Effect of Magnetic Anisotropy on Direct Chiral Discrimination in Paramagnetic NMR Spectroscopy - Supplementary Information

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EXTENSIVE DERIVATION OF INTEGRALS IN GENERALIZED SHIELDING POLARIZABILITY TENSOR

In this Section, an expression for $\mathrm{Tr}\,\rho_3$, with ρ_3 defined in the main paper, will be derived by explicitly solving the integrals.

Double Integral

The solution of double integrals of the same form of

$$\int_0^\beta \mathrm{d}\omega \int_0^\omega \mathrm{d}\omega' \;\mathrm{Tr}\left[e^{(\omega-\beta)\,H_0} V_2 e^{(\omega'-\omega)H_0} V_1 e^{-\omega' H_0}\right] \tag{SI-I}$$

and

$$\int_0^\beta \mathrm{d}\omega \int_0^\omega \mathrm{d}\omega' \;\mathrm{Tr}\left[e^{(\omega-\beta)\,H_0} V_1 e^{(\omega'-\omega)H_0} V_2 e^{-\omega' H_0}\right] \tag{SI-II}$$

has been thoroughly presented and discussed in Ref. [1]. In this Section, the procedure will be reported and applied to Eqs. SI-I–SI-II. Since both integrals can be solved via the same procedure, we will manipulate their sum in order to simplify their discussion.

Using the cyclic property of the trace, we first rearrange the integrands as:

$$\begin{aligned}\mathrm{Tr}\,\rho_3^{(2)} = &\int_0^\beta \mathrm{d}\omega \int_0^\omega \mathrm{d}\omega' \;\mathrm{Tr}\left[e^{-\beta\,H_0} V_2 e^{(\omega'-\omega)H_0} V_1 e^{(\omega-\omega')H_0}\right] \\ &+ \int_0^\beta \mathrm{d}\omega \int_0^\omega \mathrm{d}\omega' \;\mathrm{Tr}\left[e^{-\beta\,H_0} V_1 e^{(\omega'-\omega)H_0} V_2 e^{(\omega-\omega')H_0}\right]\end{aligned} \tag{SI-III}$$

where the apex in ρ_3 is used to explicit that only its double integral term is being considered. In this formulation, it can be easily noted that the integrand only depends on $\omega' - \omega$, thus suggesting the following advantageous variable substitution:

$$\begin{aligned} u &= \omega \\ v &= \omega - \omega' \end{aligned} \tag{SI-IV}$$

which gives:

$$\begin{aligned} \mathrm{Tr}\,\rho_3^{(2)} = &\int_0^\beta \mathrm{d}u \int_0^u \mathrm{d}v \;\; \mathrm{Tr}\left[e^{-\beta H_0} V_2 e^{-vH_0} V_1 e^{vH_0}\right] \\ &+ \int_0^\beta \mathrm{d}u \int_0^u \mathrm{d}v \;\; \mathrm{Tr}\left[e^{-\beta H_0} V_1 e^{-vH_0} V_2 e^{vH_0}\right] \end{aligned} \tag{SI-V}$$

Since the two double integrals feature the same integration domain and very similar integrands, it is advisable to further manipulate them in order to simplify the expression. For this reason, we apply the following variable transformation to the second integral on rhs in Eq. SI-V:

$$\begin{aligned} u &\rightarrow \beta - u \\ v &\rightarrow \beta - v \end{aligned} \tag{SI-VI}$$

and, after transforming the integration domains, we obtain:

$$\begin{aligned} \mathrm{Tr}\,\rho_3^{(2)} = &\int_0^\beta \mathrm{d}u \int_0^u \mathrm{d}v \;\; \mathrm{Tr}\left[e^{-\beta H_0} V_2 e^{-vH_0} V_1 e^{vH_0}\right] \\ &+ \int_0^\beta \mathrm{d}u \int_u^\beta \mathrm{d}v \;\; \mathrm{Tr}\left[e^{-\beta H_0} V_2 e^{-vH_0} V_1 e^{vH_0}\right] \end{aligned} \tag{SI-VII}$$

After the transformation, we notice that the two double integrals now feature the same integrand but different integration domains, thus allowing the collection in a single integral:

$$\mathrm{Tr}\,\rho_3^{(2)} = \int_0^\beta \mathrm{d}u \int_0^\beta \mathrm{d}v \;\; \mathrm{Tr}\left[e^{-\beta H_0} V_2 e^{-vH_0} V_1 e^{vH_0}\right] \tag{SI-VIII}$$

Using a well–known result of statistical mechanics [2]:

$$\int_0^\beta \mathrm{Tr}\left[e^{-\beta H_0} F\right] = \beta \langle F \rangle_0 \,\mathrm{Tr}\,\rho_0 \tag{SI-IX}$$

where

$$\langle F \rangle_0 = \frac{\mathrm{Tr}\,(F\rho_0)}{\mathrm{Tr}\,\rho_0} = \frac{\sum_{n\nu} F_{n\nu} e^{-\beta E_n}}{\sum_{n\nu} e^{-\beta E_n}} \tag{SI-X}$$

is the thermal average of F in the canonical ensemble corresponding to H_0 computed in the basis of H_0 eigenstates described in the main paper, we can further simplify Eq. SI-V:

$$\mathrm{Tr}\,\rho_3^{(2)} = \beta\,\mathrm{Tr}\,\rho_0 \left\langle \int_0^\beta \mathrm{d}v\; V_2 e^{-vH_0} V_1 e^{vH_0} \right\rangle_0 \tag{SI-XI}$$

In order to solve the integral, we carry out the ensemble averaging first:

$$\begin{aligned}\int_0^\beta \mathrm{d}v\;\left\langle V_2 e^{-vH_0} V_1 e^{vH_0}\right\rangle_0 &= \frac{1}{Z_0}\int_0^\beta \mathrm{d}u\;\left[\sum_{n\nu}\left\langle n\nu\middle|V_2 e^{-vH_0}V_1\middle|n_n u\right\rangle e^{(v-\beta)E_n}\right] \\ &= \frac{1}{Z_0}\sum_{n\nu,m\mu}\langle n\nu|V_2|m\mu\rangle\langle m\mu|V_1|n_n u\rangle\, e^{-\beta E_n}\int_0^\beta \mathrm{d}u\; e^{v(E_n-E_m)}\end{aligned} \tag{SI-XII}$$

where $Z_0 = \sum_{n\nu} e^{-\beta E_n}$ is the partition function. In the last step, the resolution of identity $\hat{I} = \sum_{m\mu}|m\mu\rangle\langle m\mu|$ has been applied. The remaining integral in Eq. SI-XII can be readily evaluated as:

$$\int_0^\beta \mathrm{d}u\; e^{v(E_n-E_m)}\begin{cases}\beta & \text{if l=m}\\ \dfrac{e^{\beta(E_n-E_m)}-1}{E_n-E_m} & \text{if l}\neq\text{m}\end{cases} \tag{SI-XIII}$$

where δ_{mn} is the Kronecker delta. Since the integral is not defined for $E_n = E_m$, its solution has been partitioned into two terms to account for the specific solution at discontinuity. The final solution of the double integral component, therefore, is:

$$\mathrm{Tr}\,\rho_3^{(2)} = \beta\sum_{n\nu} e^{-\beta E_n}\left[\beta\sum_{\nu'}\langle n\nu|V_2|n\nu'\rangle\langle n\nu'|V_1|n\nu\rangle + \sum_{m\neq n,\mu}\frac{\langle n\nu|V_2|m\mu\rangle\langle m\mu|V_1|n\nu\rangle + \text{c.c.}}{E_m-E_n}\right] \tag{SI-XIV}$$

Triple Integral

The solution of the triple integral

$$\int_0^\beta \mathrm{d}\omega\int_0^\omega \mathrm{d}\omega'\int_0^{\omega'}\mathrm{d}\omega''\,\mathrm{Tr}[e^{(\omega-\beta)H_0}V_1 e^{(\omega'-\omega)H_0}V_1 e^{(\omega''-\omega')H_0}V_1 e^{-\omega''H_0}] \tag{SI-XV}$$

is not soluble using the same integral domain symmetrization discussed above, therefore it has to be solved directly by applying variable transformations and resolution of identity. In the first step

of the solution, resolution of identity is introduced twice to give:

$$\begin{aligned}\mathrm{Tr}\,\rho_3^{(3)} &= \sum_{n\nu}\sum_{m\mu}\sum_{l\lambda}\int_0^\beta \mathrm{d}\omega \int_0^\omega \mathrm{d}\omega' \int_0^{\omega'} \mathrm{d}\omega''\; e^{-\beta E_n} e^{\omega E_n}\,\langle n\nu|V_1|m\mu\rangle\, e^{(\omega'-\omega)E_m}\,\langle m\mu|V_1|l\lambda\rangle\, e^{(\omega''-\omega')E_l}\,\langle l\lambda|V_1|n\nu\rangle\, e^{-\omega'' E_n} \\ &= \sum_{n\nu}\sum_{m\mu}\sum_{l\lambda} e^{-\beta E_n}\,\langle n\nu|V_1|m\mu\rangle\,\langle m\mu|V_1|l\lambda\rangle\,\langle l\lambda|V_1|n\nu\rangle \int_0^\beta \mathrm{d}\omega\; e^{\omega(E_n-E_m)} \int_0^\omega \mathrm{d}\omega'\; e^{\omega'(E_m-E_l)} \int_0^{\omega'} \mathrm{d}\omega''\; e^{\omega''(E_l-E_n)}\end{aligned} \tag{SI-XVI}$$

In order to obtain the explicit expression for $\mathrm{Tr}\,\rho_3^{(3)}$, therefore, we have to solve the triple integral

$$\int_0^\beta \mathrm{d}\omega e^{\omega(E_n-E_m)} \int_0^\omega \mathrm{d}\omega'\; e^{\omega'(E_m-E_l)} \int_0^{\omega'} \mathrm{d}\omega''\; e^{\omega''(E_l-E_n)} \tag{SI-XVII}$$

The first step in the solution of Eq. SI-XVII is the treatment of the integral dependent on the variable ω'', as already discussed in Sec. :

$$\int_0^{\omega'} \mathrm{d}\omega''\; e^{\omega''(E_l-E_n)} = \begin{cases} \omega' & \text{if n=l} \\ \dfrac{e^{\omega'(E_l-E_n)}-1}{E_l-E_n} & \text{if n} \neq \text{l} \end{cases} \tag{SI-XVIII}$$

which, after substitution in Eq. SI-XVII, gives:

$$\begin{aligned}&\int_0^\beta \mathrm{d}\omega\; e^{\omega(E_n-E_m)} \int_0^\omega \mathrm{d}\omega'\; e^{\omega'(E_m-E_l)} \left[\underbrace{\omega'}_{l=n} + \underbrace{\frac{e^{\omega'(E_l-E_n)}-1}{E_l-E_n}}_{l\neq n} \right] \\ &= \int_0^\beta \mathrm{d}\omega \left[\underbrace{\int_0^\omega \mathrm{d}\omega'\; \omega' e^{\omega'(E_m-E_l)}}_{n=l} + \underbrace{\int_0^\omega \mathrm{d}\omega'\; \frac{e^{\omega'(E_m-E_n)}}{E_l-E_n}}_{n\neq l} - \underbrace{\int_0^\omega \mathrm{d}\omega'\; \frac{e^{\omega'(E_m-E_l)}}{E_l-E_n}}_{n\neq l} \right]\end{aligned} \tag{SI-XIX}$$

The three components of the integral dependent on ω' are easily solved as:

$$\begin{aligned}\underbrace{\int_0^\omega \mathrm{d}\omega'\; \omega' e^{\omega'(E_m-E_l)}}_{l=m} &= \underbrace{\frac{\omega'^2}{2}}_{n=l,m=l}\Bigg|_0^\omega + \underbrace{\frac{e^{\omega'(E_m-E_l)}}{(E_m-E_l)^2}\left[\omega'(E_m-E_l)-1\right]}_{n=l,m\neq l}\Bigg|_0^\omega \\ &= \underbrace{\frac{\omega^2}{2}}_{n=l,m=l} + \underbrace{\frac{\omega e^{\omega(E_m-E_l)}}{E_m-E_l}}_{n=l,m\neq l} - \underbrace{\frac{e^{\omega(E_m-E_l)}-1}{(E_m-E_l)^2}}_{n=l,m\neq l}\end{aligned} \tag{SI-XX}$$

$$\underbrace{\int_0^\omega \mathrm{d}\omega'\; \frac{e^{\omega'(E_m-E_n)}}{E_l-E_n}}_{n\neq l} = \underbrace{\frac{\omega}{E_l-E_n}}_{n\neq l,n=m} + \underbrace{\frac{e^{\omega(E_m-E_n)}-1}{(E_l-E_n)(E_m-E_n)}}_{n\neq l,n\neq m} \tag{SI-XXI}$$

$$\underbrace{\int_0^{\omega} \mathrm{d}\omega' \, \frac{e^{\omega'(E_m-E_l)}}{E_l-E_n}}_{n\neq l} = \underbrace{\frac{\omega}{E_l-E_n}}_{n\neq l,m=l} + \underbrace{\frac{e^{\omega(E_m-E_l)}-1}{(E_l-E_n)\,(E_m-E_l)}}_{n\neq l,m\neq l} \tag{SI-XXII}$$

where we have used the well–known integral solution

$$\int \mathrm{d}x \; xe^{cx} = \begin{cases} \dfrac{x^2}{2} & \text{if c} = 0 \\ \dfrac{e^{cx}}{c^2}\,(cx-1) & \text{if c} \neq 0 \end{cases} \tag{SI-XXIII}$$

