0026
10	1	10	←	9	1	9	6837.2612	-0.0165
5	4	2	←	4	3	1	6850.2756	-0.0070
7	3	5	←	6	2	4	7175.9121	-0.0037
8	2	6	←	7	1	6	7201.7967	-0.0103
7	3	4	←	6	2	4	7233.8188	0.0074
7	3	5	←	6	2	5	7486.2073	0.0053
11	0	11	←	10	1	10	7497.4633	-0.0177
11	0	11	←	10	0	10	7513.8397	-0.0091
11	1	11	←	10	0	10	7523.2752	0.0062
10	2	9	←	9	1	8	7525.1669	-0.0010
7	3	4	←	6	2	5	7544.0899	-0.0076
6	4	3	←	5	3	2	7570.4838	-0.0077
8	3	6	←	7	2	5	7765.5313	-0.0036
13	2	11	←	12	3	9	7785.0528	-0.0026
8	3	5	←	7	2	5	7887.7060	-0.0025
							RMS	8.1 kHz

Table S30 Linelist for ^{13}C2' isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	0	3	←	2	0	2	2149.2755	0.0101
3	1	3	←	2	0	2	2464.6611	-0.0077
7	1	7	←	6	2	4	2508.4784	0.0091
8	3	6	←	7	4	3	2601.5988	0.0001
7	2	6	←	6	3	4	2631.3802	-0.0160
4	0	4	←	3	0	3	2843.9563	-0.0064
4	2	2	←	3	2	1	2936.8512	-0.0067
4	1	3	←	3	1	2	2993.2243	-0.0047
4	1	4	←	3	0	3	3086.5609	0.0031
5	1	5	←	4	1	4	3456.2113	-0.0142
3	2	2	←	2	1	1	3468.9232	0.0038
5	2	4	←	4	2	3	3604.2252	0.0123
5	3	3	←	4	3	2	3630.0873	-0.0038
3	2	2	←	2	1	2	3636.7738	0.0009
3	2	1	←	2	1	2	3661.8872	0.0017
5	2	3	←	4	2	2	3695.0736	0.0097
5	1	5	←	4	0	4	3698.8247	0.0040
7	1	6	←	6	2	4	4017.6234	-0.0024
6	0	6	←	5	1	5	4019.6544	0.0040
3	2	1	←	2	0	2	4044.2040	-0.0173
4	2	3	←	3	1	2	4107.4739	0.0144
6	1	6	←	5	1	5	4137.4587	-0.0002
6	0	6	←	5	0	5	4193.9403	0.0017
6	1	6	←	5	0	5	4311.7435	-0.0036
6	4	2	←	5	4	1	4356.1471	0.0027
10	2	9	←	9	3	7	4444.1269	-0.0107
3	3	1	←	2	2	1	4478.2251	0.0026
8	1	7	←	7	2	5	4665.4877	0.0111
9	2	7	←	8	3	5	4842.0139	-0.0122
5	2	3	←	4	1	3	4882.8294	0.0007
7	1	7	←	6	0	6	4932.9342	0.0003
7	2	6	←	6	2	5	5022.7392	0.0083
7	3	5	←	6	3	4	5087.8562	-0.0008
12	0	12	←	11	1	10	5091.6684	-0.0141
7	3	4	←	6	3	3	5121.6699	0.0007
7	1	6	←	6	1	5	5172.9149	-0.0042
4	3	2	←	3	2	1	5185.5322	-0.0077
4	3	1	←	3	2	1	5187.5574	0.0014
4	3	2	←	3	2	2	5210.6412	-0.0113
4	3	1	←	3	2	2	5212.6615	-0.0071

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
7	2	5	←	6	2	4	5225.6008	0.0041
13	1	13	←	12	2	11	5258.3770	0.0080
5	2	4	←	4	1	4	5275.9421	0.0074
6	2	5	←	5	1	4	5304.3126	0.0056
11	3	8	←	10	4	7	5338.3910	-0.0013
8	0	8	←	7	1	7	5442.9059	-0.0118
8	1	8	←	7	1	7	5489.7588	0.0131
8	0	8	←	7	0	7	5518.6508	-0.0047
8	1	8	←	7	0	7	5565.4827	-0.0008
6	2	4	←	5	1	4	5612.8468	-0.0024
8	3	6	←	7	3	5	5815.2124	0.0095
7	2	6	←	6	1	5	5869.4891	0.0072
8	1	7	←	7	1	6	5873.4578	0.0104
5	3	3	←	4	2	2	5878.7860	0.0128
8	3	5	←	7	3	4	5878.9649	0.0116
5	3	2	←	4	2	3	5960.2947	-0.0028
8	2	6	←	7	2	5	5986.0793	0.0070
9	0	9	←	8	1	8	6133.8494	-0.0019
9	1	9	←	8	1	8	6161.9494	-0.0057
9	0	9	←	8	0	8	6180.6875	0.0082
9	1	9	←	8	0	8	6208.7717	-0.0112
7	2	5	←	6	1	5	6380.8809	-0.0090
9	2	8	←	8	2	7	6420.4142	0.0150
7	1	6	←	6	0	6	6442.0875	-0.0029
6	3	4	←	5	2	3	6542.8134	0.0006
6	3	3	←	5	2	3	6566.3931	-0.0014
6	3	4	←	5	2	4	6707.2000	0.0020
6	3	3	←	5	2	4	6730.7783	-0.0014
10	0	10	←	9	1	9	6815.8980	0.0021
10	1	9	←	9	2	8	6818.7700	0.0001
10	0	10	←	9	0	9	6844.0046	0.0048
5	4	2	←	4	3	1	6844.4563	-0.0135
10	1	10	←	9	0	9	6860.4761	-0.0081
7	2	6	←	6	1	6	7020.8454	0.0008
7	3	5	←	6	2	4	7170.6421	-0.0071
7	3	4	←	6	2	4	7228.0563	0.0131
7	3	5	←	6	2	5	7479.1968	0.0052
11	0	11	←	10	1	10	7492.0600	-0.0043
10	2	9	←	9	1	8	7520.7435	0.0043
7	3	4	←	6	2	5	7536.5806	-0.0048
6	4	3	←	5	3	2	7564.0554	-0.0063
6	4	3	←	5	3	3	7572.0490	-0.0028
11	1	10	←	10	1	9	7889.2640	-0.0037
							RMS	7.7 kHz

Table S31 Linelist for ^{13}C3' isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	2	1	←	2	2	0	2178.9331	0.0121
6	2	4	←	5	3	2	2241.0342	-0.0056
9	4	5	←	8	5	4	2413.6018	0.0084
3	1	3	←	2	0	2	2457.5968	0.0078
13	1	12	←	12	4	9	2480.2113	0.0147
4	1	4	←	3	1	3	2759.9409	-0.0173
8	1	8	←	7	2	5	2775.3214	-0.0107
4	0	4	←	3	0	3	2832.2466	0.0082
4	2	3	←	3	2	2	2875.4491	-0.0058
4	1	3	←	3	1	2	2978.8304	-0.0058
6	0	6	←	5	1	4	3181.4143	0.0005
5	0	5	←	4	1	4	3265.3125	-0.0044
8	1	8	←	7	2	6	3274.0976	0.0052
6	1	5	←	5	2	3	3282.3463	0.0073
5	1	5	←	4	1	4	3442.4220	-0.0129
5	0	5	←	4	0	4	3510.5952	-0.0023
5	2	4	←	4	2	3	3588.1617	-0.0119

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	2	2	←	2	1	2	3626.7673	-0.0085
3	2	1	←	2	1	2	3651.1398	-0.0106
5	2	3	←	4	2	2	3676.5872	-0.0048
5	1	4	←	4	1	3	3712.3724	-0.0088
6	0	6	←	5	1	5	4000.7568	-0.0005
4	2	3	←	3	1	2	4097.8855	-0.0012
6	1	6	←	5	1	5	4121.1511	-0.0057
6	0	6	←	5	0	5	4177.8898	0.0145
6	1	6	←	5	0	5	4298.2830	0.0081
6	3	4	←	5	3	3	4338.9398	-0.0032
6	3	3	←	5	3	2	4353.8448	-0.0114
4	2	3	←	3	1	3	4428.4100	0.0040
6	1	5	←	5	1	4	4437.0198	-0.0027
6	2	4	←	5	2	3	4437.4857	-0.0005
4	2	2	←	3	1	3	4499.8190	-0.0093
11	1	11	←	10	2	9	4517.2337	-0.0165
7	0	7	←	6	1	6	4718.5129	-0.0017
7	1	7	←	6	1	6	4796.3787	0.0050
9	2	7	←	8	3	5	4800.9969	0.0139
7	0	7	←	6	0	6	4838.9200	0.0058
7	3	5	←	6	3	4	5064.3556	-0.0011
7	3	4	←	6	3	3	5096.7339	-0.0023
7	1	6	←	6	1	5	5149.8708	-0.0031
4	3	2	←	3	2	2	5198.9568	-0.0001
7	2	5	←	6	2	4	5199.2621	-0.0046
4	3	1	←	3	2	2	5200.8841	0.0009
9	1	8	←	8	2	6	5218.6917	-0.0096
6	2	5	←	5	1	4	5291.7470	0.0184
8	0	8	←	7	1	7	5420.1471	-0.0111
6	1	5	←	5	0	5	5433.4996	0.0154
8	1	8	←	7	1	7	5468.5768	-0.0051
8	0	8	←	7	0	7	5498.0231	0.0057
8	1	8	←	7	0	7	5546.4395	-0.0014
13	4	9	←	12	5	8	5613.3997	-0.0035
8	2	7	←	7	2	6	5699.8843	0.0064
8	3	6	←	7	3	5	5788.4560	-0.0010
13	3	11	←	12	4	8	5847.5108	-0.0044
5	3	3	←	4	2	2	5865.4077	0.0056
5	3	2	←	4	2	2	5873.0568	0.0183
5	3	3	←	4	2	3	5936.8252	0.0007
9	1	9	←	8	1	8	6138.4011	0.0064
9	1	9	←	8	0	8	6186.8314	0.0131
7	2	5	←	6	1	5	6354.4033	-0.0107
9	2	8	←	8	2	7	6393.4110	-0.0037
6	3	4	←	5	2	3	6527.7658	0.0127
9	3	6	←	8	3	5	6612.9619	-0.0170
6	3	4	←	5	2	4	6687.5892	-0.0047
9	2	7	←	8	2	6	6704.5737	-0.0022
6	3	3	←	5	2	4	6710.1357	-0.0076
10	0	10	←	9	1	9	6789.1673	-0.0108
10	0	10	←	9	0	9	6818.4253	0.0157
5	4	1	←	4	3	1	6830.6644	-0.0004
8	2	6	←	7	1	6	7160.8623	0.0053
10	1	9	←	9	1	8	7200.0672	0.0072
7	3	4	←	6	2	4	7209.5575	0.0048
10	3	8	←	9	3	7	7227.9564	0.0118
7	3	5	←	6	2	5	7455.0484	-0.0167
11	1	11	←	10	0	10	7490.4422	-0.0019
7	3	4	←	6	2	5	7509.9899	-0.0041
6	4	3	←	5	3	2	7547.0233	0.0015
6	4	2	←	5	3	2	7547.5949	-0.0006
6	4	3	←	5	3	3	7554.6603	0.0021
11	1	10	←	10	2	9	7557.9682	-0.0002
5	5	0	←	4	4	1	7753.4615	0.0065
							RMS	8.7 kHz