Substituting these results in Eq. SI-XIX gives:

$$\begin{aligned} \int_0^{\beta} \mathrm{d}\omega \, \Bigg[& \underbrace{\frac{\omega^2 e^{\omega(E_n-E_m)}}{2}}_{n=l,m=l} + \omega \underbrace{\frac{e^{\omega(E_n-E_l)}}{E_m-E_l}}_{n=l,m\neq l} - \underbrace{\frac{e^{\omega(E_n-E_l)}}{(E_m-E_l)^2}}_{n=l,m\neq l} + \underbrace{\frac{e^{\omega(E_n-E_m)}}{(E_m-E_l)^2}}_{n=l,m\neq l} - \underbrace{\frac{e^{\omega(E_n-E_m)}-1}{(E_l-E_n)\,(E_m-E_n)}}_{n\neq l,n\neq m} \\ & + \omega \underbrace{\frac{e^{\omega(E_n-E_m)}}{E_l-E_n}}_{n\neq l,n=m} - \underbrace{\frac{e^{\omega(E_n-E_l)}}{(E_l-E_n)\,(E_m-E_l)}}_{n\neq l,m\neq l} + \underbrace{\frac{e^{\omega(E_n-E_m)}}{(E_l-E_n)\,(E_m-E_l)}}_{n\neq l,m\neq l} - \omega \underbrace{\frac{e^{\omega(E_n-E_m)}}{E_l-E_n}}_{n\neq l,m=l} \Bigg] \end{aligned} \tag{SI-XXIV}$$

The remaining integral in Eq. SI-XXIV can be easily solved, thus giving the final result:

$$\begin{aligned} & \underbrace{\frac{\beta^3}{6}}_{n=l,m=l} + \frac{\beta^2}{2} \left[\underbrace{\frac{1}{(E_m-E_l)}}_{n=l,m\neq l} + \underbrace{\frac{1}{(E_l-E_n)}}_{n=m,n\neq l} \right] \\ & + \beta \left[- \underbrace{\frac{1}{(E_m-E_l)^2}}_{n=l,m\neq l} + \underbrace{\frac{1}{(E_l-E_n)\,(E_m-E_n)}}_{n\neq m,n\neq l} - \underbrace{\frac{e^{\beta(E_n-E_m)}}{(E_n-E_m)\,(E_l-E_n)}}_{m=l,n\neq l} + \underbrace{\frac{1}{(E_l-E_n)\,(E_m-E_l)}}_{n\neq m,m\neq l,n=m} \right] \\ & + \underbrace{\frac{e^{\beta(E_n-E_m)}-1}{(E_n-E_m)\,(E_m-E_l)^2}}_{m\neq l,n=l} + \underbrace{\frac{e^{\beta(E_n-E_m)}-1}{(E_l-E_n)\,(E_m-E_n)^2}}_{n\neq m,n\neq l} + \underbrace{\frac{e^{\beta(E_n-E_l)}-1}{(E_m-E_l)\,(E_l-E_n)^2}}_{n\neq l,m\neq l} \\ & + \underbrace{\frac{e^{\beta(E_n-E_m)}-1}{(E_n-E_m)\,(E_m-E_l)\,(E_l-E_n)}}_{n\neq m,n\neq l,m\neq l} + \underbrace{\frac{e^{\beta(E_n-E_m)}-1}{(E_l-E_n)\,(E_n-E_m)^2}}_{n\neq l,m=l} \end{aligned} \tag{SI-XXV}$$

Substitution of these results in Eq. SI-XVI gives the final solution of the triple integral.

MOLECULES STUDIED IN THE PAPER

	Complex
1	$[Dy(acac)_3(H_2O)_2]$ [3]
2	$[Dy(acac)_3(dppz)]$ [4]
3	$[Dy(acac)_3(dpq)]$ [4]
4	$[Dy(acac)_3(phen)]$ [5]
5	$[Dy(hfac)_3(dme)]$ [6]
6	$[Dy(paaH^*)_2(NO_3)_2(MeOH)]^+$ [7]
7	$[Dy(tfpb)_3(dppz)]$ [8]
8	$[Dy(tta)_3(bipy)]$ [9]
9	$[Dy(tta)_3(phen)]$ [9]
10	$[Dy(tta)_3(pinene{-}bipy)]$ [10]

TABLE SI-I: List of the ten Dy^{III} complexes for which the generalized shielding polarizability calculations have been performed. In this Table, the following acronyms have been adopted: acac = acetylacetonate, dppz = dipyridophenazine, dpq = dipyridoquinoxaline, phen = 1,10–phenanthroline, hfac = hexafluoroacetylacetone, dme = dimethoxyethane, paaH* = N–(2–Pyridyl)acetoacetamide, tfpb = 4,4,4–trifluoro–1–phenyl–1,3–butandionate, tta = tetradecylthioacetate, bipy = 2,20–bipyridine, pinene−bipy = 4,5–pinene bipyridine.

ATOMIC UNITS CONVERSION FACTORS

All calculations in the Paper have been performed in atomic units. All conversion factors are extracted from the latest CODATA compilation [11], and are reported hereafter. $1\,\mathrm{ppm\,au}$ of $\bar{\Phi} = 1.944690397 \cdot 10^{-18}\mathrm{m\,V^{-1}}$, $\mu_B = \frac{\alpha}{2}$, with $\alpha = 7.2973525664 \cdot 10^{-3}$, $1\,\mathrm{au}$ of $\mu = 8.478353552 \cdot 10^{-30}\mathrm{C\,m^{-1}} = 2.541746231D$, $1\,\mathrm{au}$ of magnetic dipole moment $= 1.854801999 \cdot 10^{-23}\mathrm{J\,T^{-1}}$, $\beta = (k_BT)^{-1} = 1077.730816919$ for $T = 293\mathrm{K}$, with $k_B = 1.38064852 \cdot 10^{-23}\mathrm{J\,K^{-1}}$, $1a_0 = 0.52917721067\text{Å}$ and $1\mathrm{cm^{-1}} = 4.556335252767 \cdot 10^{-6}E_h$.

CRYSTAL FIELD ENERGIES FOR THE $^6H_{\frac{15}{2}}$ MULTIPLET

KD	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_6	ϵ_7	ϵ_8	ϵ_9	ϵ_{10}
0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1	167.114	160.585	132.818	144.687	118.562	114.832	135.421	149.639	137.060	90.714
2	251.895	240.389	203.068	214.397	166.204	197.379	168.256	165.279	185.713	155.315
3	308.527	279.328	241.492	266.756	197.717	253.659	213.212	206.806	221.888	180.729
4	336.973	323.028	285.131	315.382	229.401	312.313	246.892	240.195	249.418	209.621
5	431.446	366.999	313.903	353.697	273.840	339.187	276.017	309.595	303.290	277.471
6	475.343	450.357	444.832	462.612	346.426	394.822	339.002	417.183	418.623	404.501
7	551.534	522.215	545.131	536.457	460.123	442.516	478.593	471.496	520.697	467.483

TABLE SI-II: Energy levels for the eight KDs arising from the crystal field splitting of the ground state Russell–Saunders term, expressed in cm^{-1}, for the ten Dy^{III} complexes presented in Table SI-I.

STUDY OF THE RELATIVE SIGNS OF PSEUDOSCALAR CONTRIBUTIONS FOR $B_0^{(2)} > 0$ AND $B_2^{(2)} = 0$

In this section, the relative sign of the relevant pseudoscalar contributions to the model Hamiltonian studied in the paper for a purely axial crystal field, with $B_0^{(2)} > 0$, will be derived. The procedure outlined below follows that of the corresponding analysis for $B_0^{(2)} < 0$ introduced in the main paper.

The crystal field states generated by this perturbation, still correspondent to pure M_J states, are arranged into a set of KDs of increasing energy as M_J^2 increases. Within this framework, the ground Kramers Doublet is characterized by a magnetic anisotropy of easy–axis type ($g_{xx} = g_{yy} > 0$, $g_{zz} = 0$), while the other doublets of interest for our analysis are characterized by a purely axial magnetic anisotropy along the z axis ($g_{xx} = g_{yy} = 0$, $g_{zz} > 0$). The transition g–tensor between the ground KD and the first excited KD, introduced in Eq. (42) of the main paper, also displays non–zero g_{xx} and g_{yy} contributions, while it has to be noted that, since the magnetic moment operator only allows M_J–mixing for $\Delta M_J = 0, \pm 1$ [12], given the pure M_J character of the crystal field states under application of a purely axial crystal field, $\boldsymbol{g}_{\frac{1}{2},\frac{5}{2}} = \mathbf{0}$ and, consequently, $\bar{\Phi}^{p(1)}_{\frac{1}{2},\frac{5}{2}} = 0$.

	xx	yy	zz
$g_{\rm g}$	10.67	10.67	1.33
$g_{\rm e}$	0	0	4
$g_{\rm ee}$	0	0	6.67
$g_{\rm g,e}$	10.58	10.58	0

TABLE SI-III: Non–zero values of the g–tensors for $B_0^{(2)} > 0$ and $B_2^{(2)} = 0$. In the Table, the subscripts g, e and ee represent, respectively, the ground, first excited and second excited KD.

Substitution of the non–zero components of the g–tensors into Eqs. (31) and (41) gives:

$$\begin{aligned}\bar{\Phi}^{p(2)}_{\frac{1}{2}} &= \frac{1}{6}\left(\Phi^{p(2)}_{\frac{1}{2},xyz} - \Phi^{p(2)}_{\frac{1}{2},xzy} + \Phi^{p(2)}_{\frac{1}{2},yzx} - \Phi^{p(2)}_{\frac{1}{2},yxz} + \Phi^{p(2)}_{\frac{1}{2},zxy} - \Phi^{p(2)}_{\frac{1}{2},zyx}\right)\\ &= \frac{\beta^2\mu_B^2}{8R^5}\left[\mu_x R_y R_z\left(g_{yy}^2 - g_{zz}^2\right) + \mu_y R_x R_z\left(g_{zz}^2 - g_{xx}^2\right) + \mu_z R_x R_y\left(g_{xx}^2 - g_{yy}^2\right)\right]\\ &= \frac{\beta^2\mu_B^2}{8R^5} R_z\left(R_x\mu_y - R_y\mu_x\right)\left(g^2_{\frac{1}{2},\parallel} - g^2_{\frac{1}{2},\perp}\right) \qquad \text{(SI-XXVI)}\end{aligned}$$

$$\begin{aligned}\bar{\Phi}^{p(2)}_{\frac{3}{2}} &= \frac{1}{6}\left(\Phi^{p(2)}_{\frac{3}{2},zxy} - \Phi^{p(2)}_{\frac{3}{2},zyx}\right)\\ &= \frac{\beta^2\mu_B^2}{8R^5} g^2_{\frac{3}{2},\parallel} R_z\left(R_x\mu_y - R_y\mu_x\right) \qquad \text{(SI-XXVII)}\end{aligned}$$

$$\begin{aligned}\bar{\Phi}^{p(2)}_{\frac{5}{2}} &= \frac{1}{6}\left(\Phi^{p(2)}_{\frac{5}{2},zxy} - \Phi^{p(2)}_{\frac{5}{2},zyx}\right)\\ &= \frac{\beta^2\mu_B^2}{8R^5} g^2_{\frac{5}{2},\parallel} R_z\left(R_x\mu_y - R_y\mu_x\right) \qquad \text{(SI-XXVIII)}\end{aligned}$$

$$\begin{aligned}\bar{\Phi}^{p(1)}_{\frac{1}{2},\frac{3}{2}} &= \frac{1}{6}\left(\Phi^{p(1)}_{\frac{1}{2},\frac{3}{2},xyz} - \Phi^{p(1)}_{\frac{1}{2},\frac{3}{2},xzy} + \Phi^{p(1)}_{\frac{1}{2},\frac{3}{2},yzx} - \Phi^{p(1)}_{\frac{1}{2},\frac{3}{2},yxz}\right)\\ &= \frac{\beta\mu_B^2}{4R^5\left(E_{\frac{3}{2}} - E_{\frac{1}{2}}\right)}\left[g^2_{\frac{1}{2},\frac{3}{2},xx}\left(R_x R_y\mu_z - R_x R_z\mu_y\right) + g^2_{\frac{1}{2},\frac{3}{2},yy}\left(R_y R_z\mu_x - R_y R_x\mu_z\right)\right]\\ &= \frac{\beta\mu_B^2}{4R^5\left(E_{\frac{3}{2}} - E_{\frac{1}{2}}\right)} g^2_{\frac{1}{2},\frac{3}{2},\perp} R_z\left(R_y\mu_x - R_x\mu_y\right) \qquad \text{(SI-XXIX)}\end{aligned}$$

where $g_\perp = g_{xx} = g_{yy}$ and $g_\parallel = g_{zz}$. It is now trivial to observe that, regardless of the position of the probe atom, $\bar{\Phi}^{p(2)}_{\frac{1}{2}}$ and $\bar{\Phi}^{p(1)}_{\frac{1}{2},\frac{3}{2}}$ will always have the same sign, but will always have opposite sign with respect to $\bar{\Phi}^{p(2)}_{\frac{3}{2}}$ and $\bar{\Phi}^{p(2)}_{\frac{5}{2}}$.