Table S32 Linelist for ^{13}C4' isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	0	3	←	2	0	2	2131.4670	0.0111
5	1	4	←	4	2	2	2499.3388	-0.0004
8	1	8	←	7	2	5	2746.2332	0.0132
3	1	2	←	2	0	2	2782.2709	-0.0075
4	0	4	←	3	0	3	2820.9293	0.0047
4	3	2	←	3	3	1	2876.7255	0.0126
4	1	3	←	3	1	2	2967.3115	0.0104
7	2	5	←	6	3	4	3072.7123	-0.0007
5	0	5	←	4	1	4	3248.7112	-0.0038
5	1	5	←	4	1	4	3428.0734	0.0040
9	3	6	←	8	4	4	3457.4080	0.0016
3	2	2	←	2	1	1	3461.4004	0.0041
5	0	5	←	4	0	4	3496.5732	-0.0011
5	2	4	←	4	2	3	3573.7492	-0.0025
5	3	3	←	4	3	2	3598.7577	0.0048
5	3	2	←	4	3	1	3604.3799	-0.0106
3	2	2	←	2	1	2	3626.7673	-0.0026
3	2	1	←	2	1	2	3650.9839	-0.0052
5	2	3	←	4	2	2	3661.7055	0.0032
5	1	5	←	4	0	4	3675.9255	-0.0031
5	1	4	←	4	1	3	3698.0471	0.0000
9	2	8	←	8	3	6	3811.8463	-0.0037
6	0	6	←	5	1	5	3981.7592	0.0010
6	1	6	←	5	1	5	4103.9644	0.0033
6	2	5	←	5	2	4	4279.6412	0.0052
6	1	6	←	5	0	5	4283.3185	0.0031
10	3	7	←	9	4	5	4306.9469	-0.0050
6	3	3	←	5	3	2	4336.1846	-0.0047
13	5	9	←	12	6	6	4362.3661	-0.0102
13	5	8	←	12	6	6	4383.4258	-0.0035
6	2	4	←	5	2	3	4419.6275	0.0110
6	1	5	←	5	1	4	4419.9656	0.0029
5	1	4	←	4	0	4	4495.2331	-0.0131
4	2	2	←	3	1	3	4496.4886	0.0062
10	0	10	←	9	1	8	4496.8992	-0.0034
7	1	7	←	6	1	6	4776.3508	-0.0016
7	0	7	←	6	0	6	4819.3383	-0.0008
5	2	3	←	4	1	3	4860.4251	0.0150
7	1	7	←	6	0	6	4898.5515	-0.0037
7	2	6	←	6	2	5	4980.8975	0.0002
7	3	4	←	6	3	3	5075.9847	0.0092
7	1	6	←	6	1	5	5130.1874	0.0054
4	3	1	←	3	2	1	5179.4734	-0.0022
4	3	2	←	3	2	2	5201.7816	-0.0117
4	3	1	←	3	2	2	5203.6916	-0.0032
5	2	4	←	4	1	4	5250.8158	0.0030
6	2	5	←	5	1	4	5283.0546	-0.0071
8	0	8	←	7	1	7	5396.3396	-0.0062
8	1	8	←	7	1	7	5445.7253	-0.0076
8	0	8	←	7	0	7	5475.5640	0.0020
8	1	8	←	7	0	7	5524.9365	-0.0125
6	2	4	←	5	1	4	5581.9749	-0.0045
8	4	5	←	7	4	4	5768.1033	0.0176
7	2	6	←	6	1	5	5843.9915	-0.0048
5	3	3	←	4	2	2	5865.6735	-0.0004
8	2	6	←	7	2	5	5932.8390	0.0042
5	3	2	←	4	2	3	5944.1947	-0.0051
6	2	5	←	5	1	5	6102.3817	0.0024
9	0	9	←	8	0	8	6132.2046	-0.0082
9	1	9	←	8	0	8	6162.0900	-0.0075
14	2	13	←	13	3	11	6318.0373	0.0083
7	2	5	←	6	1	5	6340.5549	0.0085
9	1	8	←	8	1	7	6506.5269	0.0137
6	3	3	←	5	2	3	6547.7109	0.0105

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
9	2	7	←	8	2	6	6678.4793	0.0177
6	3	4	←	5	2	4	6684.3680	-0.0020
6	3	3	←	5	2	4	6706.6366	-0.0008
10	0	10	←	9	0	9	6790.0944	-0.0111
10	1	10	←	9	0	9	6807.7589	-0.0193
7	3	5	←	6	2	4	7149.8088	0.0102
10	3	8	←	9	3	7	7199.1086	0.0055
7	3	4	←	6	2	4	7204.0588	-0.0005
10	4	6	←	9	4	5	7243.3352	0.0087
7	3	4	←	6	2	5	7502.9863	0.0092
6	4	3	←	5	3	3	7557.5071	-0.0117
6	4	2	←	5	3	3	7558.0764	-0.0053
8	3	6	←	7	2	5	7736.4865	-0.0021
8	3	5	←	7	2	5	7851.2279	-0.0064
8	2	7	←	7	1	7	7880.0132	-0.0021
11	4	8	←	10	4	7	7951.9484	-0.0059
							RMS	7.6 kHz

Table S33 Linelist for ^{13}C5' isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
4	0	4	←	3	1	3	2506.2897	-0.0014
4	1	4	←	3	1	3	2751.7401	-0.0066
4	2	3	←	3	2	2	2867.9271	0.0035
4	1	3	←	3	1	2	2971.8755	-0.0021
5	0	5	←	4	1	4	3255.0405	-0.0005
9	3	7	←	8	4	4	3261.2555	-0.0030
5	1	5	←	4	1	4	3432.1103	0.0011
3	2	1	←	2	1	1	3483.6296	0.0045
5	0	5	←	4	0	4	3500.4849	-0.0117
5	2	4	←	4	2	3	3578.7001	-0.0053
5	3	2	←	4	3	1	3609.8431	-0.0027
5	1	5	←	4	0	4	3677.5636	-0.0011
5	1	4	←	4	1	3	3703.5713	-0.0074
6	0	6	←	5	1	5	3988.4484	-0.0085
6	1	6	←	5	1	5	4108.6923	0.0025
7	1	6	←	6	2	5	4281.4980	-0.0073
6	2	5	←	5	2	4	4285.4406	-0.0051
6	1	6	←	5	0	5	4285.7581	0.0003
6	5	2	←	5	5	1	4320.1083	0.0084
6	5	1	←	5	5	0	4320.1083	0.0030
6	3	4	←	5	3	3	4327.8702	0.0160
6	1	5	←	5	1	4	4426.2924	0.0021
6	2	4	←	5	2	3	4427.1490	0.0053
4	2	2	←	3	1	3	4497.6403	-0.0123
5	2	4	←	4	1	3	4700.0247	0.0071
7	0	7	←	6	1	6	4704.0754	-0.0056
5	2	3	←	4	1	3	4861.2097	0.0081
7	1	7	←	6	0	6	4901.9760	0.0000
7	2	6	←	6	2	5	4987.5027	0.0055
7	1	6	←	6	1	5	5137.1006	0.0010
4	3	2	←	3	2	2	5197.8303	0.0009
4	3	1	←	3	2	2	5199.7870	0.0085
8	0	8	←	7	1	7	5403.5284	0.0020
8	1	8	←	7	1	7	5451.7562	-0.0156
8	0	8	←	7	0	7	5481.1876	-0.0008
8	1	8	←	7	0	7	5529.4341	0.0002
8	4	5	←	7	4	4	5776.7548	-0.0007
8	4	4	←	7	4	3	5780.9053	-0.0052
8	3	5	←	7	3	4	5835.5102	0.0115
7	2	6	←	6	1	5	5843.0928	0.0013
5	3	3	←	4	2	2	5861.9357	-0.0002
5	3	3	←	4	2	3	5933.9700	-0.0041
5	3	2	←	4	2	3	5941.6949	-0.0057
8	2	6	←	7	2	5	5942.5884	0.0014

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
9	1	8	←	8	2	7	5957.0379	0.0136
9	0	9	←	8	0	8	6138.5487	-0.0012
9	1	9	←	8	0	8	6167.6417	0.0010
9	6	3	←	8	6	2	6486.1794	-0.0080
9	1	8	←	8	1	7	6514.0080	0.0035
6	3	4	←	5	2	3	6521.9400	0.0013
9	3	6	←	8	3	5	6597.3608	0.0020
6	3	4	←	5	2	4	6683.1183	-0.0044
6	3	3	←	5	2	4	6705.9234	-0.0131
10	1	9	←	9	2	8	6761.6914	-0.0078
10	0	10	←	9	1	9	6768.0840	-0.0024
5	4	2	←	4	3	1	6829.9503	-0.0041
7	3	4	←	6	2	4	7201.7969	0.0158
10	4	7	←	9	4	6	7234.5523	0.0153
7	3	5	←	6	2	5	7449.0915	-0.0081
7	3	4	←	6	2	5	7504.6592	-0.0037
11	1	10	←	10	2	9	7536.9499	0.0058
6	4	2	←	5	3	2	7545.0899	-0.0054
6	4	3	←	5	3	3	7552.2415	0.0018
6	4	2	←	5	3	3	7552.8340	0.0120
8	3	5	←	7	2	5	7850.0029	-0.0034
							RMS	6.9 kHz