TEMPERATURE–DEPENDENT COMPONENTS OF $\bar{\Phi}$ AND INDUCED POLARIZATION AND VOLTAGES

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
H1	$-1.77 \cdot 10^{5}$	$-3.33 \cdot 10^{5}$	$1.56 \cdot 10^{5}$	$1.29 \cdot 10^{2}$	$2.03 \cdot 10^{-16}$	0.37
H2	$-3.40 \cdot 10^{4}$	$-6.16 \cdot 10^{4}$	$2.76 \cdot 10^{4}$	$7.84 \cdot 10^{1}$	$3.89 \cdot 10^{-17}$	0.07
H3	$-1.78 \cdot 10^{5}$	$-3.29 \cdot 10^{5}$	$1.51 \cdot 10^{5}$	$1.44 \cdot 10^{2}$	$2.03 \cdot 10^{-16}$	0.37
H4	$2.23 \cdot 10^{5}$	$4.22 \cdot 10^{5}$	$-1.99 \cdot 10^{5}$	$1.02 \cdot 10^{1}$	$2.56 \cdot 10^{-16}$	0.46
H5	$2.42 \cdot 10^{5}$	$4.50 \cdot 10^{5}$	$-2.08 \cdot 10^{5}$	$-6.07 \cdot 10^{1}$	$2.77 \cdot 10^{-16}$	0.50
H6	$2.32 \cdot 10^{5}$	$4.35 \cdot 10^{5}$	$-2.03 \cdot 10^{5}$	$-6.16 \cdot 10^{1}$	$2.66 \cdot 10^{-16}$	0.48
H7	$2.78 \cdot 10^{5}$	$5.17 \cdot 10^{5}$	$-2.39 \cdot 10^{5}$	$-1.14 \cdot 10^{2}$	$3.18 \cdot 10^{-16}$	0.57
H8	$-7.33 \cdot 10^{2}$	$9.69 \cdot 10^{2}$	$-1.63 \cdot 10^{3}$	$-7.04 \cdot 10^{1}$	$8.40 \cdot 10^{-19}$	0.00
H9	$1.10 \cdot 10^{5}$	$2.08 \cdot 10^{5}$	$-9.87 \cdot 10^{4}$	$-9.86 \cdot 10^{1}$	$1.26 \cdot 10^{-16}$	0.23
H10	$1.80 \cdot 10^{5}$	$3.37 \cdot 10^{5}$	$-1.57 \cdot 10^{5}$	$-1.31 \cdot 10^{2}$	$2.06 \cdot 10^{-16}$	0.37
H11	$1.31 \cdot 10^{5}$	$2.52 \cdot 10^{5}$	$-1.20 \cdot 10^{5}$	$-1.36 \cdot 10^{2}$	$1.50 \cdot 10^{-16}$	0.27
H12	$-2.83 \cdot 10^{4}$	$-5.88 \cdot 10^{4}$	$3.05 \cdot 10^{4}$	$-2.97 \cdot 10^{1}$	$3.24 \cdot 10^{-17}$	0.06
H13	$2.64 \cdot 10^{4}$	$4.95 \cdot 10^{4}$	$-2.31 \cdot 10^{4}$	$-5.16 \cdot 10^{1}$	$3.02 \cdot 10^{-17}$	0.05
H14	$1.50 \cdot 10^{3}$	$2.55 \cdot 10^{3}$	$-1.01 \cdot 10^{3}$	$-4.10 \cdot 10^{1}$	$1.71 \cdot 10^{-18}$	0.00
H15	$3.19 \cdot 10^{5}$	$6.01 \cdot 10^{5}$	$-2.81 \cdot 10^{5}$	$-7.01 \cdot 10^{1}$	$3.66 \cdot 10^{-16}$	0.66
H16	$1.31 \cdot 10^{5}$	$2.47 \cdot 10^{5}$	$-1.16 \cdot 10^{5}$	8.63	$1.50 \cdot 10^{-16}$	0.27
H17	$2.03 \cdot 10^{5}$	$3.84 \cdot 10^{5}$	$-1.80 \cdot 10^{5}$	7.54	$2.33 \cdot 10^{-16}$	0.42
H18	$-9.50 \cdot 10^{4}$	$-1.78 \cdot 10^{5}$	$8.27 \cdot 10^{4}$	$1.15 \cdot 10^{2}$	$1.09 \cdot 10^{-16}$	0.20
H19	$-2.72 \cdot 10^{5}$	$-5.12 \cdot 10^{5}$	$2.41 \cdot 10^{5}$	$1.09 \cdot 10^{2}$	$3.11 \cdot 10^{-16}$	0.56
H20	$-1.87 \cdot 10^{5}$	$-3.55 \cdot 10^{5}$	$1.68 \cdot 10^{5}$	$8.98 \cdot 10^{1}$	$2.15 \cdot 10^{-16}$	0.39
H21	$-2.55 \cdot 10^{5}$	$-4.88 \cdot 10^{5}$	$2.33 \cdot 10^{5}$	$8.90 \cdot 10^{1}$	$2.92 \cdot 10^{-16}$	0.53
H22	$-2.63 \cdot 10^{5}$	$-5.33 \cdot 10^{5}$	$2.70 \cdot 10^{5}$	$1.40 \cdot 10^{1}$	$3.01 \cdot 10^{-16}$	0.54
H23	$1.37 \cdot 10^{5}$	$2.86 \cdot 10^{5}$	$-1.48 \cdot 10^{5}$	$-4.12 \cdot 10^{2}$	$1.57 \cdot 10^{-16}$	0.28
H24	$2.65 \cdot 10^{5}$	$4.47 \cdot 10^{5}$	$-1.82 \cdot 10^{5}$	$-1.34 \cdot 10^{2}$	$3.03 \cdot 10^{-16}$	0.55
H25	$-5.26 \cdot 10^{4}$	$-7.29 \cdot 10^{4}$	$2.05 \cdot 10^{4}$	$-2.33 \cdot 10^{2}$	$6.03 \cdot 10^{-17}$	0.11

TABLE SI-IV: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **1**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$-1.38 \cdot 10^{5}$	$-2.57 \cdot 10^{5}$	$1.18 \cdot 10^{5}$	$1.45 \cdot 10^{2}$	$1.00 \cdot 10^{-17}$	0.02
C2	$-3.61 \cdot 10^{4}$	$-5.75 \cdot 10^{4}$	$2.11 \cdot 10^{4}$	$2.96 \cdot 10^{2}$	$2.62 \cdot 10^{-18}$	0.00
C3	$4.25 \cdot 10^{5}$	$8.03 \cdot 10^{5}$	$-3.78 \cdot 10^{5}$	$2.68 \cdot 10^{1}$	$3.07 \cdot 10^{-17}$	0.06
C4	$9.16 \cdot 10^{5}$	$1.72 \cdot 10^{6}$	$-8.01 \cdot 10^{5}$	$-1.87 \cdot 10^{2}$	$6.63 \cdot 10^{-17}$	0.12
C5	$3.34 \cdot 10^{5}$	$6.23 \cdot 10^{5}$	$-2.89 \cdot 10^{5}$	$-9.71 \cdot 10^{1}$	$2.42 \cdot 10^{-17}$	0.04
C6	$1.18 \cdot 10^{5}$	$2.25 \cdot 10^{5}$	$-1.06 \cdot 10^{5}$	$-1.31 \cdot 10^{2}$	$8.58 \cdot 10^{-18}$	0.02
C7	$2.66 \cdot 10^{5}$	$5.13 \cdot 10^{5}$	$-2.48 \cdot 10^{5}$	$-3.57 \cdot 10^{2}$	$1.92 \cdot 10^{-17}$	0.03
C8	$2.13 \cdot 10^{5}$	$4.12 \cdot 10^{5}$	$-1.99 \cdot 10^{5}$	$-2.55 \cdot 10^{2}$	$1.54 \cdot 10^{-17}$	0.03
C9	$1.07 \cdot 10^{5}$	$2.08 \cdot 10^{5}$	$-1.00 \cdot 10^{5}$	$-2.35 \cdot 10^{2}$	$7.77 \cdot 10^{-18}$	0.01
C10	$1.02 \cdot 10^{4}$	$1.77 \cdot 10^{4}$	$-7.41 \cdot 10^{3}$	$-6.07 \cdot 10^{1}$	$7.41 \cdot 10^{-19}$	0.00
C11	$2.57 \cdot 10^{5}$	$4.85 \cdot 10^{5}$	$-2.28 \cdot 10^{5}$	-7.56	$1.86 \cdot 10^{-17}$	0.03
C12	$3.76 \cdot 10^{5}$	$7.15 \cdot 10^{5}$	$-3.39 \cdot 10^{5}$	$1.39 \cdot 10^{2}$	$2.72 \cdot 10^{-17}$	0.05
C13	$-2.07 \cdot 10^{5}$	$-3.87 \cdot 10^{5}$	$1.80 \cdot 10^{5}$	$2.39 \cdot 10^{2}$	$1.50 \cdot 10^{-17}$	0.03
C14	$-7.84 \cdot 10^{5}$	$-1.48 \cdot 10^{6}$	$6.95 \cdot 10^{5}$	$4.06 \cdot 10^{2}$	$5.68 \cdot 10^{-17}$	0.10
C15	$-3.10 \cdot 10^{5}$	$-5.88 \cdot 10^{5}$	$2.78 \cdot 10^{5}$	$1.32 \cdot 10^{2}$	$2.25 \cdot 10^{-17}$	0.04

TABLE SI-V: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **1**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$-1.46 \cdot 10^{6}$	$-2.73 \cdot 10^{6}$	$1.26 \cdot 10^{6}$	$1.23 \cdot 10^{3}$	$3.60 \cdot 10^{-16}$	0.65
O2	$2.52 \cdot 10^{6}$	$4.69 \cdot 10^{6}$	$-2.17 \cdot 10^{6}$	$-7.38 \cdot 10^{2}$	$6.19 \cdot 10^{-16}$	1.12
O3	$-1.78 \cdot 10^{5}$	$-3.11 \cdot 10^{5}$	$1.33 \cdot 10^{5}$	$-5.97 \cdot 10^{2}$	$4.38 \cdot 10^{-17}$	0.08
O4	$-1.23 \cdot 10^{3}$	$-1.51 \cdot 10^{4}$	$1.42 \cdot 10^{4}$	$-3.96 \cdot 10^{2}$	$3.01 \cdot 10^{-19}$	0.00
O5	$2.02 \cdot 10^{6}$	$3.82 \cdot 10^{6}$	$-1.80 \cdot 10^{6}$	$6.24 \cdot 10^{1}$	$4.97 \cdot 10^{-16}$	0.90
O6	$-2.52 \cdot 10^{6}$	$-4.77 \cdot 10^{6}$	$2.24 \cdot 10^{6}$	$9.78 \cdot 10^{2}$	$6.19 \cdot 10^{-16}$	1.12
O7	$-6.10 \cdot 10^{4}$	$-1.99 \cdot 10^{5}$	$1.39 \cdot 10^{5}$	$-9.47 \cdot 10^{1}$	$1.50 \cdot 10^{-17}$	0.03
O8	$5.40 \cdot 10^{4}$	$1.66 \cdot 10^{5}$	$-1.11 \cdot 10^{5}$	$-6.95 \cdot 10^{2}$	$1.33 \cdot 10^{-17}$	0.02

TABLE SI-VI: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **1**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
H1	$4.70 \cdot 10^{3}$	$6.35 \cdot 10^{3}$	$-1.65 \cdot 10^{3}$	-7.52	$5.38 \cdot 10^{-18}$	0.01
H2	$-1.49 \cdot 10^{3}$	$-1.24 \cdot 10^{3}$	$-2.38 \cdot 10^{2}$	-4.87	$1.70 \cdot 10^{-18}$	0.00
H3	$3.28 \cdot 10^{5}$	$5.46 \cdot 10^{5}$	$-2.18 \cdot 10^{5}$	$-1.23 \cdot 10^{2}$	$3.76 \cdot 10^{-16}$	0.68
H4	$1.04 \cdot 10^{5}$	$1.85 \cdot 10^{5}$	$-8.03 \cdot 10^{4}$	$-5.26 \cdot 10^{1}$	$1.20 \cdot 10^{-16}$	0.22
H5	$1.96 \cdot 10^{5}$	$3.36 \cdot 10^{5}$	$-1.40 \cdot 10^{5}$	$-6.98 \cdot 10^{1}$	$2.25 \cdot 10^{-16}$	0.41
H6	$-3.27 \cdot 10^{3}$	$-2.29 \cdot 10^{3}$	$-9.65 \cdot 10^{2}$	-7.96	$3.74 \cdot 10^{-18}$	0.01
H7	$2.41 \cdot 10^{3}$	$2.15 \cdot 10^{4}$	$-1.90 \cdot 10^{4}$	$-2.97 \cdot 10^{1}$	$2.76 \cdot 10^{-18}$	0.00
H8	$4.50 \cdot 10^{4}$	$5.74 \cdot 10^{4}$	$-1.24 \cdot 10^{4}$	$-1.72 \cdot 10^{1}$	$5.15 \cdot 10^{-17}$	0.09
H9	$1.39 \cdot 10^{5}$	$2.45 \cdot 10^{5}$	$-1.06 \cdot 10^{5}$	$-4.21 \cdot 10^{1}$	$1.59 \cdot 10^{-16}$	0.29
H10	$6.00 \cdot 10^{4}$	$1.23 \cdot 10^{5}$	$-6.31 \cdot 10^{4}$	$-4.10 \cdot 10^{1}$	$6.87 \cdot 10^{-17}$	0.12
H11	$4.94 \cdot 10^{5}$	$8.82 \cdot 10^{5}$	$-3.88 \cdot 10^{5}$	$-1.82 \cdot 10^{2}$	$5.66 \cdot 10^{-16}$	1.02
H12	$5.94 \cdot 10^{2}$	$1.01 \cdot 10^{3}$	$-4.07 \cdot 10^{2}$	-4.71	$6.80 \cdot 10^{-19}$	0.00
H13	$1.27 \cdot 10^{5}$	$1.59 \cdot 10^{5}$	$-3.15 \cdot 10^{4}$	$-3.01 \cdot 10^{1}$	$1.46 \cdot 10^{-16}$	0.26
H14	$1.08 \cdot 10^{5}$	$1.46 \cdot 10^{5}$	$-3.74 \cdot 10^{4}$	$-1.14 \cdot 10^{1}$	$1.24 \cdot 10^{-16}$	0.22
H15	$-1.40 \cdot 10^{4}$	$-7.28 \cdot 10^{3}$	$-6.61 \cdot 10^{3}$	$-6.94 \cdot 10^{1}$	$1.60 \cdot 10^{-17}$	0.03
H16	$1.33 \cdot 10^{4}$	$2.24 \cdot 10^{4}$	$-9.05 \cdot 10^{3}$	$-5.55 \cdot 10^{1}$	$1.53 \cdot 10^{-17}$	0.03
H17	$3.41 \cdot 10^{3}$	$-7.37 \cdot 10^{3}$	$1.08 \cdot 10^{4}$	$-2.74 \cdot 10^{1}$	$3.90 \cdot 10^{-18}$	0.01
H18	$-2.67 \cdot 10^{5}$	$-4.12 \cdot 10^{5}$	$1.46 \cdot 10^{5}$	$7.25 \cdot 10^{1}$	$3.05 \cdot 10^{-16}$	0.55
H19	$-8.31 \cdot 10^{4}$	$-1.21 \cdot 10^{5}$	$3.82 \cdot 10^{4}$	$2.04 \cdot 10^{1}$	$9.52 \cdot 10^{-17}$	0.17
H20	$-2.29 \cdot 10^{5}$	$-3.71 \cdot 10^{5}$	$1.41 \cdot 10^{5}$	$9.70 \cdot 10^{1}$	$2.63 \cdot 10^{-16}$	0.47
H21	$2.50 \cdot 10^{5}$	$4.39 \cdot 10^{5}$	$-1.89 \cdot 10^{5}$	$-1.01 \cdot 10^{2}$	$2.86 \cdot 10^{-16}$	0.52
H22	$2.10 \cdot 10^{5}$	$3.60 \cdot 10^{5}$	$-1.50 \cdot 10^{5}$	$-7.20 \cdot 10^{1}$	$2.40 \cdot 10^{-16}$	0.43
H23	$3.04 \cdot 10^{5}$	$5.16 \cdot 10^{5}$	$-2.12 \cdot 10^{5}$	$-1.00 \cdot 10^{2}$	$3.48 \cdot 10^{-16}$	0.63
H24	$4.47 \cdot 10^{5}$	$6.20 \cdot 10^{5}$	$-1.72 \cdot 10^{5}$	-9.85	$5.12 \cdot 10^{-16}$	0.93
H25	$-3.35 \cdot 10^{5}$	$-5.50 \cdot 10^{5}$	$2.15 \cdot 10^{5}$	$1.51 \cdot 10^{2}$	$3.83 \cdot 10^{-16}$	0.69
H26	$-2.73 \cdot 10^{5}$	$-4.46 \cdot 10^{5}$	$1.73 \cdot 10^{5}$	$1.16 \cdot 10^{2}$	$3.13 \cdot 10^{-16}$	0.56
H27	$-2.79 \cdot 10^{5}$	$-4.38 \cdot 10^{5}$	$1.59 \cdot 10^{5}$	$8.64 \cdot 10^{1}$	$3.20 \cdot 10^{-16}$	0.58
H28	$-2.03 \cdot 10^{5}$	$-3.06 \cdot 10^{5}$	$1.03 \cdot 10^{5}$	$4.87 \cdot 10^{1}$	$2.32 \cdot 10^{-16}$	0.42
H29	$-2.39 \cdot 10^{4}$	$-7.78 \cdot 10^{4}$	$5.39 \cdot 10^{4}$	$7.69 \cdot 10^{1}$	$2.73 \cdot 10^{-17}$	0.05
H30	$5.92 \cdot 10^{4}$	$6.06 \cdot 10^{4}$	$-1.42 \cdot 10^{3}$	$2.35 \cdot 10^{1}$	$6.78 \cdot 10^{-17}$	0.12
H31	$1.90 \cdot 10^{5}$	$2.81 \cdot 10^{5}$	$-9.14 \cdot 10^{4}$	$-1.57 \cdot 10^{1}$	$2.17 \cdot 10^{-16}$	0.39

TABLE SI-VII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **2**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$6.83 \cdot 10^{4}$	$7.56 \cdot 10^{4}$	$-7.20 \cdot 10^{3}$	$-1.32 \cdot 10^{2}$	$4.95 \cdot 10^{-18}$	0.01
C2	$2.22 \cdot 10^{3}$	$3.17 \cdot 10^{3}$	$-9.43 \cdot 10^{2}$	-8.15	$1.61 \cdot 10^{-19}$	0.00
C3	$1.11 \cdot 10^{3}$	$2.00 \cdot 10^{3}$	$-8.78 \cdot 10^{2}$	$-1.27 \cdot 10^{1}$	$8.02 \cdot 10^{-20}$	0.00
C4	$4.64 \cdot 10^{4}$	$5.61 \cdot 10^{4}$	$-9.61 \cdot 10^{3}$	$-5.19 \cdot 10^{1}$	$3.36 \cdot 10^{-18}$	0.01
C5	$-1.56 \cdot 10^{3}$	$-1.31 \cdot 10^{3}$	$-2.50 \cdot 10^{2}$	-6.12	$1.13 \cdot 10^{-19}$	0.00
C6	$2.39 \cdot 10^{5}$	$4.09 \cdot 10^{5}$	$-1.70 \cdot 10^{5}$	$-9.60 \cdot 10^{1}$	$1.73 \cdot 10^{-17}$	0.03
C7	$-2.82 \cdot 10^{5}$	$-4.09 \cdot 10^{5}$	$1.28 \cdot 10^{5}$	$8.80 \cdot 10^{1}$	$2.04 \cdot 10^{-17}$	0.04
C8	$9.19 \cdot 10^{5}$	$1.57 \cdot 10^{6}$	$-6.50 \cdot 10^{5}$	$-3.10 \cdot 10^{2}$	$6.66 \cdot 10^{-17}$	0.12
C9	$2.30 \cdot 10^{5}$	$2.19 \cdot 10^{5}$	$1.01 \cdot 10^{4}$	$9.46 \cdot 10^{1}$	$1.66 \cdot 10^{-17}$	0.03
C10	$-2.97 \cdot 10^{3}$	$-2.43 \cdot 10^{3}$	$-5.30 \cdot 10^{2}$	-8.46	$2.15 \cdot 10^{-19}$	0.00
C11	$-9.90 \cdot 10^{3}$	$-7.67 \cdot 10^{3}$	$-2.20 \cdot 10^{3}$	$-3.46 \cdot 10^{1}$	$7.17 \cdot 10^{-19}$	0.00
C12	$-1.95 \cdot 10^{4}$	$-4.05 \cdot 10^{3}$	$-1.54 \cdot 10^{4}$	$-6.61 \cdot 10^{1}$	$1.41 \cdot 10^{-18}$	0.00
C13	$4.43 \cdot 10^{3}$	$3.56 \cdot 10^{4}$	$-3.11 \cdot 10^{4}$	$-4.84 \cdot 10^{1}$	$3.20 \cdot 10^{-19}$	0.00
C14	$7.15 \cdot 10^{4}$	$9.05 \cdot 10^{4}$	$-1.90 \cdot 10^{4}$	$-2.70 \cdot 10^{1}$	$5.17 \cdot 10^{-18}$	0.01
C15	$-1.06 \cdot 10^{6}$	$-1.70 \cdot 10^{6}$	$6.42 \cdot 10^{5}$	$3.99 \cdot 10^{2}$	$7.67 \cdot 10^{-17}$	0.14
C16	$6.58 \cdot 10^{3}$	$8.91 \cdot 10^{3}$	$-2.29 \cdot 10^{3}$	$-3.22 \cdot 10^{1}$	$4.77 \cdot 10^{-19}$	0.00
C17	$-4.15 \cdot 10^{4}$	$-1.14 \cdot 10^{4}$	$-2.99 \cdot 10^{4}$	$-1.73 \cdot 10^{2}$	$3.00 \cdot 10^{-18}$	0.01
C18	$2.82 \cdot 10^{5}$	$4.97 \cdot 10^{5}$	$-2.15 \cdot 10^{5}$	$-8.84 \cdot 10^{1}$	$2.04 \cdot 10^{-17}$	0.04
C19	$-3.74 \cdot 10^{3}$	$-3.12 \cdot 10^{3}$	$-6.08 \cdot 10^{2}$	$-1.32 \cdot 10^{1}$	$2.71 \cdot 10^{-19}$	0.00
C20	$5.97 \cdot 10^{4}$	$1.38 \cdot 10^{5}$	$-7.83 \cdot 10^{4}$	$-6.46 \cdot 10^{1}$	$4.32 \cdot 10^{-18}$	0.01
C21	$2.58 \cdot 10^{5}$	$4.82 \cdot 10^{5}$	$-2.24 \cdot 10^{5}$	$-1.28 \cdot 10^{2}$	$1.87 \cdot 10^{-17}$	0.03
C22	$1.03 \cdot 10^{5}$	$1.05 \cdot 10^{5}$	$-2.25 \cdot 10^{3}$	$-1.42 \cdot 10^{2}$	$7.45 \cdot 10^{-18}$	0.01
C23	$2.50 \cdot 10^{5}$	$5.11 \cdot 10^{5}$	$-2.61 \cdot 10^{5}$	$-1.80 \cdot 10^{2}$	$1.81 \cdot 10^{-17}$	0.03
C24	$1.64 \cdot 10^{2}$	$5.55 \cdot 10^{2}$	$-3.85 \cdot 10^{2}$	-5.96	$1.19 \cdot 10^{-20}$	0.00
C25	$2.06 \cdot 10^{5}$	$2.34 \cdot 10^{5}$	$-2.81 \cdot 10^{4}$	$-3.35 \cdot 10^{1}$	$1.49 \cdot 10^{-17}$	0.03
C26	$1.42 \cdot 10^{5}$	$1.87 \cdot 10^{5}$	$-4.43 \cdot 10^{4}$	$-2.26 \cdot 10^{1}$	$1.03 \cdot 10^{-17}$	0.02
C27	$7.29 \cdot 10^{3}$	$8.10 \cdot 10^{3}$	$-7.50 \cdot 10^{2}$	$-6.32 \cdot 10^{1}$	$5.28 \cdot 10^{-19}$	0.00
C28	$-2.24 \cdot 10^{5}$	$-3.47 \cdot 10^{5}$	$1.24 \cdot 10^{5}$	$7.35 \cdot 10^{1}$	$1.62 \cdot 10^{-17}$	0.03
C29	$3.37 \cdot 10^{5}$	$5.80 \cdot 10^{5}$	$-2.42 \cdot 10^{5}$	$-1.19 \cdot 10^{2}$	$2.44 \cdot 10^{-17}$	0.04
C30	$3.82 \cdot 10^{5}$	$5.01 \cdot 10^{5}$	$-1.19 \cdot 10^{5}$	$-3.75 \cdot 10^{1}$	$2.77 \cdot 10^{-17}$	0.05
C31	$-3.91 \cdot 10^{5}$	$-6.32 \cdot 10^{5}$	$2.40 \cdot 10^{5}$	$1.53 \cdot 10^{2}$	$2.83 \cdot 10^{-17}$	0.05
C32	$-4.07 \cdot 10^{5}$	$-6.20 \cdot 10^{5}$	$2.13 \cdot 10^{5}$	$1.12 \cdot 10^{2}$	$2.95 \cdot 10^{-17}$	0.05
C33	$9.65 \cdot 10^{4}$	$1.09 \cdot 10^{5}$	$-1.28 \cdot 10^{4}$	$3.70 \cdot 10^{1}$	$6.98 \cdot 10^{-18}$	0.01