Table S34 Linelist for ^{13}C6' isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
6	1	6	←	5	2	4	2314.7798	-0.0091
3	1	3	←	2	0	2	2459.8650	-0.0081
8	3	6	←	7	4	4	2597.4437	0.0135
3	1	2	←	2	0	2	2793.3706	-0.0190
4	0	4	←	3	0	3	2838.0095	-0.0120
2	2	1	←	1	1	1	2851.5503	0.0131
4	2	3	←	3	2	2	2882.0985	-0.0003
4	2	2	←	3	2	1	2930.0913	0.0032
5	0	5	←	4	1	4	3274.6708	0.0093
5	1	5	←	4	1	4	3449.2176	-0.0038
5	2	4	←	4	2	3	3596.3525	0.0027
5	3	2	←	4	3	1	3627.8990	0.0032
3	2	2	←	2	1	2	3628.6830	0.0098
3	2	1	←	2	1	2	3653.5403	-0.0149
5	2	3	←	4	2	2	3686.4296	0.0057
5	1	5	←	4	0	4	3691.9066	0.0032
5	1	4	←	4	1	3	3721.4808	-0.0045
8	0	8	←	7	1	6	3930.7566	-0.0043
6	0	6	←	5	1	5	4010.9819	-0.0034
10	3	8	←	9	4	6	4024.3501	0.0175
8	2	6	←	7	3	5	4028.9074	-0.0020
6	1	6	←	5	1	5	4129.1329	-0.0015
6	0	6	←	5	0	5	4185.5450	-0.0002
6	1	6	←	5	0	5	4303.6929	-0.0015
6	2	5	←	5	2	4	4306.5131	0.0013
6	3	4	←	5	3	3	4349.3775	0.0015
6	3	3	←	5	3	2	4364.7648	-0.0067
11	3	9	←	10	4	7	4712.9635	-0.0145
7	0	7	←	6	1	6	4729.4355	-0.0058
11	0	11	←	10	1	9	4805.1971	0.0053
7	1	7	←	6	1	6	4805.5067	0.0037
7	0	7	←	6	0	6	4847.5966	0.0061
5	2	3	←	4	1	3	4872.1796	0.0114
7	2	6	←	6	2	5	5011.9269	-0.0059
7	4	3	←	6	4	2	5076.5123	0.0142
7	3	5	←	6	3	4	5076.5123	0.0039
7	3	4	←	6	3	3	5109.8982	-0.0066
7	1	6	←	6	1	5	5161.5041	0.0119
8	1	7	←	7	2	6	5163.5935	-0.0024

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
4	3	2	←	3	2	1	5174.5577	0.0114
4	3	1	←	3	2	1	5176.5429	0.0064
4	3	2	←	3	2	2	5199.4353	0.0068
7	2	5	←	6	2	4	5213.2755	-0.0003
6	2	5	←	5	1	4	5294.2637	0.0146
12	3	10	←	11	4	7	5300.2235	0.0020
11	3	8	←	10	4	7	5321.7247	0.0014
13	4	10	←	12	5	8	5398.7499	0.0086
5	2	3	←	4	1	4	5426.4999	-0.0125
6	1	5	←	5	0	5	5448.6857	-0.0064
8	1	8	←	7	1	7	5478.8364	-0.0044
8	1	8	←	7	0	7	5554.8973	-0.0052
6	2	4	←	5	1	4	5600.1987	0.0068
8	3	6	←	7	3	5	5802.2686	0.0100
7	2	6	←	6	1	5	5858.6691	0.0112
5	3	3	←	4	2	2	5866.4633	0.0072
5	3	2	←	4	2	2	5874.3486	0.0043
3	3	1	←	2	1	2	5932.8390	0.0066
5	3	3	←	4	2	3	5939.3335	0.0061
8	2	6	←	7	2	5	5972.0352	-0.0057
9	1	8	←	8	2	7	5995.7298	0.0137
6	2	5	←	5	1	5	6120.8580	0.0007
9	0	9	←	8	1	8	6121.4621	-0.0131
9	0	9	←	8	0	8	6168.5584	-0.0099
7	2	5	←	6	1	5	6365.9460	0.0023
9	2	8	←	8	2	7	6406.8379	-0.0027
8	2	7	←	7	1	6	6409.2812	-0.0119
6	3	3	←	5	2	3	6552.6981	0.0061
6	3	4	←	5	2	4	6692.3544	0.0008
6	3	3	←	5	2	4	6715.6356	-0.0017
9	2	7	←	8	2	6	6721.7395	0.0118
9	2	8	←	8	1	7	6955.3673	-0.0048
7	3	5	←	6	2	4	7156.3952	-0.0122
8	2	6	←	7	1	6	7176.4742	-0.0184
7	3	4	←	6	2	4	7213.0885	0.0007
10	1	9	←	9	1	8	7213.6187	0.0011
10	3	8	←	9	3	7	7244.7397	-0.0010
10	2	8	←	9	2	7	7459.4570	0.0056
7	3	5	←	6	2	5	7462.3527	0.0025
11	1	11	←	10	1	10	7486.8376	-0.0070
10	2	9	←	9	1	8	7507.2090	-0.0105
7	3	4	←	6	2	5	7519.0221	-0.0083
6	4	3	←	5	3	2	7547.9081	0.0006
6	4	2	←	5	3	2	7548.5125	0.0050
6	4	3	←	5	3	3	7555.7937	-0.0020
6	4	2	←	5	3	3	7556.3987	0.0031
8	3	6	←	7	2	5	7745.3996	0.0094
8	3	5	←	7	2	5	7865.0584	-0.0074
8	2	7	←	7	1	7	7910.2672	-0.0129
							RMS	8.2 kHz

Table S35 Linelist for ^{13}C1" isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	1	3	←	2	1	2	2084.7785	-0.0010
3	1	2	←	2	1	1	2253.0106	-0.0131
3	1	3	←	2	0	2	2466.9326	-0.0038
4	0	4	←	3	1	3	2532.3159	-0.0166
3	1	2	←	2	0	2	2803.7175	-0.0012
2	2	0	←	1	1	0	2809.0419	0.0194
4	0	4	←	3	0	3	2847.3460	-0.0012
4	2	2	←	3	2	1	2940.9311	-0.0104
4	1	3	←	3	1	2	2997.3422	-0.0021
4	1	4	←	3	0	3	3089.3769	-0.0148
5	0	5	←	4	1	4	3286.5199	-0.0059

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
2	2	0	←	1	0	1	3298.4355	0.0136
5	1	5	←	4	1	4	3460.2023	0.0028
3	2	2	←	2	1	1	3471.7667	0.0073
3	2	1	←	2	1	1	3497.0670	-0.0008
5	0	5	←	4	0	4	3528.5710	0.0005
7	0	7	←	6	1	5	3589.4112	0.0105
5	2	4	←	4	2	3	3608.8176	0.0061
3	2	2	←	2	1	2	3640.2898	-0.0075
4	1	3	←	3	0	3	3649.1300	-0.0111
3	2	1	←	2	1	2	3665.6065	0.0005
5	2	3	←	4	2	2	3700.3125	0.0027
5	1	5	←	4	0	4	3702.2500	0.0060
9	2	8	←	8	3	6	3878.5114	-0.0061
8	0	8	←	7	1	6	3934.4852	-0.0168
6	0	6	←	5	1	5	4024.9325	0.0001
4	2	3	←	3	1	2	4110.8838	-0.0065
6	1	6	←	5	1	5	4142.1722	0.0104
6	1	6	←	5	0	5	4315.8328	-0.0024
6	2	5	←	5	2	4	4321.3189	0.0087
4	2	3	←	3	1	3	4447.6589	-0.0136
10	2	9	←	9	3	7	4449.5281	-0.0055
6	2	4	←	5	2	3	4466.4232	0.0061
3	3	0	←	2	2	1	4481.9619	-0.0056
5	1	4	←	4	0	4	4536.8306	-0.0085
8	1	7	←	7	2	5	4671.3164	0.0035
7	0	7	←	6	1	6	4745.2731	-0.0104
7	1	7	←	6	1	6	4820.5414	0.0013
9	2	7	←	8	3	5	4852.5564	0.0136
5	2	3	←	4	1	3	4887.9642	0.0130
7	2	6	←	6	2	5	5028.9798	-0.0104
7	3	5	←	6	3	4	5094.5750	0.0008
7	4	3	←	6	4	2	5094.6780	-0.0017
7	3	4	←	6	3	3	5128.7615	-0.0010
7	1	6	←	6	1	5	5179.5667	0.0123
4	3	2	←	3	2	1	5189.8048	0.0002
4	3	1	←	3	2	1	5191.8542	0.0099
4	3	2	←	3	2	2	5215.1172	0.0040
4	3	1	←	3	2	2	5217.1693	0.0164
7	2	5	←	6	2	4	5233.0810	0.0046
9	1	8	←	8	2	6	5242.6529	0.0088
5	2	4	←	4	1	4	5282.1127	0.0058
8	0	8	←	7	1	7	5449.3949	-0.0043
8	0	8	←	7	0	7	5524.6607	0.0050
8	1	8	←	7	0	7	5571.1214	0.0030
6	2	4	←	5	1	4	5619.3191	-0.0039
8	2	7	←	7	2	6	5731.3627	0.0000
8	4	5	←	7	4	4	5826.3655	-0.0147
8	4	4	←	7	4	3	5830.7900	-0.0049
7	2	6	←	6	1	5	5874.1699	0.0067
5	3	3	←	4	2	2	5883.7465	-0.0001
5	3	2	←	4	2	3	5965.9173	-0.0076
9	0	9	←	8	1	8	6140.9250	0.0014
6	2	5	←	5	1	5	6143.2092	-0.0083
9	1	9	←	8	1	8	6168.7759	0.0077
9	1	9	←	8	0	8	6215.2301	-0.0009
7	2	5	←	6	1	5	6388.9357	-0.0142
8	2	7	←	7	1	6	6425.9692	-0.0022
9	2	8	←	8	2	7	6428.1872	0.0120
9	1	8	←	8	1	7	6565.8766	0.0047
6	3	4	←	5	2	4	6713.8914	-0.0038
6	3	3	←	5	2	4	6737.7560	0.0077
10	0	10	←	9	1	9	6823.5804	0.0000
7	2	6	←	6	1	6	7030.0485	0.0023
8	2	6	←	7	1	6	7203.9355	-0.0007
10	2	8	←	9	2	7	7486.6706	0.0097
7	3	5	←	6	2	5	7487.1605	0.0012
11	1	11	←	10	0	10	7526.0709	-0.0065