TABLE SI-VIII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **2**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
O1	$-3.86 \cdot 10^{4}$	$-1.86 \cdot 10^{4}$	$-1.94 \cdot 10^{4}$	$-5.34 \cdot 10^{2}$	$9.48 \cdot 10^{-18}$	0.02
O2	$2.83 \cdot 10^{6}$	$4.83 \cdot 10^{6}$	$-2.00 \cdot 10^{6}$	$-9.58 \cdot 10^{2}$	$6.96 \cdot 10^{-16}$	1.26
O3	$-2.01 \cdot 10^{6}$	$-3.10 \cdot 10^{6}$	$1.09 \cdot 10^{6}$	$5.78 \cdot 10^{2}$	$4.93 \cdot 10^{-16}$	0.89
O4	$2.13 \cdot 10^{6}$	$3.64 \cdot 10^{6}$	$-1.51 \cdot 10^{6}$	$-7.58 \cdot 10^{2}$	$5.24 \cdot 10^{-16}$	0.95
O5	$-1.83 \cdot 10^{5}$	$-6.85 \cdot 10^{5}$	$5.01 \cdot 10^{5}$	$6.79 \cdot 10^{2}$	$4.50 \cdot 10^{-17}$	0.08
O6	$-3.08 \cdot 10^{6}$	$-5.09 \cdot 10^{6}$	$2.01 \cdot 10^{6}$	$1.40 \cdot 10^{3}$	$7.56 \cdot 10^{-16}$	1.37
N1	$5.59 \cdot 10^{5}$	$6.59 \cdot 10^{5}$	$-9.95 \cdot 10^{4}$	$-1.87 \cdot 10^{2}$	$8.92 \cdot 10^{-18}$	0.02
N2	$1.58 \cdot 10^{5}$	$4.98 \cdot 10^{5}$	$-3.40 \cdot 10^{5}$	$-4.59 \cdot 10^{2}$	$2.51 \cdot 10^{-18}$	0.00
N3	$8.21 \cdot 10^{3}$	$1.08 \cdot 10^{4}$	$-2.55 \cdot 10^{3}$	$-1.80 \cdot 10^{1}$	$1.31 \cdot 10^{-19}$	0.00
N4	$-7.46 \cdot 10^{3}$	$-5.46 \cdot 10^{3}$	$-1.98 \cdot 10^{3}$	$-2.01 \cdot 10^{1}$	$1.19 \cdot 10^{-19}$	0.00

TABLE SI-IX: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **2**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
H1	$-1.84 \cdot 10^{5}$	$-1.63 \cdot 10^{5}$	$-2.15 \cdot 10^{4}$	$1.60 \cdot 10^{2}$	$2.11 \cdot 10^{-16}$	0.38
H2	$-6.81 \cdot 10^{4}$	$-6.23 \cdot 10^{4}$	$-5.83 \cdot 10^{3}$	$1.92 \cdot 10^{1}$	$7.80 \cdot 10^{-17}$	0.14
H3	$-4.08 \cdot 10^{4}$	$-3.04 \cdot 10^{4}$	$-1.04 \cdot 10^{4}$	-6.34	$4.67 \cdot 10^{-17}$	0.08
H4	$-4.71 \cdot 10^{3}$	$-5.72 \cdot 10^{2}$	$-4.14 \cdot 10^{3}$	-3.63	$5.40 \cdot 10^{-18}$	0.01
H5	$1.09 \cdot 10^{3}$	$2.52 \cdot 10^{3}$	$-1.42 \cdot 10^{3}$	-2.75	$1.25 \cdot 10^{-18}$	0.00
H6	$3.29 \cdot 10^{4}$	$2.26 \cdot 10^{4}$	$1.03 \cdot 10^{4}$	$8.58 \cdot 10^{-1}$	$3.77 \cdot 10^{-17}$	0.07
H7	$6.38 \cdot 10^{4}$	$4.14 \cdot 10^{4}$	$2.24 \cdot 10^{4}$	$2.57 \cdot 10^{1}$	$7.31 \cdot 10^{-17}$	0.13
H8	$1.57 \cdot 10^{5}$	$3.42 \cdot 10^{4}$	$1.22 \cdot 10^{5}$	$1.89 \cdot 10^{2}$	$1.79 \cdot 10^{-16}$	0.32
H9	$-3.28 \cdot 10^{5}$	$-5.53 \cdot 10^{5}$	$2.24 \cdot 10^{5}$	$8.51 \cdot 10^{1}$	$3.76 \cdot 10^{-16}$	0.68
H10	$-1.67 \cdot 10^{5}$	$-2.67 \cdot 10^{5}$	$1.00 \cdot 10^{5}$	$3.82 \cdot 10^{1}$	$1.91 \cdot 10^{-16}$	0.34
H11	$-2.25 \cdot 10^{5}$	$-3.94 \cdot 10^{5}$	$1.69 \cdot 10^{5}$	$-2.38 \cdot 10^{1}$	$2.58 \cdot 10^{-16}$	0.47
H12	$5.26 \cdot 10^{4}$	$1.18 \cdot 10^{5}$	$-6.54 \cdot 10^{4}$	$-1.44 \cdot 10^{1}$	$6.02 \cdot 10^{-17}$	0.11
H13	$3.26 \cdot 10^{5}$	$5.28 \cdot 10^{5}$	$-2.02 \cdot 10^{5}$	$-4.43 \cdot 10^{1}$	$3.73 \cdot 10^{-16}$	0.67
H14	$1.93 \cdot 10^{5}$	$3.55 \cdot 10^{5}$	$-1.63 \cdot 10^{5}$	-1.95	$2.21 \cdot 10^{-16}$	0.40
H15	$2.83 \cdot 10^{5}$	$5.49 \cdot 10^{5}$	$-2.66 \cdot 10^{5}$	$4.33 \cdot 10^{1}$	$3.24 \cdot 10^{-16}$	0.59
H16	$-2.10 \cdot 10^{5}$	$-3.80 \cdot 10^{5}$	$1.70 \cdot 10^{5}$	$1.03 \cdot 10^{2}$	$2.41 \cdot 10^{-16}$	0.43
H17	$-2.21 \cdot 10^{5}$	$-3.81 \cdot 10^{5}$	$1.60 \cdot 10^{5}$	$9.24 \cdot 10^{1}$	$2.53 \cdot 10^{-16}$	0.46
H18	$-1.87 \cdot 10^{5}$	$-3.54 \cdot 10^{5}$	$1.66 \cdot 10^{5}$	$1.44 \cdot 10^{2}$	$2.14 \cdot 10^{-16}$	0.39
H19	$-3.24 \cdot 10^{5}$	$-5.57 \cdot 10^{5}$	$2.33 \cdot 10^{5}$	9.53	$3.71 \cdot 10^{-16}$	0.67
H20	$-5.72 \cdot 10^{2}$	$1.56 \cdot 10^{5}$	$-1.57 \cdot 10^{5}$	$8.20 \cdot 10^{1}$	$6.55 \cdot 10^{-19}$	0.00
H21	$1.11 \cdot 10^{5}$	$1.35 \cdot 10^{5}$	$-2.43 \cdot 10^{4}$	$-1.37 \cdot 10^{2}$	$1.27 \cdot 10^{-16}$	0.23
H22	$-5.72 \cdot 10^{4}$	$-1.32 \cdot 10^{5}$	$7.48 \cdot 10^{4}$	$-9.64 \cdot 10^{1}$	$6.55 \cdot 10^{-17}$	0.12
H23	$4.65 \cdot 10^{4}$	$-1.31 \cdot 10^{4}$	$5.98 \cdot 10^{4}$	$-2.14 \cdot 10^{2}$	$5.32 \cdot 10^{-17}$	0.10
H24	$1.31 \cdot 10^{5}$	$2.57 \cdot 10^{5}$	$-1.26 \cdot 10^{5}$	$6.66 \cdot 10^{1}$	$1.50 \cdot 10^{-16}$	0.27
H25	$5.88 \cdot 10^{4}$	$1.71 \cdot 10^{5}$	$-1.12 \cdot 10^{5}$	$5.30 \cdot 10^{1}$	$6.73 \cdot 10^{-17}$	0.12
H26	$2.09 \cdot 10^{5}$	$4.18 \cdot 10^{5}$	$-2.09 \cdot 10^{5}$	$5.26 \cdot 10^{1}$	$2.39 \cdot 10^{-16}$	0.43
H27	$-2.66 \cdot 10^{4}$	$1.38 \cdot 10^{4}$	$-4.05 \cdot 10^{4}$	$3.82 \cdot 10^{1}$	$3.05 \cdot 10^{-17}$	0.06
H28	$-2.13 \cdot 10^{4}$	$-1.56 \cdot 10^{4}$	$-5.71 \cdot 10^{3}$	$-4.87 \cdot 10^{1}$	$2.44 \cdot 10^{-17}$	0.04
H29	$2.81 \cdot 10^{4}$	$3.06 \cdot 10^{4}$	$-2.48 \cdot 10^{3}$	$-3.75 \cdot 10^{1}$	$3.21 \cdot 10^{-17}$	0.06

TABLE SI-X: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **3**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$-2.48 \cdot 10^{5}$	$-1.97 \cdot 10^{5}$	$-5.17 \cdot 10^{4}$	$7.11 \cdot 10^{1}$	$1.80 \cdot 10^{-17}$	0.03
C2	$-1.01 \cdot 10^{5}$	$-8.27 \cdot 10^{4}$	$-1.78 \cdot 10^{4}$	$1.41 \cdot 10^{1}$	$7.28 \cdot 10^{-18}$	0.01
C3	$-6.47 \cdot 10^{4}$	$-4.64 \cdot 10^{4}$	$-1.82 \cdot 10^{4}$	-9.30	$4.68 \cdot 10^{-18}$	0.01
C4	$-5.65 \cdot 10^{4}$	$-2.90 \cdot 10^{4}$	$-2.74 \cdot 10^{4}$	$-2.84 \cdot 10^{1}$	$4.09 \cdot 10^{-18}$	0.01
C5	$-1.58 \cdot 10^{4}$	$-3.15 \cdot 10^{3}$	$-1.26 \cdot 10^{4}$	$-1.64 \cdot 10^{1}$	$1.14 \cdot 10^{-18}$	0.00
C6	$-5.08 \cdot 10^{3}$	$-1.11 \cdot 10^{2}$	$-4.96 \cdot 10^{3}$	-5.17	$3.67 \cdot 10^{-19}$	0.00
C7	$3.53 \cdot 10^{2}$	$2.88 \cdot 10^{3}$	$-2.52 \cdot 10^{3}$	-4.47	$2.55 \cdot 10^{-20}$	0.00
C8	$5.19 \cdot 10^{3}$	$9.58 \cdot 10^{3}$	$-4.38 \cdot 10^{3}$	$-1.41 \cdot 10^{1}$	$3.76 \cdot 10^{-19}$	0.00
C9	$4.01 \cdot 10^{4}$	$3.42 \cdot 10^{4}$	$5.87 \cdot 10^{3}$	$-1.91 \cdot 10^{1}$	$2.90 \cdot 10^{-18}$	0.01
C10	$5.32 \cdot 10^{4}$	$3.66 \cdot 10^{4}$	$1.66 \cdot 10^{4}$	1.18	$3.85 \cdot 10^{-18}$	0.01
C11	$8.96 \cdot 10^{4}$	$5.64 \cdot 10^{4}$	$3.31 \cdot 10^{4}$	$2.70 \cdot 10^{1}$	$6.48 \cdot 10^{-18}$	0.01
C12	$2.12 \cdot 10^{5}$	$1.10 \cdot 10^{5}$	$1.03 \cdot 10^{5}$	$1.07 \cdot 10^{2}$	$1.54 \cdot 10^{-17}$	0.03
C13	$6.97 \cdot 10^{4}$	$7.11 \cdot 10^{4}$	$-1.31 \cdot 10^{3}$	$-6.28 \cdot 10^{1}$	$5.05 \cdot 10^{-18}$	0.01
C14	$-1.14 \cdot 10^{5}$	$-4.88 \cdot 10^{4}$	$-6.49 \cdot 10^{4}$	$-8.60 \cdot 10^{1}$	$8.24 \cdot 10^{-18}$	0.01
C15	$-2.93 \cdot 10^{5}$	$-4.92 \cdot 10^{5}$	$1.99 \cdot 10^{5}$	$3.53 \cdot 10^{1}$	$2.12 \cdot 10^{-17}$	0.04
C16	$-5.46 \cdot 10^{5}$	$-8.98 \cdot 10^{5}$	$3.52 \cdot 10^{5}$	$2.27 \cdot 10^{1}$	$3.95 \cdot 10^{-17}$	0.07
C17	$1.01 \cdot 10^{5}$	$2.19 \cdot 10^{5}$	$-1.18 \cdot 10^{5}$	$-4.07 \cdot 10^{1}$	$7.34 \cdot 10^{-18}$	0.01
C18	$7.73 \cdot 10^{5}$	$1.37 \cdot 10^{6}$	$-5.94 \cdot 10^{5}$	$-9.10 \cdot 10^{1}$	$5.59 \cdot 10^{-17}$	0.10
C19	$3.41 \cdot 10^{5}$	$6.07 \cdot 10^{5}$	$-2.66 \cdot 10^{5}$	-8.34	$2.47 \cdot 10^{-17}$	0.04
C20	$-2.91 \cdot 10^{5}$	$-5.18 \cdot 10^{5}$	$2.27 \cdot 10^{5}$	$1.45 \cdot 10^{2}$	$2.11 \cdot 10^{-17}$	0.04
C21	$-9.48 \cdot 10^{5}$	$-1.63 \cdot 10^{6}$	$6.82 \cdot 10^{5}$	$3.32 \cdot 10^{2}$	$6.86 \cdot 10^{-17}$	0.12
C22	$-6.28 \cdot 10^{5}$	$-1.08 \cdot 10^{6}$	$4.51 \cdot 10^{5}$	$2.20 \cdot 10^{1}$	$4.55 \cdot 10^{-17}$	0.08
C23	$-3.34 \cdot 10^{5}$	$-6.83 \cdot 10^{5}$	$3.49 \cdot 10^{5}$	$-3.34 \cdot 10^{2}$	$2.42 \cdot 10^{-17}$	0.04
C24	$-1.25 \cdot 10^{5}$	$3.32 \cdot 10^{4}$	$-1.58 \cdot 10^{5}$	$2.05 \cdot 10^{1}$	$9.03 \cdot 10^{-18}$	0.02
C25	$-1.89 \cdot 10^{4}$	$2.64 \cdot 10^{5}$	$-2.83 \cdot 10^{5}$	$1.42 \cdot 10^{2}$	$1.37 \cdot 10^{-18}$	0.00
C26	$2.43 \cdot 10^{5}$	$7.47 \cdot 10^{5}$	$-5.04 \cdot 10^{5}$	$2.28 \cdot 10^{2}$	$1.76 \cdot 10^{-17}$	0.03
C27	$9.65 \cdot 10^{3}$	$-5.47 \cdot 10^{4}$	$6.45 \cdot 10^{4}$	$-1.81 \cdot 10^{2}$	$6.99 \cdot 10^{-19}$	0.00
C28	$1.58 \cdot 10^{5}$	$3.53 \cdot 10^{5}$	$-1.95 \cdot 10^{5}$	$7.72 \cdot 10^{1}$	$1.14 \cdot 10^{-17}$	0.02
C29	$-2.02 \cdot 10^{4}$	$7.94 \cdot 10^{3}$	$-2.81 \cdot 10^{4}$	$-1.50 \cdot 10^{1}$	$1.46 \cdot 10^{-18}$	0.00

TABLE SI-XI: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **3**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
O1	$6.82 \cdot 10^{5}$	$5.47 \cdot 10^{5}$	$1.37 \cdot 10^{5}$	$-1.50 \cdot 10^{3}$	$1.68 \cdot 10^{-16}$	0.30
O2	$-2.02 \cdot 10^{6}$	$-3.68 \cdot 10^{6}$	$1.66 \cdot 10^{6}$	$1.19 \cdot 10^{3}$	$4.96 \cdot 10^{-16}$	0.90
O3	$5.81 \cdot 10^{3}$	$2.95 \cdot 10^{4}$	$-2.31 \cdot 10^{4}$	$-6.08 \cdot 10^{2}$	$1.43 \cdot 10^{-18}$	0.00
O4	$1.18 \cdot 10^{6}$	$2.49 \cdot 10^{6}$	$-1.31 \cdot 10^{6}$	$5.80 \cdot 10^{2}$	$2.91 \cdot 10^{-16}$	0.53
O5	$-2.51 \cdot 10^{6}$	$-4.28 \cdot 10^{6}$	$1.77 \cdot 10^{6}$	$2.29 \cdot 10^{2}$	$6.17 \cdot 10^{-16}$	1.11
O6	$3.06 \cdot 10^{6}$	$5.08 \cdot 10^{6}$	$-2.02 \cdot 10^{6}$	$-3.46 \cdot 10^{2}$	$7.52 \cdot 10^{-16}$	1.36
N1	$-5.38 \cdot 10^{5}$	$-3.40 \cdot 10^{5}$	$-1.98 \cdot 10^{5}$	$-6.00 \cdot 10^{1}$	$8.59 \cdot 10^{-18}$	0.02
N2	$4.23 \cdot 10^{5}$	$2.61 \cdot 10^{5}$	$1.62 \cdot 10^{5}$	$5.37 \cdot 10^{1}$	$6.74 \cdot 10^{-18}$	0.01
N3	$-1.27 \cdot 10^{4}$	$-3.92 \cdot 10^{3}$	$-8.73 \cdot 10^{3}$	-7.93	$2.02 \cdot 10^{-19}$	0.00
N4	$6.22 \cdot 10^{3}$	$6.98 \cdot 10^{3}$	$-7.63 \cdot 10^{2}$	-5.80	$9.91 \cdot 10^{-20}$	0.00

TABLE SI-XII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **3**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
H1	$-3.74 \cdot 10^{5}$	$-6.39 \cdot 10^{5}$	$2.64 \cdot 10^{5}$	$1.97 \cdot 10^{2}$	$4.28 \cdot 10^{-16}$	0.77
H2	$-2.17 \cdot 10^{4}$	$-5.72 \cdot 10^{4}$	$3.56 \cdot 10^{4}$	$4.29 \cdot 10^{1}$	$2.48 \cdot 10^{-17}$	0.04
H3	$1.98 \cdot 10^{4}$	$8.02 \cdot 10^{3}$	$1.17 \cdot 10^{4}$	$2.22 \cdot 10^{1}$	$2.26 \cdot 10^{-17}$	0.04
H4	$1.38 \cdot 10^{4}$	$7.27 \cdot 10^{3}$	$6.50 \cdot 10^{3}$	$1.16 \cdot 10^{1}$	$1.58 \cdot 10^{-17}$	0.03
H5	$-6.74 \cdot 10^{3}$	$-1.29 \cdot 10^{4}$	$6.10 \cdot 10^{3}$	8.64	$7.72 \cdot 10^{-18}$	0.01
H6	$-4.06 \cdot 10^{4}$	$-4.55 \cdot 10^{4}$	$4.93 \cdot 10^{3}$	$1.04 \cdot 10^{1}$	$4.65 \cdot 10^{-17}$	0.08
H7	$-7.48 \cdot 10^{4}$	$-6.95 \cdot 10^{4}$	$-5.26 \cdot 10^{3}$	$1.91 \cdot 10^{1}$	$8.56 \cdot 10^{-17}$	0.15
H8	$-2.46 \cdot 10^{5}$	$-1.76 \cdot 10^{5}$	$-6.98 \cdot 10^{4}$	$8.32 \cdot 10^{1}$	$2.81 \cdot 10^{-16}$	0.51
H9	$-2.56 \cdot 10^{5}$	$-4.54 \cdot 10^{5}$	$1.98 \cdot 10^{5}$	$-1.63 \cdot 10^{1}$	$2.93 \cdot 10^{-16}$	0.53
H10	$-1.83 \cdot 10^{5}$	$-3.50 \cdot 10^{5}$	$1.66 \cdot 10^{5}$	$-9.64 \cdot 10^{1}$	$2.10 \cdot 10^{-16}$	0.38
H11	$-4.45 \cdot 10^{5}$	$-7.71 \cdot 10^{5}$	$3.26 \cdot 10^{5}$	$-6.15 \cdot 10^{1}$	$5.09 \cdot 10^{-16}$	0.92
H12	$1.68 \cdot 10^{5}$	$2.25 \cdot 10^{5}$	$-5.67 \cdot 10^{4}$	$-1.52 \cdot 10^{2}$	$1.92 \cdot 10^{-16}$	0.35
H13	$4.42 \cdot 10^{5}$	$7.42 \cdot 10^{5}$	$-3.00 \cdot 10^{5}$	$-9.30 \cdot 10^{1}$	$5.06 \cdot 10^{-16}$	0.91
H14	$3.04 \cdot 10^{5}$	$5.00 \cdot 10^{5}$	$-1.96 \cdot 10^{5}$	$-8.16 \cdot 10^{1}$	$3.48 \cdot 10^{-16}$	0.63
H15	$3.86 \cdot 10^{5}$	$6.91 \cdot 10^{5}$	$-3.05 \cdot 10^{5}$	$-2.40 \cdot 10^{1}$	$4.42 \cdot 10^{-16}$	0.80
H16	$-1.37 \cdot 10^{5}$	$-1.56 \cdot 10^{5}$	$1.98 \cdot 10^{4}$	$2.70 \cdot 10^{1}$	$1.56 \cdot 10^{-16}$	0.28
H17	$3.01 \cdot 10^{3}$	$7.89 \cdot 10^{4}$	$-7.59 \cdot 10^{4}$	$3.25 \cdot 10^{1}$	$3.45 \cdot 10^{-18}$	0.01
H18	$1.41 \cdot 10^{5}$	$3.24 \cdot 10^{5}$	$-1.83 \cdot 10^{5}$	$2.51 \cdot 10^{1}$	$1.61 \cdot 10^{-16}$	0.29
H19	$-1.43 \cdot 10^{5}$	$-1.72 \cdot 10^{5}$	$2.91 \cdot 10^{4}$	$1.58 \cdot 10^{1}$	$1.64 \cdot 10^{-16}$	0.30
H20	$1.09 \cdot 10^{4}$	$-5.40 \cdot 10^{3}$	$1.63 \cdot 10^{4}$	$1.94 \cdot 10^{1}$	$1.25 \cdot 10^{-17}$	0.02
H21	$-4.25 \cdot 10^{4}$	$-8.50 \cdot 10^{4}$	$4.25 \cdot 10^{4}$	$-3.16 \cdot 10^{1}$	$4.87 \cdot 10^{-17}$	0.09
H22	$4.38 \cdot 10^{4}$	4.60	$4.39 \cdot 10^{4}$	$-1.10 \cdot 10^{2}$	$5.02 \cdot 10^{-17}$	0.09
H23	$1.62 \cdot 10^{5}$	$2.03 \cdot 10^{5}$	$-4.03 \cdot 10^{4}$	$-1.74 \cdot 10^{2}$	$1.86 \cdot 10^{-16}$	0.34
H24	$-3.28 \cdot 10^{4}$	$-1.16 \cdot 10^{5}$	$8.36 \cdot 10^{4}$	$-1.48 \cdot 10^{2}$	$3.76 \cdot 10^{-17}$	0.07
H25	$1.40 \cdot 10^{5}$	$1.25 \cdot 10^{5}$	$1.46 \cdot 10^{4}$	$-2.41 \cdot 10^{2}$	$1.60 \cdot 10^{-16}$	0.29
H26	$-3.67 \cdot 10^{5}$	$-6.58 \cdot 10^{5}$	$2.91 \cdot 10^{5}$	$-8.40 \cdot 10^{1}$	$4.21 \cdot 10^{-16}$	0.76
H27	$-3.54 \cdot 10^{5}$	$-5.81 \cdot 10^{5}$	$2.27 \cdot 10^{5}$	$5.65 \cdot 10^{1}$	$4.06 \cdot 10^{-16}$	0.73
H28	$-3.05 \cdot 10^{5}$	$-5.16 \cdot 10^{5}$	$2.11 \cdot 10^{5}$	$4.15 \cdot 10^{1}$	$3.49 \cdot 10^{-16}$	0.63
H29	$-3.42 \cdot 10^{5}$	$-5.79 \cdot 10^{5}$	$2.37 \cdot 10^{5}$	$1.17 \cdot 10^{2}$	$3.92 \cdot 10^{-16}$	0.71