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
7	3	4	←	6	2	5	7545.1951	-0.0055
6	4	2	←	5	3	3	7579.1970	-0.0164
8	3	5	←	7	2	5	7888.7038	0.0004
11	1	10	←	10	1	9	7898.1241	0.0061
							RMS	8.2 kHz

Table S36 Linelist for ^{13}C2" isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	1	2	←	2	1	1	2252.5927	0.0001
6	2	4	←	5	3	3	2297.0696	0.0006
3	1	3	←	2	0	2	2462.1085	0.0052
4	1	4	←	3	1	3	2771.7516	-0.0092
4	0	4	←	3	0	3	2844.8509	-0.0173
2	2	0	←	1	1	1	2857.7976	-0.0197
4	2	2	←	3	2	1	2940.4399	-0.0036
4	1	3	←	3	1	2	2996.6025	-0.0062
10	1	10	←	9	2	7	3010.3592	-0.0039
7	2	5	←	6	3	4	3166.8595	-0.0101
5	1	5	←	4	1	4	3456.7757	-0.0020
3	2	1	←	2	1	1	3488.7878	-0.0089
5	0	5	←	4	0	4	3524.9541	-0.0047
5	2	4	←	4	2	3	3606.7654	0.0132
5	4	1	←	4	4	0	3630.0871	0.0070
3	2	2	←	2	1	2	3632.9262	0.0031
3	2	1	←	2	1	2	3658.7936	0.0003
5	1	5	←	4	0	4	3695.3805	-0.0001
5	2	3	←	4	2	2	3700.0557	0.0030
5	1	4	←	4	1	3	3733.8279	-0.0076
6	0	6	←	5	1	5	4023.4192	-0.0042
4	2	2	←	3	1	2	4176.6508	0.0030
6	0	6	←	5	0	5	4193.8435	-0.0017
10	2	9	←	9	3	6	4210.4490	-0.0021
6	1	6	←	5	0	5	4308.3016	0.0026
6	2	5	←	5	2	4	4318.6315	-0.0029
6	4	2	←	5	4	1	4360.1622	0.0079
6	3	4	←	5	3	3	4363.0868	0.0152
6	2	4	←	5	2	3	4466.3182	0.0060
3	3	0	←	2	2	1	4469.2769	0.0157
4	2	2	←	3	1	3	4516.3286	-0.0073
5	1	4	←	4	0	4	4536.9643	-0.0101
5	2	4	←	4	1	3	4711.0946	-0.0046
7	0	7	←	6	1	6	4742.2583	-0.0048
7	1	7	←	6	1	6	4815.3510	-0.0026
7	0	7	←	6	0	6	4856.7255	0.0085
7	1	7	←	6	0	6	4929.8141	0.0067
7	3	5	←	6	3	4	5092.4516	0.0013
7	3	4	←	6	3	3	5127.8037	-0.0096
4	3	2	←	3	2	1	5176.3631	-0.0029
4	3	2	←	3	2	2	5202.2347	-0.0015
4	3	1	←	3	2	2	5204.3562	0.0058
7	2	5	←	6	2	4	5232.8775	0.0053
6	2	5	←	5	1	4	5295.8943	-0.0037
8	0	8	←	7	1	7	5444.8646	-0.0009
6	1	5	←	5	0	5	5473.5245	-0.0124
8	1	8	←	7	1	7	5489.7588	0.0041
8	0	8	←	7	0	7	5517.9459	-0.0100
8	1	8	←	7	0	7	5562.8380	-0.0069
6	2	4	←	5	1	4	5612.5741	0.0058
8	3	6	←	7	3	5	5820.3198	0.0045
7	2	6	←	6	1	5	5859.9860	0.0115
8	1	7	←	7	1	6	5876.3970	0.0112
5	3	3	←	4	2	3	5944.9883	0.0004
5	3	2	←	4	2	3	5953.3623	-0.0015
9	0	9	←	8	1	8	6134.9903	0.0144

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
6	2	5	←	5	1	5	6137.4989	0.0070
9	1	9	←	8	1	8	6161.7415	0.0038
9	0	9	←	8	0	8	6179.8680	0.0031
7	2	5	←	6	1	5	6383.9260	0.0069
6	2	4	←	5	1	5	6454.1608	-0.0013
6	3	3	←	5	2	3	6557.0278	0.0072
6	3	4	←	5	2	4	6701.3062	-0.0010
6	3	3	←	5	2	4	6726.0099	-0.0031
7	3	5	←	6	2	4	7158.4419	-0.0108
7	3	5	←	6	2	5	7475.1293	0.0062
7	3	4	←	6	2	5	7535.1857	-0.0062
6	4	3	←	5	3	2	7551.8377	0.0003
6	4	2	←	5	3	2	7552.4916	0.0034
6	4	3	←	5	3	3	7560.2143	0.0008
6	4	2	←	5	3	3	7560.8618	-0.0024
8	3	6	←	7	2	5	7745.8863	-0.0094
8	3	5	←	7	2	5	7872.4830	-0.0060
							RMS	7.3 kHz

Table S37 Linelist for ^{13}C3" isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	1	2	←	2	1	1	2244.8135	0.0050
6	1	6	←	5	2	4	2310.0136	-0.0099
3	1	3	←	2	0	2	2452.5935	-0.0102
4	0	4	←	3	1	3	2524.5518	-0.0004
4	1	4	←	3	1	3	2761.5987	0.0100
2	2	0	←	1	1	0	2790.1334	-0.0127
4	0	4	←	3	0	3	2834.5021	-0.0029
4	2	3	←	3	2	2	2880.3489	-0.0035
9	0	9	←	8	2	6	2880.6086	0.0106
4	3	2	←	3	3	1	2894.0759	0.0098
9	1	9	←	8	2	6	2907.0059	-0.0128
4	1	3	←	3	1	2	2986.2085	-0.0023
11	1	11	←	10	2	8	3006.2985	-0.0056
4	1	4	←	3	0	3	3071.5249	-0.0165
5	0	5	←	4	1	4	3274.9429	0.0052
6	1	5	←	5	2	3	3304.6756	-0.0030
5	1	5	←	4	1	4	3444.0494	0.0000
3	2	2	←	2	1	1	3449.4092	0.0117
5	0	5	←	4	0	4	3511.9682	-0.0058
5	4	1	←	4	4	0	3617.2740	-0.0103
3	2	2	←	2	1	2	3619.2260	-0.0064
5	3	3	←	4	3	2	3620.5833	0.0077
3	2	1	←	2	1	2	3645.1499	-0.0125
5	1	5	←	4	0	4	3681.0979	0.0121
5	2	3	←	4	2	2	3687.3602	0.0003
5	1	4	←	4	1	3	3720.7990	-0.0037
8	0	8	←	7	1	6	3900.3309	-0.0053
8	2	6	←	7	3	4	3997.5796	-0.0107
6	0	6	←	5	1	5	4009.1605	0.0024
7	1	6	←	6	2	4	4011.8015	-0.0167
3	2	1	←	2	0	2	4022.4898	0.0035
6	1	6	←	5	1	5	4122.5975	0.0069
6	0	6	←	5	0	5	4178.2710	0.0011
6	1	6	←	5	0	5	4291.7157	0.0134
6	2	5	←	5	2	4	4303.1910	0.0008
6	3	4	←	5	3	3	4347.7028	-0.0066
6	3	3	←	5	3	2	4364.1229	-0.0060
4	2	3	←	3	1	3	4424.2981	-0.0068
6	1	5	←	5	1	4	4445.8394	0.0173
3	3	1	←	2	2	0	4446.1606	-0.0062
3	3	1	←	2	2	1	4451.4053	-0.0061
3	3	0	←	2	2	1	4451.7080	-0.0086
10	0	10	←	9	1	8	4483.2946	0.0054

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
5	1	4	←	4	0	4	4521.8368	0.0119
5	2	4	←	4	1	3	4692.6430	0.0124
7	0	7	←	6	1	6	4725.1686	0.0032
11	3	9	←	10	4	7	4726.5056	-0.0166
7	1	7	←	6	1	6	4797.5135	0.0034
7	0	7	←	6	0	6	4838.6051	0.0072
7	1	7	←	6	0	6	4910.9473	0.0047
7	3	5	←	6	3	4	5074.5162	0.0033
7	3	4	←	6	3	3	5110.0504	-0.0098
7	1	6	←	6	1	5	5158.1982	0.0094
4	3	1	←	3	2	1	5158.3606	0.0191
4	3	2	←	3	2	2	5182.1328	-0.0125
7	2	5	←	6	2	4	5214.9754	-0.0001
8	0	8	←	7	1	7	5424.9814	-0.0040
5	2	3	←	4	1	4	5425.9247	-0.0070
8	1	8	←	7	1	7	5469.3615	0.0023
8	1	8	←	7	0	7	5541.6934	-0.0106
8	3	6	←	7	3	5	5799.7850	-0.0016
8	4	4	←	7	4	3	5808.4551	0.0111
7	2	6	←	6	1	5	5836.7567	0.0089
5	3	3	←	4	2	2	5846.5068	-0.0061
5	3	2	←	4	2	2	5854.9521	0.0155
8	2	6	←	7	2	5	5973.3415	0.0101
9	1	8	←	8	2	7	6006.2608	0.0058
9	1	9	←	8	1	8	6138.7986	0.0012
9	0	9	←	8	0	8	6156.7467	-0.0035
9	1	9	←	8	0	8	6183.1777	0.0065
7	2	5	←	6	1	5	6361.3527	0.0066
6	3	4	←	5	2	3	6506.8649	0.0024
9	7	3	←	8	7	2	6510.9902	-0.0051
9	7	2	←	8	7	1	6510.9902	-0.0052
9	3	7	←	8	3	6	6522.2542	0.0075
6	3	3	←	5	2	3	6531.7048	-0.0007
9	4	6	←	8	4	5	6535.7835	-0.0136
6	3	4	←	5	2	4	6676.1668	-0.0109
6	3	3	←	5	2	4	6701.0094	-0.0115
9	2	7	←	8	2	6	6722.0254	0.0141
10	0	10	←	9	1	9	6791.1103	0.0197
7	2	6	←	6	1	6	7000.7047	-0.0135
7	3	5	←	6	2	4	7130.3331	0.0070
7	3	4	←	6	2	4	7190.7188	0.0022
10	1	9	←	9	1	8	7202.7401	0.0050
10	2	9	←	9	1	8	7480.9746	-0.0076
7	3	4	←	6	2	5	7507.8873	-0.0037
6	4	2	←	5	3	2	7523.2752	-0.0043
6	4	3	←	5	3	3	7531.0424	-0.0040
8	3	5	←	7	2	5	7842.3624	-0.0069
11	1	10	←	10	1	9	7860.0208	0.0014
							RMS	8.9 kHz