TABLE SI-XIII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **4**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$-1.35 \cdot 10^{5}$	$-3.14 \cdot 10^{5}$	$1.79 \cdot 10^{5}$	$2.02 \cdot 10^{2}$	$9.77 \cdot 10^{-18}$	0.02
C2	$-8.19 \cdot 10^{3}$	$-5.54 \cdot 10^{4}$	$4.72 \cdot 10^{4}$	$6.49 \cdot 10^{1}$	$5.93 \cdot 10^{-19}$	0.00
C3	$2.73 \cdot 10^{4}$	$6.01 \cdot 10^{3}$	$2.12 \cdot 10^{4}$	$3.93 \cdot 10^{1}$	$1.97 \cdot 10^{-18}$	0.00
C4	$4.14 \cdot 10^{4}$	$2.04 \cdot 10^{4}$	$2.10 \cdot 10^{4}$	$4.58 \cdot 10^{1}$	$3.00 \cdot 10^{-18}$	0.01
C5	$1.61 \cdot 10^{4}$	$6.46 \cdot 10^{3}$	$9.60 \cdot 10^{3}$	$1.86 \cdot 10^{1}$	$1.16 \cdot 10^{-18}$	0.00
C6	$-4.46 \cdot 10^{3}$	$-1.32 \cdot 10^{4}$	$8.70 \cdot 10^{3}$	$1.50 \cdot 10^{1}$	$3.23 \cdot 10^{-19}$	0.00
C7	$-4.28 \cdot 10^{4}$	$-5.50 \cdot 10^{4}$	$1.22 \cdot 10^{4}$	$2.69 \cdot 10^{1}$	$3.10 \cdot 10^{-18}$	0.01
C8	$-6.33 \cdot 10^{4}$	$-6.89 \cdot 10^{4}$	$5.55 \cdot 10^{3}$	$1.85 \cdot 10^{1}$	$4.59 \cdot 10^{-18}$	0.01
C9	$-1.06 \cdot 10^{5}$	$-1.02 \cdot 10^{5}$	$-4.27 \cdot 10^{3}$	$2.83 \cdot 10^{1}$	$7.69 \cdot 10^{-18}$	0.01
C10	$-2.66 \cdot 10^{5}$	$-2.24 \cdot 10^{5}$	$-4.19 \cdot 10^{4}$	$8.34 \cdot 10^{1}$	$1.93 \cdot 10^{-17}$	0.03
C11	$-6.65 \cdot 10^{4}$	$-8.82 \cdot 10^{4}$	$2.17 \cdot 10^{4}$	$9.92 \cdot 10^{1}$	$4.81 \cdot 10^{-18}$	0.01
C12	$7.96 \cdot 10^{4}$	$2.68 \cdot 10^{4}$	$5.27 \cdot 10^{4}$	$1.42 \cdot 10^{2}$	$5.76 \cdot 10^{-18}$	0.01
C13	$-3.48 \cdot 10^{5}$	$-6.27 \cdot 10^{5}$	$2.80 \cdot 10^{5}$	$-8.29 \cdot 10^{1}$	$2.52 \cdot 10^{-17}$	0.05
C14	$-5.31 \cdot 10^{5}$	$-1.04 \cdot 10^{6}$	$5.08 \cdot 10^{5}$	$-2.92 \cdot 10^{2}$	$3.84 \cdot 10^{-17}$	0.07
C15	$3.25 \cdot 10^{5}$	$4.38 \cdot 10^{5}$	$-1.14 \cdot 10^{5}$	$-2.83 \cdot 10^{2}$	$2.35 \cdot 10^{-17}$	0.04
C16	$1.18 \cdot 10^{6}$	$1.92 \cdot 10^{6}$	$-7.45 \cdot 10^{5}$	$-3.40 \cdot 10^{2}$	$8.53 \cdot 10^{-17}$	0.15
C17	$4.87 \cdot 10^{5}$	$8.25 \cdot 10^{5}$	$-3.38 \cdot 10^{5}$	$-9.53 \cdot 10^{1}$	$3.53 \cdot 10^{-17}$	0.06
C18	$-6.33 \cdot 10^{3}$	$9.49 \cdot 10^{4}$	$-1.01 \cdot 10^{5}$	$4.05 \cdot 10^{1}$	$4.58 \cdot 10^{-19}$	0.00
C19	$-8.82 \cdot 10^{4}$	$1.58 \cdot 10^{5}$	$-2.46 \cdot 10^{5}$	$1.38 \cdot 10^{2}$	$6.39 \cdot 10^{-18}$	0.01
C20	$-2.38 \cdot 10^{5}$	$-2.59 \cdot 10^{5}$	$2.07 \cdot 10^{4}$	$5.14 \cdot 10^{1}$	$1.72 \cdot 10^{-17}$	0.03
C21	$-1.75 \cdot 10^{5}$	$-2.84 \cdot 10^{5}$	$1.09 \cdot 10^{5}$	$-1.23 \cdot 10^{1}$	$1.27 \cdot 10^{-17}$	0.02
C22	$-1.24 \cdot 10^{4}$	$-5.87 \cdot 10^{4}$	$4.63 \cdot 10^{4}$	$-4.19 \cdot 10^{1}$	$8.96 \cdot 10^{-19}$	0.00
C23	$8.05 \cdot 10^{4}$	$3.53 \cdot 10^{4}$	$4.54 \cdot 10^{4}$	$-2.37 \cdot 10^{2}$	$5.83 \cdot 10^{-18}$	0.01
C24	$-1.72 \cdot 10^{5}$	$-5.08 \cdot 10^{5}$	$3.36 \cdot 10^{5}$	$-5.22 \cdot 10^{2}$	$1.25 \cdot 10^{-17}$	0.02
C25	$-6.99 \cdot 10^{5}$	$-1.25 \cdot 10^{6}$	$5.55 \cdot 10^{5}$	$-1.56 \cdot 10^{2}$	$5.06 \cdot 10^{-17}$	0.09
C26	$-1.28 \cdot 10^{6}$	$-2.16 \cdot 10^{6}$	$8.88 \cdot 10^{5}$	$1.16 \cdot 10^{2}$	$9.23 \cdot 10^{-17}$	0.17
C27	$-4.48 \cdot 10^{5}$	$-7.51 \cdot 10^{5}$	$3.03 \cdot 10^{5}$	$8.41 \cdot 10^{1}$	$3.24 \cdot 10^{-17}$	0.06

TABLE SI-XIV: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **4**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$-3.19 \cdot 10^{6}$	$-5.63 \cdot 10^{6}$	$2.43 \cdot 10^{6}$	$-3.50 \cdot 10^{2}$	$7.84 \cdot 10^{-16}$	1.42
O2	$3.98 \cdot 10^{6}$	$6.81 \cdot 10^{6}$	$-2.82 \cdot 10^{6}$	$-7.05 \cdot 10^{2}$	$9.78 \cdot 10^{-16}$	1.77
O3	$1.28 \cdot 10^{6}$	$3.01 \cdot 10^{6}$	$-1.73 \cdot 10^{6}$	$3.25 \cdot 10^{2}$	$3.15 \cdot 10^{-16}$	0.57
O4	$1.35 \cdot 10^{5}$	$-6.15 \cdot 10^{4}$	$1.97 \cdot 10^{5}$	$3.76 \cdot 10^{1}$	$3.32 \cdot 10^{-17}$	0.06
O5	$1.52 \cdot 10^{6}$	$1.82 \cdot 10^{6}$	$-3.05 \cdot 10^{5}$	$-1.77 \cdot 10^{3}$	$3.72 \cdot 10^{-16}$	0.67
O6	$-3.37 \cdot 10^{6}$	$-5.66 \cdot 10^{6}$	$2.29 \cdot 10^{6}$	$8.26 \cdot 10^{2}$	$8.28 \cdot 10^{-16}$	1.50
N1	$6.58 \cdot 10^{3}$	$-2.96 \cdot 10^{5}$	$3.02 \cdot 10^{5}$	$5.24 \cdot 10^{2}$	$1.05 \cdot 10^{-19}$	0.00
N2	$-4.53 \cdot 10^{5}$	$-3.79 \cdot 10^{5}$	$-7.46 \cdot 10^{4}$	$2.50 \cdot 10^{2}$	$7.23 \cdot 10^{-18}$	0.01

TABLE SI-XV: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **4**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
H1	$-4.65 \cdot 10^{5}$	$-4.73 \cdot 10^{5}$	$7.78 \cdot 10^{3}$	$5.49 \cdot 10^{1}$	$5.32 \cdot 10^{-16}$	0.96
H2	$6.41 \cdot 10^{5}$	$1.14 \cdot 10^{6}$	$-4.97 \cdot 10^{5}$	$-1.86 \cdot 10^{2}$	$7.35 \cdot 10^{-16}$	1.33
H3	$8.91 \cdot 10^{4}$	$2.84 \cdot 10^{5}$	$-1.95 \cdot 10^{5}$	-7.35	$1.02 \cdot 10^{-16}$	0.18
H4	$-6.61 \cdot 10^{5}$	$-5.06 \cdot 10^{5}$	$-1.55 \cdot 10^{5}$	$4.08 \cdot 10^{2}$	$7.57 \cdot 10^{-16}$	1.37
H5	$-1.59 \cdot 10^{5}$	$-6.70 \cdot 10^{4}$	$-9.26 \cdot 10^{4}$	$9.17 \cdot 10^{1}$	$1.83 \cdot 10^{-16}$	0.33
H6	$7.20 \cdot 10^{4}$	$1.13 \cdot 10^{5}$	$-4.06 \cdot 10^{4}$	$-1.74 \cdot 10^{1}$	$8.25 \cdot 10^{-17}$	0.15
H7	$5.10 \cdot 10^{4}$	$-1.15 \cdot 10^{5}$	$1.66 \cdot 10^{5}$	$-1.42 \cdot 10^{2}$	$5.85 \cdot 10^{-17}$	0.11
H8	$-1.69 \cdot 10^{5}$	$-7.15 \cdot 10^{5}$	$5.46 \cdot 10^{5}$	$-3.19 \cdot 10^{2}$	$1.93 \cdot 10^{-16}$	0.35
H9	$2.65 \cdot 10^{5}$	$2.44 \cdot 10^{3}$	$2.63 \cdot 10^{5}$	$-4.60 \cdot 10^{2}$	$3.04 \cdot 10^{-16}$	0.55
H10	$2.27 \cdot 10^{5}$	$1.48 \cdot 10^{5}$	$7.95 \cdot 10^{4}$	$-2.06 \cdot 10^{2}$	$2.60 \cdot 10^{-16}$	0.47
H11	$-2.04 \cdot 10^{5}$	$-2.18 \cdot 10^{5}$	$1.35 \cdot 10^{4}$	$1.83 \cdot 10^{2}$	$2.34 \cdot 10^{-16}$	0.42
H12	$1.99 \cdot 10^{5}$	$2.05 \cdot 10^{5}$	$-6.13 \cdot 10^{3}$	$-1.13 \cdot 10^{2}$	$2.28 \cdot 10^{-16}$	0.41
H13	$4.18 \cdot 10^{5}$	$7.08 \cdot 10^{5}$	$-2.90 \cdot 10^{5}$	$5.28 \cdot 10^{1}$	$4.78 \cdot 10^{-16}$	0.86