Table S38 Linelist for ^{13}C4" isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	0	3	←	2	0	2	2134.4359	0.0012
5	0	5	←	4	1	3	2700.6402	-0.0076
4	1	4	←	3	1	3	2751.5678	0.0047
3	1	2	←	2	0	2	2785.1065	-0.0136
2	2	1	←	1	1	0	2793.1697	0.0098
2	2	1	←	1	1	1	2848.9542	-0.0129
4	2	3	←	3	2	2	2868.5120	-0.0150
4	1	3	←	3	1	2	2973.0743	-0.0038
7	2	5	←	6	3	3	3080.6469	0.0068
6	0	6	←	5	1	4	3160.5127	0.0054
5	0	5	←	4	1	4	3256.7078	-0.0105
5	1	5	←	4	1	4	3431.7785	0.0013

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	2	2	←	2	1	1	3455.4742	0.0091
3	2	1	←	2	1	1	3480.4298	0.0020
5	0	5	←	4	0	4	3500.1106	0.0063
5	3	3	←	4	3	2	3605.1077	0.0121
5	3	2	←	4	3	1	3611.0106	-0.0027
3	2	2	←	2	1	2	3622.8923	0.0057
3	2	1	←	2	1	2	3647.8436	-0.0057
5	2	3	←	4	2	2	3669.7174	-0.0112
5	1	5	←	4	0	4	3675.1748	0.0117
6	0	6	←	5	1	5	3989.6816	-0.0068
6	1	6	←	5	1	5	4108.1706	0.0009
6	0	6	←	5	0	5	4164.7497	0.0024
6	1	6	←	5	0	5	4283.2327	0.0042
6	2	5	←	5	2	4	4286.1114	0.0113
6	3	4	←	5	3	3	4329.0973	-0.0051
6	3	3	←	5	3	2	4344.5458	-0.0040
6	1	5	←	5	1	4	4427.5465	-0.0007
6	2	4	←	5	2	3	4429.5564	0.0013
4	2	2	←	3	1	3	4496.8992	-0.0043
5	2	4	←	4	1	3	4695.5442	0.0166
7	0	7	←	6	1	6	4704.7288	-0.0059
7	1	7	←	6	1	6	4781.0096	0.0031
4	2	2	←	3	0	3	4813.0145	-0.0191
7	0	7	←	6	0	6	4823.2131	-0.0028
12	1	12	←	11	2	10	4842.6826	-0.0106
5	2	3	←	4	1	3	4858.9881	-0.0104
7	1	7	←	6	0	6	4899.4894	0.0018
7	2	6	←	6	2	5	4988.0882	0.0089
7	4	3	←	6	4	2	5052.8515	-0.0027
7	3	5	←	6	3	4	5052.8515	-0.0110
7	1	6	←	6	1	5	5138.0959	-0.0007
4	3	2	←	3	2	1	5167.8255	0.0079
4	3	1	←	3	2	1	5169.8202	0.0057
4	3	2	←	3	2	2	5192.7854	0.0050
13	1	13	←	12	2	11	5198.9568	-0.0074
6	2	5	←	5	1	4	5276.7497	0.0098
8	0	8	←	7	0	7	5479.8601	0.0060
8	1	8	←	7	0	7	5527.0771	0.0021
6	2	4	←	5	1	4	5583.6624	-0.0034
8	2	7	←	7	2	6	5684.8009	-0.0144
8	4	4	←	7	4	3	5782.8609	0.0019
8	3	5	←	7	3	4	5838.4375	-0.0035
10	2	8	←	9	3	7	5844.7048	-0.0003
5	3	3	←	4	2	2	5856.2411	-0.0008
5	3	2	←	4	2	2	5864.1521	-0.0045
5	3	3	←	4	2	3	5929.3451	-0.0037
9	1	8	←	8	2	7	5963.7803	0.0017
9	0	9	←	8	1	8	6089.8065	-0.0072
9	0	9	←	8	0	8	6137.0347	0.0000
9	1	9	←	8	0	8	6165.4087	-0.0031
3	3	0	←	2	0	2	6317.1550	-0.0062
7	2	5	←	6	1	5	6346.1834	0.0019
7	1	6	←	6	0	6	6405.1210	-0.0154
9	3	7	←	8	3	6	6494.9809	-0.0060
9	5	5	←	8	5	4	6496.0504	-0.0060
9	1	8	←	8	1	7	6513.8711	0.0018
6	3	4	←	5	2	3	6515.6222	0.0064
6	3	3	←	5	2	3	6538.9888	0.0109
6	3	4	←	5	2	4	6679.0931	0.0063
9	2	7	←	8	2	6	6691.9323	0.0022
6	3	3	←	5	2	4	6702.4437	-0.0051
10	1	9	←	9	2	8	6767.4200	0.0141
10	1	10	←	9	0	9	6812.1862	0.0160
5	4	1	←	4	3	1	6822.6535	-0.0055
7	3	5	←	6	2	4	7138.9279	0.0046
10	1	9	←	9	1	8	7179.6854	0.0055
7	3	4	←	6	2	4	7195.7975	0.0037

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
10	2	8	←	9	2	7	7426.3213	0.0144
7	3	5	←	6	2	5	7445.8499	0.0006
6	4	3	←	5	3	2	7537.1795	-0.0002
6	4	2	←	5	3	2	7537.7761	-0.0056
6	4	3	←	5	3	3	7545.0899	-0.0046
6	4	2	←	5	3	3	7545.6993	0.0028
8	3	6	←	7	2	5	7724.0941	-0.0017
8	3	5	←	7	2	5	7844.1650	-0.0070
							RMS	7.6 kHz

Table S39 Linelist for ^{13}C5" isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	0	3	←	2	0	2	2135.8955	-0.0149
4	0	4	←	3	1	3	2507.1478	0.0108
4	1	4	←	3	1	3	2754.0701	0.0000
4	2	3	←	3	2	2	2870.0144	-0.0019
4	1	3	←	3	1	2	2973.8182	-0.0015
4	1	4	←	3	0	3	3073.6266	-0.0004
8	1	8	←	7	2	6	3251.1757	-0.0067
5	0	5	←	4	1	4	3256.6461	-0.0002
2	2	0	←	1	0	1	3298.4355	0.0149
3	2	2	←	2	1	1	3464.7879	0.0068
3	2	1	←	2	1	1	3489.2273	0.0148
7	0	7	←	6	1	5	3567.6921	0.0171
5	2	4	←	4	2	3	3581.3562	-0.0050
5	4	2	←	4	4	1	3603.2696	0.0039
5	3	3	←	4	3	2	3606.5540	-0.0178
5	3	2	←	4	3	1	3612.2837	-0.0021
3	2	1	←	2	1	2	3655.2577	-0.0075
5	2	3	←	4	2	2	3670.0034	-0.0070
5	1	5	←	4	0	4	3681.9923	0.0044
8	2	6	←	7	3	4	3923.8804	0.0049
4	2	3	←	3	1	2	4099.6149	0.0108
6	0	6	←	5	0	5	4169.3294	-0.0018
6	2	5	←	5	2	4	4288.6984	0.0085
6	1	6	←	5	0	5	4290.6853	0.0039
6	3	4	←	5	3	3	4330.8555	0.0007
6	1	5	←	5	1	4	4429.4378	0.0011
6	2	4	←	5	2	3	4429.6898	-0.0004
3	3	1	←	2	2	1	4479.0138	0.0060
5	2	4	←	4	1	3	4707.1444	-0.0011
7	0	7	←	6	1	6	4707.4488	-0.0011
7	0	7	←	6	0	6	4828.7967	-0.0034
5	2	3	←	4	1	3	4867.3871	-0.0013
7	1	7	←	6	0	6	4907.3187	-0.0046
7	3	5	←	6	3	4	5054.9441	0.0092
7	3	4	←	6	3	3	5087.3376	-0.0048
7	1	6	←	6	1	5	5140.9714	-0.0012
4	3	2	←	3	2	1	5182.1328	0.0025
4	3	1	←	3	2	1	5184.0629	0.0052
7	2	5	←	6	2	4	5190.2816	-0.0078
9	1	8	←	8	2	6	5200.6116	-0.0086
4	3	2	←	3	2	2	5206.5732	0.0117
6	2	5	←	5	1	4	5289.7592	0.0119
8	0	8	←	7	1	7	5407.7733	-0.0113
5	2	3	←	4	1	4	5418.9622	-0.0040
8	0	8	←	7	0	7	5486.3094	0.0015
8	1	8	←	7	0	7	5535.1711	-0.0042
6	2	4	←	5	1	4	5590.9937	0.0031
8	2	7	←	7	2	6	5688.8808	0.0020
8	3	6	←	7	3	5	5777.7050	0.0007
8	4	4	←	7	4	3	5784.7807	-0.0002
8	1	7	←	7	1	6	5838.0726	-0.0070
5	3	3	←	4	2	2	5871.5274	0.0039

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
5	3	2	←	4	2	2	5879.1564	-0.0084
5	3	3	←	4	2	3	5943.1080	-0.0090
8	2	6	←	7	2	5	5946.1786	0.0073
5	3	2	←	4	2	3	5950.7509	-0.0076
9	0	9	←	8	1	8	6095.3971	-0.0092
9	0	9	←	8	0	8	6144.2664	-0.0075
9	1	9	←	8	0	8	6173.8002	0.0084
7	2	5	←	6	1	5	6351.8493	0.0060
9	2	8	←	8	2	7	6380.9806	-0.0108
6	2	4	←	5	1	5	6413.6066	0.0049
9	1	8	←	8	1	7	6519.5955	0.0130
6	3	4	←	5	2	4	6692.6077	-0.0029
9	2	7	←	8	2	6	6693.2677	0.0109
6	3	3	←	5	2	4	6715.1695	-0.0065
10	0	10	←	9	1	9	6773.9749	-0.0023
10	1	10	←	9	0	9	6820.9171	-0.0031
7	2	6	←	6	1	6	6991.4421	-0.0007
8	2	6	←	7	1	6	7157.0424	0.0005
10	1	9	←	9	1	8	7186.9686	0.0186
7	3	4	←	6	2	4	7212.5782	-0.0071
10	3	8	←	9	3	7	7214.5301	0.0029
10	5	5	←	9	5	4	7227.9564	0.0022
10	2	8	←	9	2	7	7428.6858	0.0148
7	3	5	←	6	2	5	7458.8554	-0.0001
6	4	3	←	5	3	2	7557.0806	-0.0056
6	4	2	←	5	3	2	7557.6634	0.0039
6	4	2	←	5	3	3	7565.2968	-0.0040
8	3	6	←	7	2	5	7745.0180	-0.0091
11	2	10	←	10	2	9	7749.2860	-0.0089
8	3	5	←	7	2	5	7861.2306	-0.0020
8	2	7	←	7	1	7	7894.3383	-0.0101
11	3	9	←	10	3	8	7926.4076	0.0020
							RMS	8.2 kHz

Table S40 Linelist for ^{13}C6" isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
4	1	4	←	3	1	3	2766.6197	-0.0071
2	2	1	←	1	1	0	2801.2145	0.0063
4	0	4	←	3	0	3	2839.2818	0.0002
4	3	1	←	3	3	0	2898.0854	0.0057
4	1	3	←	3	1	2	2987.5176	-0.0162
5	0	5	←	4	1	4	3274.9429	-0.0022
5	1	5	←	4	1	4	3450.6388	-0.0091
3	2	1	←	2	1	1	3492.1553	-0.0031
9	3	6	←	8	4	5	3533.2449	0.0161
5	3	3	←	4	3	2	3623.3931	0.0034
3	2	2	←	2	1	2	3634.3090	0.0114
4	1	3	←	3	0	3	3637.8394	0.0088
3	2	1	←	2	1	2	3659.1205	0.0084
5	1	5	←	4	0	4	3694.6801	0.0124
5	1	4	←	4	1	3	3723.0428	0.0100
6	0	6	←	5	1	5	4011.8015	-0.0038
6	1	6	←	5	1	5	4130.8726	0.0091
4	2	2	←	3	1	2	4177.7129	-0.0020
6	0	6	←	5	0	5	4187.5124	0.0042
10	2	9	←	9	3	6	4208.5482	-0.0075
6	1	6	←	5	0	5	4306.5793	0.0129
6	2	5	←	5	2	4	4308.3016	0.0189
6	3	4	←	5	3	3	4351.0490	0.0007
6	3	3	←	5	3	2	4366.3608	0.0040
10	3	7	←	9	4	6	4400.6693	0.0009
6	1	5	←	5	1	4	4449.4348	-0.0094
6	2	4	←	5	2	3	4451.0297	-0.0007
3	3	0	←	2	2	1	4477.7312	0.0187

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
7	0	7	←	6	1	6	4730.7859	-0.0120
7	1	7	←	6	1	6	4807.5424	0.0070
7	0	7	←	6	0	6	4849.8536	-0.0024
5	2	3	←	4	1	3	4877.8620	-0.0018
7	2	6	←	6	2	5	5014.0277	-0.0031
7	4	4	←	6	4	3	5076.8365	-0.0098
7	3	5	←	6	3	4	5078.4617	-0.0094
12	0	12	←	11	1	10	5089.8441	-0.0164
8	1	7	←	7	2	6	5162.2260	-0.0138
7	1	6	←	6	1	5	5163.8208	-0.0063
4	3	2	←	3	2	1	5183.6254	-0.0030
4	3	2	←	3	2	2	5208.4564	0.0135
4	3	1	←	3	2	2	5210.4257	0.0043
7	2	5	←	6	2	4	5215.1172	0.0010
5	2	4	←	4	1	4	5269.8189	-0.0132
6	2	5	←	5	1	4	5300.5628	0.0098
8	0	8	←	7	1	7	5433.6057	-0.0007
8	1	8	←	7	1	7	5481.1872	0.0127
8	0	8	←	7	0	7	5510.3443	0.0003
8	1	8	←	7	0	7	5557.9129	0.0009
6	2	4	←	5	1	4	5605.8548	-0.0067
8	2	7	←	7	2	6	5714.5606	-0.0028
8	3	5	←	7	3	4	5867.2078	0.0030
5	3	3	←	4	2	2	5875.9147	0.0144
10	2	8	←	9	3	7	5877.1199	0.0122
5	3	2	←	4	2	2	5883.7465	0.0039
5	3	3	←	4	2	3	5948.5734	-0.0098
8	2	6	←	7	2	5	5974.2569	-0.0018
9	0	9	←	8	1	8	6123.7932	0.0072
6	2	5	←	5	1	5	6127.4630	-0.0040
9	1	9	←	8	1	8	6152.4041	-0.0025
9	0	9	←	8	0	8	6171.3526	-0.0013
12	3	9	←	11	4	8	6263.5710	-0.0098
7	2	5	←	6	1	5	6371.5172	-0.0163
9	2	8	←	8	2	7	6409.6192	-0.0041
6	3	3	←	5	2	3	6562.4285	0.0119
9	3	6	←	8	3	5	6633.3029	-0.0021
6	3	4	←	5	2	4	6701.8177	-0.0089
9	2	7	←	8	2	6	6724.3589	-0.0158
6	3	3	←	5	2	4	6724.9604	-0.0170
13	1	12	←	12	2	10	6777.1632	0.0022
10	0	10	←	9	1	9	6805.0103	-0.0124
10	0	10	←	9	0	9	6833.6396	-0.0038
5	4	2	←	4	3	1	6842.3590	0.0000
5	4	1	←	4	3	1	6842.4694	-0.0090
5	4	1	←	4	3	2	6844.4563	-0.0006
10	1	10	←	9	0	9	6850.4892	0.0156
10	2	9	←	9	2	8	7099.2381	0.0090
13	3	10	←	12	4	8	7101.3803	0.0157
12	2	10	←	11	3	8	7140.7446	0.0082
8	2	6	←	7	1	6	7181.9482	-0.0170
10	1	9	←	9	1	8	7217.3373	0.0103
8	1	7	←	7	0	7	7442.0594	-0.0168
11	1	11	←	10	0	10	7506.8777	-0.0017
6	4	3	←	5	3	2	7560.7070	0.0000
6	4	2	←	5	3	2	7561.2952	-0.0064
6	4	2	←	5	3	3	7569.1524	0.0085
5	3	2	←	4	0	4	7872.4830	0.0104
11	1	10	←	10	1	9	7877.3372	0.0101
							RMS	9.4 kHz

Table S41 Linelist for $H_2^{18}O1$ isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	1	3	←	2	1	2	2070.0726	-0.0052
3	0	3	←	2	0	2	2136.8779	0.0013
4	3	1	←	4	2	2	2157.7066	-0.0033
3	2	1	←	2	2	0	2179.4088	-0.0015
3	3	0	←	3	2	1	2192.9364	0.0115
14	3	11	←	14	2	12	2194.4911	-0.0053
3	3	1	←	3	2	2	2219.2623	-0.0054
3	1	2	←	2	1	1	2239.4417	0.0059
5	3	3	←	5	2	4	2260.7127	-0.0095
6	3	4	←	6	2	5	2306.3116	-0.0048
6	3	3	←	6	2	5	2332.6096	0.0021
3	1	3	←	2	0	2	2433.8449	0.0012
4	0	4	←	3	1	3	2529.3067	-0.0022
5	1	4	←	4	2	2	2575.2746	-0.0040
8	0	8	←	7	2	5	2718.0440	-0.0133
2	2	1	←	1	1	0	2740.1225	0.0099
2	2	0	←	1	1	0	2745.5186	0.0089
4	1	4	←	3	1	3	2754.5109	-0.0020
3	1	2	←	2	0	2	2772.8933	0.0099
2	2	1	←	1	1	1	2796.6859	0.0126
2	2	0	←	1	1	1	2802.0853	0.0150
4	0	4	←	3	0	3	2826.2805	0.0044
4	2	3	←	3	2	2	2873.3119	0.0004
4	3	2	←	3	3	1	2887.3973	-0.0025
4	3	1	←	3	3	0	2889.3322	0.0021
4	2	2	←	3	2	1	2924.5449	-0.0001
14	1	13	←	13	4	10	2962.5774	-0.0075
4	1	3	←	3	1	2	2978.8266	0.0017
10	0	10	←	9	2	7	2987.9784	-0.0043
4	1	4	←	3	0	3	3051.4781	-0.0018
7	2	5	←	6	3	4	3222.3621	0.0099
5	0	5	←	4	1	4	3275.9754	-0.0061
3	2	2	←	2	1	1	3402.9457	0.0168
3	2	1	←	2	1	1	3429.6119	0.0165
5	1	5	←	4	1	4	3435.0234	-0.0029
5	0	5	←	4	0	4	3501.1821	-0.0033
6	1	5	←	5	2	4	3501.8251	-0.0049
3	2	2	←	2	1	2	3572.6224	0.0119
5	2	4	←	4	2	3	3584.9095	-0.0006
3	2	1	←	2	1	2	3599.2898	0.0126
5	4	2	←	4	4	1	3608.8445	-0.0082
5	4	1	←	4	4	0	3608.9786	-0.0023
5	3	3	←	4	3	2	3612.2770	0.0006
4	1	3	←	3	0	3	3614.8391	0.0074
5	3	2	←	4	3	1	3618.9470	0.0004
9	3	6	←	8	4	4	3658.9469	0.0113
5	1	5	←	4	0	4	3660.2316	0.0011
5	2	3	←	4	2	2	3680.5026	0.0030
5	1	4	←	4	1	3	3711.1583	0.0000
9	5	5	←	9	4	6	3945.1095	-0.0093
6	0	6	←	5	1	5	4006.0753	-0.0041
7	1	6	←	6	2	4	4028.4758	-0.0132
4	2	3	←	3	1	2	4036.8178	0.0133
11	4	8	←	10	5	6	4051.0100	-0.0136
8	2	6	←	7	3	4	4056.1222	-0.0177
6	1	6	←	5	1	5	4111.5695	-0.0026
4	2	2	←	3	1	2	4114.7151	0.0105
8	2	6	←	7	3	5	4119.9495	0.0142
6	0	6	←	5	0	5	4165.1193	-0.0051
6	1	6	←	5	0	5	4270.6144	-0.0027
6	2	5	←	5	2	4	4292.1350	0.0005
6	4	3	←	5	4	2	4334.4125	0.0042
6	4	2	←	5	4	1	4334.9819	0.0008
6	3	4	←	5	3	3	4337.7276	-0.0010

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
7	1	6	←	6	2	5	4352.5541	-0.0048
6	3	3	←	5	3	2	4355.0935	-0.0019
3	3	1	←	2	2	0	4371.9976	-0.0139
3	3	0	←	2	2	0	4372.3233	-0.0118
3	3	1	←	2	2	1	4377.3990	-0.0096
3	3	0	←	2	2	1	4377.7208	-0.0114
6	1	5	←	5	1	4	4433.5626	0.0011
6	2	4	←	5	2	3	4442.7145	-0.0004
4	2	2	←	3	1	3	4453.7535	0.0091
5	1	4	←	4	0	4	4499.7233	0.0092
5	2	4	←	4	1	3	4642.9021	0.0123
7	0	7	←	6	1	6	4717.9702	-0.0056
7	1	7	←	6	1	6	4784.4848	0.0016
5	2	3	←	4	1	3	4816.3841	0.0049
7	0	7	←	6	0	6	4823.4639	-0.0046
7	6	2	←	7	5	3	4858.4796	0.0100
7	1	7	←	6	0	6	4889.9744	-0.0014
16	2	15	←	15	3	12	4945.1116	0.0062
7	2	6	←	6	2	5	4994.3059	0.0003
9	2	7	←	8	3	6	5039.7109	-0.0025
7	4	4	←	6	4	3	5061.7535	-0.0038
7	3	5	←	6	3	4	5062.7413	-0.0063
4	3	2	←	3	2	1	5079.9956	-0.0053
4	3	1	←	3	2	1	5082.2493	-0.0056
7	3	4	←	6	3	3	5100.2540	0.0020
4	3	2	←	3	2	2	5106.6621	-0.0054
4	3	1	←	3	2	2	5108.9165	-0.0049
7	1	6	←	6	1	5	5142.8660	0.0025
7	2	5	←	6	2	4	5204.6038	0.0051
5	2	4	←	4	1	4	5206.2578	0.0163
6	2	5	←	5	1	4	5223.8727	0.0069
5	2	3	←	4	1	4	5379.7199	-0.0110
8	0	8	←	7	1	7	5414.0151	-0.0049
8	1	8	←	7	1	7	5454.3411	-0.0026
11	3	8	←	10	4	7	5462.7788	0.0060
8	0	8	←	7	0	7	5480.5269	-0.0004
12	2	11	←	11	3	9	5486.1580	-0.0123
8	1	8	←	7	0	7	5520.8483	-0.0028
6	2	4	←	5	1	4	5547.9407	0.0048
8	2	7	←	7	2	6	5690.9470	0.0064
9	7	3	←	9	6	4	5738.5142	0.0112
5	3	3	←	4	2	2	5767.7282	-0.0041
8	6	3	←	7	6	2	5775.3375	-0.0019
5	3	2	←	4	2	2	5776.6493	-0.0071
8	5	4	←	7	5	3	5781.4099	0.0092
8	5	3	←	7	5	2	5781.5643	0.0071
7	2	6	←	6	1	5	5784.6179	0.0079
8	3	6	←	7	3	5	5786.0859	0.0026
8	4	5	←	7	4	4	5790.8352	-0.0015
8	4	4	←	7	4	3	5795.9357	0.0014
13	4	9	←	12	5	7	5814.6634	-0.0060
8	1	7	←	7	1	6	5836.4336	0.0000
5	3	3	←	4	2	3	5845.6280	-0.0044
5	3	2	←	4	2	3	5854.5533	-0.0032
8	3	5	←	7	3	4	5856.3231	0.0016
8	2	6	←	7	2	5	5960.3275	-0.0032
9	1	8	←	8	2	7	6017.3748	-0.0022
9	0	9	←	8	1	8	6098.0993	-0.0020
9	1	9	←	8	1	8	6121.8347	-0.0023
9	0	9	←	8	0	8	6138.4271	0.0020
9	1	9	←	8	0	8	6162.1628	0.0020
11	4	8	←	11	1	10	6291.8597	0.0032
7	2	5	←	6	1	5	6318.9788	0.0058
12	3	9	←	11	4	7	6330.1732	0.0009
8	2	7	←	7	1	6	6332.6945	0.0072
9	2	8	←	8	2	7	6381.8233	0.0006
6	2	4	←	5	1	5	6387.4117	-0.0078

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
7	1	6	←	6	0	6	6409.8473	0.0182
6	3	4	←	5	2	3	6424.9510	-0.0104
6	3	3	←	5	2	3	6451.2420	-0.0103
9	3	7	←	8	3	6	6506.4180	0.0050
9	5	5	←	8	5	4	6509.7439	-0.0009
9	1	8	←	8	1	7	6513.6330	0.0022
9	4	6	←	8	4	5	6521.3155	0.0017
9	4	5	←	8	4	4	6533.2202	0.0001
6	3	4	←	5	2	4	6598.4436	-0.0073
9	3	6	←	8	3	5	6623.1626	0.0018
6	3	3	←	5	2	4	6624.7371	-0.0047
12	3	10	←	12	0	12	6694.9845	0.0053
9	2	7	←	8	2	6	6705.8538	-0.0076
15	3	13	←	14	4	10	6723.7315	0.0012
10	0	10	←	9	1	9	6773.9581	0.0011
10	1	10	←	9	1	9	6787.6094	-0.0054
10	0	10	←	9	0	9	6797.6870	-0.0056
10	1	10	←	9	0	9	6811.3474	-0.0030
10	1	9	←	9	2	8	6812.5300	-0.0094
9	2	8	←	8	1	7	6878.0953	0.0189
11	2	9	←	10	3	8	6904.0363	0.0001
4	3	2	←	3	0	3	6906.1642	-0.0031
14	1	13	←	13	2	11	6942.5598	0.0034
7	3	5	←	6	2	4	7044.9893	-0.0048
13	4	9	←	13	2	12	7060.2666	-0.0045
10	2	9	←	9	2	8	7067.0558	0.0087
7	3	4	←	6	2	4	7108.7785	-0.0109
11	5	6	←	11	3	9	7112.2871	-0.0014
8	2	6	←	7	1	6	7136.4482	0.0078
10	1	9	←	9	1	8	7176.9893	0.0041
10	7	4	←	9	7	3	7221.4063	0.0090
10	3	8	←	9	3	7	7222.5074	0.0081
10	6	5	←	9	6	4	7228.4896	0.0078
10	4	7	←	9	4	6	7252.5374	-0.0039
7	3	5	←	6	2	5	7369.0571	-0.0069
10	3	7	←	9	3	6	7397.3397	-0.0064
10	2	9	←	9	1	8	7431.5041	0.0113
7	3	4	←	6	2	5	7432.8514	-0.0080
10	2	8	←	9	2	7	7438.2625	0.0031
11	0	11	←	10	1	10	7444.5018	0.0000
11	1	11	←	10	1	10	7452.2239	0.0021
11	0	11	←	10	0	10	7458.1515	-0.0081
11	1	11	←	10	0	10	7465.8801	0.0004
8	3	6	←	7	2	5	7626.4790	0.0002
11	2	10	←	10	2	9	7747.0305	0.0099
8	3	5	←	7	2	5	7760.4996	-0.0126
12	2	10	←	11	3	9	7824.6189	-0.0124
11	1	10	←	10	1	9	7831.6611	0.0061
14	5	9	←	14	2	12	7931.9827	-0.0181
11	6	5	←	10	6	4	7957.4599	0.0094
							RMS	7.4 kHz

Table S42 Linelist for $H_2^{18}O2$ isotopologue of DPE-2w OHO complex. OMC is the difference between the observed and calculated transition.

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
5	3	3	←	5	2	3	2041.9614	0.0008
6	2	5	←	5	3	2	2044.2500	-0.0129
3	1	3	←	2	1	2	2066.1544	-0.0048
3	2	2	←	2	2	1	2159.6088	-0.0039
3	2	1	←	2	2	0	2183.6910	-0.0140
4	3	2	←	4	2	3	2205.8920	-0.0138
6	3	4	←	6	2	5	2287.8751	0.0057
7	3	5	←	7	2	6	2364.2585	0.0046
9	1	8	←	9	1	9	2395.9101	0.0163
9	1	8	←	9	0	9	2415.3016	-0.0034

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
3	1	3	←	2	0	2	2419.7507	0.0041
4	0	4	←	3	1	3	2537.5025	-0.0087
9	3	7	←	9	2	8	2607.2874	0.0098
9	4	5	←	8	5	4	2657.3846	-0.0077
7	2	6	←	6	3	3	2672.5317	0.0073
7	2	6	←	6	3	4	2704.3934	0.0035
2	2	1	←	1	1	0	2721.6199	0.0078
2	2	0	←	1	1	0	2727.7466	0.0077
4	1	4	←	3	1	3	2748.5858	-0.0014
3	1	2	←	2	0	2	2778.5886	0.0095
2	2	1	←	1	1	1	2781.4923	0.0090
2	2	0	←	1	1	1	2787.6193	0.0092
10	1	9	←	10	0	10	2802.2685	-0.0056
4	0	4	←	3	0	3	2821.7277	-0.0037
4	2	3	←	3	2	2	2874.7010	-0.0025
4	3	2	←	3	3	1	2890.6263	-0.0027
4	3	1	←	3	3	0	2892.9794	0.0006
8	4	4	←	8	3	5	2900.6002	-0.0169
4	2	2	←	3	2	1	2932.4420	0.0015
4	1	3	←	3	1	2	2985.7208	-0.0011
4	1	4	←	3	0	3	3032.8055	-0.0018
6	4	2	←	6	3	4	3044.8841	-0.0117
11	4	8	←	11	3	9	3168.4995	0.0058
7	2	5	←	6	3	3	3263.7640	-0.0050
5	0	5	←	4	1	4	3281.2900	-0.0094
6	1	5	←	5	2	3	3350.8187	-0.0119
10	4	7	←	9	5	5	3376.9350	-0.0165
3	2	2	←	2	1	1	3381.6201	0.0120
3	2	1	←	2	1	1	3411.8407	0.0135
5	1	5	←	4	1	4	3426.6672	-0.0044
5	0	5	←	4	0	4	3492.3724	-0.0029
3	2	2	←	2	1	2	3561.2281	0.0066
5	2	4	←	4	2	3	3585.7425	-0.0023
3	2	1	←	2	1	2	3591.4502	0.0097
5	4	2	←	4	4	1	3612.9248	0.0043
5	4	1	←	4	4	0	3613.0916	0.0036
5	3	3	←	4	3	2	3616.5716	0.0014
5	3	2	←	4	3	1	3624.6716	-0.0020
4	1	3	←	3	0	3	3628.7780	0.0034
5	1	5	←	4	0	4	3637.7468	-0.0007
9	1	9	←	8	2	7	3658.3484	0.0056
5	2	3	←	4	2	2	3692.5556	-0.0041
5	1	4	←	4	1	3	3717.9205	-0.0024
4	3	1	←	4	1	4	3829.8363	0.0077
3	3	0	←	3	0	3	3969.6641	0.0069
4	2	3	←	3	1	2	4010.9475	0.0140
5	3	2	←	5	1	5	4027.8217	-0.0087
4	2	2	←	3	1	2	4098.8967	0.0074
6	1	6	←	5	1	5	4100.4297	-0.0063
11	4	8	←	10	5	5	4118.8218	0.0060
8	2	6	←	7	3	4	4128.2104	-0.0021
6	0	6	←	5	0	5	4151.9853	-0.0045
6	1	6	←	5	0	5	4245.8161	0.0077
6	2	5	←	5	2	4	4291.8379	-0.0037
6	5	2	←	5	5	1	4334.5391	0.0029
6	4	3	←	5	4	2	4339.7742	0.0002
6	4	2	←	5	4	1	4340.5229	0.0011
6	3	4	←	5	3	3	4342.9809	0.0012
3	3	1	←	2	2	0	4343.4625	-0.0039
3	3	0	←	2	2	0	4343.8431	-0.0176
3	3	1	←	2	2	1	4349.5883	-0.0048
3	3	0	←	2	2	1	4349.9812	-0.0062
6	3	3	←	5	3	2	4363.9981	0.0004
4	2	3	←	3	1	3	4369.7825	0.0167
15	7	8	←	14	8	6	4396.2883	-0.0020
6	1	5	←	5	1	4	4438.6323	-0.0024
6	2	4	←	5	2	3	4458.3137	-0.0138

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
5	1	4	←	4	0	4	4524.9656	-0.0003
5	2	4	←	4	1	3	4610.9642	0.0079
10	2	8	←	10	1	10	4632.8620	-0.0041
8	1	7	←	7	2	5	4646.8077	0.0103
10	3	7	←	9	4	6	4654.6054	-0.0143
7	0	7	←	6	1	6	4712.8119	-0.0078
13	5	9	←	12	6	6	4732.6528	0.0180
7	1	7	←	6	1	6	4770.3213	-0.0065
5	2	3	←	4	1	3	4805.7347	0.0076
7	0	7	←	6	0	6	4806.6348	-0.0034
7	1	7	←	6	0	6	4864.1410	-0.0054
9	2	7	←	8	3	5	4974.5053	0.0012
7	2	6	←	6	2	5	4992.2582	-0.0010
4	3	2	←	3	2	1	5050.3875	-0.0028
4	3	1	←	3	2	1	5053.1265	-0.0079
7	5	3	←	6	5	2	5060.8322	-0.0030
7	5	2	←	6	5	1	5060.8941	0.0035
7	3	5	←	6	3	4	5068.6400	-0.0036
7	4	3	←	6	4	2	5071.0683	0.0035
4	3	2	←	3	2	2	5080.6088	-0.0006
4	3	1	←	3	2	2	5083.3503	-0.0032
7	3	4	←	6	3	3	5113.7291	-0.0005
7	1	6	←	6	1	5	5144.2846	0.0000
6	2	5	←	5	1	4	5184.8857	0.0107
5	2	4	←	4	1	4	5206.9344	0.0110
7	2	5	←	6	2	4	5222.2426	-0.0046
8	1	7	←	7	2	6	5238.0268	-0.0152
5	4	1	←	5	2	4	5284.0665	-0.0186
5	2	3	←	4	1	4	5401.6985	0.0043
8	0	8	←	7	1	7	5403.1405	-0.0081
8	1	8	←	7	1	7	5437.0514	-0.0012
8	0	8	←	7	0	7	5460.6490	-0.0077
6	1	5	←	5	0	5	5471.2234	-0.0020
8	1	8	←	7	0	7	5494.5632	0.0023
6	2	4	←	5	1	4	5546.1333	0.0016
8	2	7	←	7	2	6	5686.5143	0.0032
5	3	3	←	4	2	2	5734.5134	-0.0067
7	2	6	←	6	1	5	5738.5142	0.0148
13	5	9	←	13	3	10	5739.2510	-0.0061
5	3	2	←	4	2	2	5745.3619	-0.0057
8	7	1	←	7	7	0	5777.9032	0.0016
8	5	4	←	7	5	3	5788.9096	0.0089
8	5	3	←	7	5	2	5789.1234	0.0035
8	3	6	←	7	3	5	5792.1044	-0.0008
8	4	5	←	7	4	4	5799.2867	0.0073
8	4	4	←	7	4	3	5805.9041	0.0015
5	3	3	←	4	2	3	5822.4768	0.0007
8	1	7	←	7	1	6	5832.2552	-0.0015
5	3	2	←	4	2	3	5833.3276	0.0040
8	3	5	←	7	3	4	5875.6404	-0.0105
8	2	6	←	7	2	5	5978.1651	-0.0079
6	2	5	←	5	1	5	6072.1102	0.0168
6	4	2	←	6	1	5	6078.9904	-0.0149
9	0	9	←	8	1	8	6081.9777	-0.0007
9	1	9	←	8	1	8	6101.3896	-0.0001
9	0	9	←	8	0	8	6115.8787	-0.0037
9	1	9	←	8	0	8	6135.2954	0.0016
8	2	7	←	7	1	6	6280.7420	0.0161
7	2	5	←	6	1	5	6329.7455	0.0014
9	2	8	←	8	2	7	6374.4443	0.0031
6	3	4	←	5	2	3	6384.9415	0.0013
18	8	10	←	18	7	11	6387.4117	-0.0024
6	3	3	←	5	2	3	6416.8061	0.0004
17	8	10	←	17	7	10	6421.5439	-0.0050
17	8	9	←	17	7	11	6425.2166	0.0034
7	1	6	←	6	0	6	6463.5265	0.0063
15	3	12	←	15	2	14	6487.0746	0.0023

J'	$K_{a'}$	$K_{c'}$		J	K_a	K_c	Observed (MHz)	OMC (MHz)
9	1	8	←	8	1	7	6502.7050	-0.0005
9	7	3	←	8	7	2	6503.4149	0.0120
9	3	7	←	8	3	6	6511.8783	0.0074
9	5	5	←	8	5	4	6518.9411	0.0128
9	5	4	←	8	5	3	6519.6310	-0.0006
9	4	6	←	8	4	5	6531.3387	0.0106
9	4	5	←	8	4	4	6546.7436	0.0149
6	3	4	←	5	2	4	6579.7115	0.0005
6	3	3	←	5	2	4	6611.5722	-0.0042
9	3	6	←	8	3	5	6648.6759	-0.0156
9	2	7	←	8	2	6	6721.9295	-0.0127
10	1	10	←	9	1	9	6764.0506	0.0002
10	0	10	←	9	0	9	6772.5917	-0.0026
10	1	10	←	9	0	9	6783.4597	-0.0020
9	2	8	←	8	1	7	6822.9281	0.0177
10	1	9	←	9	2	8	6839.3448	-0.0137
7	3	5	←	6	2	4	6995.2530	-0.0033
10	2	9	←	9	2	8	7056.2686	0.0015
5	4	1	←	5	1	5	7064.3355	-0.0013
7	3	4	←	6	2	4	7072.2087	0.0009
10	1	9	←	9	1	8	7159.5689	0.0055
8	2	6	←	7	1	6	7163.6284	-0.0041
10	9	1	←	9	9	0	7221.3203	-0.0093
10	8	2	←	9	8	1	7224.8871	0.0062
10	3	8	←	9	3	7	7226.5923	0.0004
16	1	15	←	15	2	13	7242.0382	-0.0047
6	4	3	←	6	1	6	7303.4942	0.0080
7	3	5	←	6	2	5	7356.5189	0.0058
11	0	11	←	10	1	10	7419.6207	-0.0050
11	1	11	←	10	1	10	7425.6039	0.0003
10	3	7	←	9	3	6	7427.8404	-0.0140
11	0	11	←	10	0	10	7430.4884	-0.0046
7	3	4	←	6	2	5	7433.4593	-0.0051
11	1	11	←	10	0	10	7436.4704	-0.0004
5	3	3	←	4	1	4	7443.6424	-0.0122
10	2	8	←	9	2	7	7450.3990	-0.0111
8	1	7	←	7	0	7	7489.1399	0.0011
8	3	6	←	7	2	5	7565.1246	0.0102
11	1	10	←	10	2	9	7592.1976	-0.0109
8	3	5	←	7	2	5	7725.6020	-0.0094
11	2	10	←	10	2	9	7732.5696	0.0119
11	1	10	←	10	1	9	7809.1214	0.0043
11	3	9	←	10	3	8	7935.2069	0.0111
11	7	5	←	10	7	4	7958.0331	0.0094
8	4	5	←	8	1	8	7963.9945	0.0043
							RMS	7.8 kHz

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