TABLE SI-XVI: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **5**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$4.31 \cdot 10^{4}$	$3.52 \cdot 10^{5}$	$-3.08 \cdot 10^{5}$	$-2.27 \cdot 10^{1}$	$3.12 \cdot 10^{-18}$	0.01
C2	$-3.94 \cdot 10^{5}$	$-2.15 \cdot 10^{5}$	$-1.79 \cdot 10^{5}$	$2.36 \cdot 10^{2}$	$2.85 \cdot 10^{-17}$	0.05
C3	$6.55 \cdot 10^{4}$	$3.55 \cdot 10^{4}$	$3.01 \cdot 10^{4}$	$-7.74 \cdot 10^{1}$	$4.74 \cdot 10^{-18}$	0.01
C4	$2.04 \cdot 10^{5}$	$-1.66 \cdot 10^{5}$	$3.70 \cdot 10^{5}$	$-4.37 \cdot 10^{2}$	$1.48 \cdot 10^{-17}$	0.03
C5	$-1.46 \cdot 10^{6}$	$-2.14 \cdot 10^{6}$	$6.85 \cdot 10^{5}$	$4.17 \cdot 10^{2}$	$1.05 \cdot 10^{-16}$	0.19
C6	$-3.86 \cdot 10^{5}$	$-4.25 \cdot 10^{5}$	$3.80 \cdot 10^{4}$	$3.45 \cdot 10^{2}$	$2.80 \cdot 10^{-17}$	0.05
C7	$6.31 \cdot 10^{5}$	$1.22 \cdot 10^{6}$	$-5.88 \cdot 10^{5}$	$3.31 \cdot 10^{2}$	$4.57 \cdot 10^{-17}$	0.08
C8	$-6.15 \cdot 10^{5}$	$-9.38 \cdot 10^{5}$	$3.23 \cdot 10^{5}$	$1.09 \cdot 10^{2}$	$4.45 \cdot 10^{-17}$	0.08
C9	$4.23 \cdot 10^{5}$	$7.35 \cdot 10^{5}$	$-3.12 \cdot 10^{5}$	$6.90 \cdot 10^{1}$	$3.06 \cdot 10^{-17}$	0.06
C10	$1.93 \cdot 10^{5}$	$3.34 \cdot 10^{5}$	$-1.41 \cdot 10^{5}$	$-1.25 \cdot 10^{1}$	$1.39 \cdot 10^{-17}$	0.03
C11	$3.47 \cdot 10^{5}$	$3.16 \cdot 10^{5}$	$3.12 \cdot 10^{4}$	$-2.30 \cdot 10^{2}$	$2.51 \cdot 10^{-17}$	0.05
C12	$2.36 \cdot 10^{5}$	$-1.79 \cdot 10^{5}$	$4.15 \cdot 10^{5}$	$-5.22 \cdot 10^{2}$	$1.71 \cdot 10^{-17}$	0.03
C13	$-3.03 \cdot 10^{4}$	$5.68 \cdot 10^{4}$	$-8.72 \cdot 10^{4}$	$7.17 \cdot 10^{1}$	$2.20 \cdot 10^{-18}$	0.00
C14	$1.10 \cdot 10^{4}$	$-1.66 \cdot 10^{5}$	$1.77 \cdot 10^{5}$	$-1.87 \cdot 10^{2}$	$7.96 \cdot 10^{-19}$	0.00
C15	$1.60 \cdot 10^{6}$	$2.55 \cdot 10^{6}$	$-9.57 \cdot 10^{5}$	$-1.34 \cdot 10^{2}$	$1.15 \cdot 10^{-16}$	0.21
C16	$8.11 \cdot 10^{5}$	$1.37 \cdot 10^{6}$	$-5.60 \cdot 10^{5}$	$1.03 \cdot 10^{2}$	$5.87 \cdot 10^{-17}$	0.11
C17	$1.54 \cdot 10^{5}$	$5.18 \cdot 10^{5}$	$-3.64 \cdot 10^{5}$	$4.37 \cdot 10^{2}$	$1.12 \cdot 10^{-17}$	0.02
C18	$5.41 \cdot 10^{5}$	$8.63 \cdot 10^{5}$	$-3.22 \cdot 10^{5}$	$-8.51 \cdot 10^{1}$	$3.92 \cdot 10^{-17}$	0.07
C19	$-1.73 \cdot 10^{5}$	$-1.38 \cdot 10^{5}$	$-3.53 \cdot 10^{4}$	$2.02 \cdot 10^{2}$	$1.25 \cdot 10^{-17}$	0.02

TABLE SI-XVII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **5**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
O1	$-2.04 \cdot 10^{5}$	$5.65 \cdot 10^{5}$	$-7.69 \cdot 10^{5}$	$2.17 \cdot 10^{2}$	$5.01 \cdot 10^{-17}$	0.09
O2	$9.19 \cdot 10^{5}$	$6.09 \cdot 10^{5}$	$3.10 \cdot 10^{5}$	$-7.69 \cdot 10^{2}$	$2.26 \cdot 10^{-16}$	0.41
O3	$-4.77 \cdot 10^{6}$	$-7.60 \cdot 10^{6}$	$2.83 \cdot 10^{6}$	$5.70 \cdot 10^{2}$	$1.17 \cdot 10^{-15}$	2.12
O4	$3.81 \cdot 10^{6}$	$6.36 \cdot 10^{6}$	$-2.55 \cdot 10^{6}$	$2.86 \cdot 10^{2}$	$9.36 \cdot 10^{-16}$	1.69
O5	$-5.11 \cdot 10^{5}$	$-4.36 \cdot 10^{4}$	$-4.68 \cdot 10^{5}$	$4.72 \cdot 10^{2}$	$1.25 \cdot 10^{-16}$	0.23
O6	$-1.08 \cdot 10^{6}$	$-3.22 \cdot 10^{6}$	$2.15 \cdot 10^{6}$	$-1.34 \cdot 10^{3}$	$2.65 \cdot 10^{-16}$	0.48
O7	$3.95 \cdot 10^{6}$	$6.38 \cdot 10^{6}$	$-2.43 \cdot 10^{6}$	$-6.53 \cdot 10^{2}$	$9.69 \cdot 10^{-16}$	1.75
O8	$-2.13 \cdot 10^{6}$	$-2.37 \cdot 10^{6}$	$2.44 \cdot 10^{5}$	$1.60 \cdot 10^{3}$	$5.22 \cdot 10^{-16}$	0.94
F1	$-5.06 \cdot 10^{5}$	$-7.17 \cdot 10^{5}$	$2.11 \cdot 10^{5}$	$8.69 \cdot 10^{1}$	$5.13 \cdot 10^{-16}$	0.93
F2	$-3.08 \cdot 10^{5}$	$-4.53 \cdot 10^{5}$	$1.45 \cdot 10^{5}$	$8.11 \cdot 10^{1}$	$3.13 \cdot 10^{-16}$	0.57
F3	$-4.25 \cdot 10^{5}$	$-7.43 \cdot 10^{5}$	$3.18 \cdot 10^{5}$	2.56	$4.31 \cdot 10^{-16}$	0.78
F4	$4.27 \cdot 10^{5}$	$6.93 \cdot 10^{5}$	$-2.66 \cdot 10^{5}$	$-9.60 \cdot 10^{-1}$	$4.34 \cdot 10^{-16}$	0.78
F5	$3.92 \cdot 10^{5}$	$6.65 \cdot 10^{5}$	$-2.74 \cdot 10^{5}$	$1.97 \cdot 10^{1}$	$3.97 \cdot 10^{-16}$	0.72
F6	$1.49 \cdot 10^{5}$	$2.80 \cdot 10^{5}$	$-1.31 \cdot 10^{5}$	$6.07 \cdot 10^{1}$	$1.51 \cdot 10^{-16}$	0.27
F7	$-1.33 \cdot 10^{5}$	$-3.49 \cdot 10^{4}$	$-9.84 \cdot 10^{4}$	$1.45 \cdot 10^{2}$	$1.35 \cdot 10^{-16}$	0.24
F8	$3.49 \cdot 10^{4}$	$7.88 \cdot 10^{4}$	$-4.39 \cdot 10^{4}$	$1.18 \cdot 10^{1}$	$3.54 \cdot 10^{-17}$	0.06
F9	$-5.96 \cdot 10^{4}$	$-1.96 \cdot 10^{4}$	$-4.00 \cdot 10^{4}$	$4.23 \cdot 10^{1}$	$6.04 \cdot 10^{-17}$	0.11
F10	$2.00 \cdot 10^{3}$	$-9.30 \cdot 10^{4}$	$9.51 \cdot 10^{4}$	$-1.43 \cdot 10^{2}$	$2.03 \cdot 10^{-18}$	0.00
F11	$-1.39 \cdot 10^{5}$	$-3.69 \cdot 10^{5}$	$2.30 \cdot 10^{5}$	$-1.15 \cdot 10^{2}$	$1.41 \cdot 10^{-16}$	0.26
F12	$8.74 \cdot 10^{4}$	$4.26 \cdot 10^{4}$	$4.49 \cdot 10^{4}$	$-1.05 \cdot 10^{2}$	$8.87 \cdot 10^{-17}$	0.16
F13	$3.16 \cdot 10^{5}$	$5.08 \cdot 10^{5}$	$-1.92 \cdot 10^{5}$	$-9.69 \cdot 10^{1}$	$3.21 \cdot 10^{-16}$	0.58
F14	$3.44 \cdot 10^{5}$	$5.55 \cdot 10^{5}$	$-2.11 \cdot 10^{5}$	$-4.48 \cdot 10^{1}$	$3.49 \cdot 10^{-16}$	0.63
F15	$3.25 \cdot 10^{5}$	$5.16 \cdot 10^{5}$	$-1.91 \cdot 10^{5}$	$-4.08 \cdot 10^{1}$	$3.30 \cdot 10^{-16}$	0.60
F16	$-2.61 \cdot 10^{5}$	$-3.65 \cdot 10^{5}$	$1.04 \cdot 10^{5}$	$1.28 \cdot 10^{2}$	$2.64 \cdot 10^{-16}$	0.48
F17	$-2.69 \cdot 10^{5}$	$-2.50 \cdot 10^{5}$	$-1.96 \cdot 10^{4}$	$2.00 \cdot 10^{2}$	$2.73 \cdot 10^{-16}$	0.49
F18	$2.64 \cdot 10^{3}$	$7.15 \cdot 10^{4}$	$-6.89 \cdot 10^{4}$	$9.67 \cdot 10^{1}$	$2.67 \cdot 10^{-18}$	0.00

TABLE SI-XVIII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **5**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
H1	$3.23 \cdot 10^{5}$	$5.39 \cdot 10^{5}$	$-2.16 \cdot 10^{5}$	$-2.72 \cdot 10^{1}$	$3.70 \cdot 10^{-16}$	0.67
H2	$-5.70 \cdot 10^{5}$	$-7.30 \cdot 10^{5}$	$1.61 \cdot 10^{5}$	$6.50 \cdot 10^{1}$	$6.52 \cdot 10^{-16}$	1.18
H3	$-3.19 \cdot 10^{4}$	$-1.67 \cdot 10^{4}$	$-1.53 \cdot 10^{4}$	$2.17 \cdot 10^{1}$	$3.65 \cdot 10^{-17}$	0.07
H4	$-5.12 \cdot 10^{5}$	$-7.61 \cdot 10^{5}$	$2.48 \cdot 10^{5}$	$1.28 \cdot 10^{2}$	$5.86 \cdot 10^{-16}$	1.06
H5	$1.94 \cdot 10^{5}$	$3.37 \cdot 10^{5}$	$-1.43 \cdot 10^{5}$	$1.33 \cdot 10^{1}$	$2.22 \cdot 10^{-16}$	0.40
H6	$-4.97 \cdot 10^{5}$	$-7.64 \cdot 10^{5}$	$2.67 \cdot 10^{5}$	$1.95 \cdot 10^{2}$	$5.69 \cdot 10^{-16}$	1.03
H7	$-4.67 \cdot 10^{5}$	$-7.17 \cdot 10^{5}$	$2.50 \cdot 10^{5}$	$1.35 \cdot 10^{2}$	$5.35 \cdot 10^{-16}$	0.97
H8	$-8.22 \cdot 10^{5}$	$-1.26 \cdot 10^{6}$	$4.36 \cdot 10^{5}$	$2.33 \cdot 10^{2}$	$9.41 \cdot 10^{-16}$	1.70
H9	$-2.64 \cdot 10^{5}$	$-3.83 \cdot 10^{5}$	$1.19 \cdot 10^{5}$	$7.68 \cdot 10^{1}$	$3.02 \cdot 10^{-16}$	0.55
H10	$7.06 \cdot 10^{4}$	$1.21 \cdot 10^{5}$	$-5.02 \cdot 10^{4}$	$2.51 \cdot 10^{1}$	$8.09 \cdot 10^{-17}$	0.15
H11	$3.82 \cdot 10^{5}$	$7.78 \cdot 10^{5}$	$-3.96 \cdot 10^{5}$	$-4.77 \cdot 10^{1}$	$4.38 \cdot 10^{-16}$	0.79
H12	$2.36 \cdot 10^{5}$	$3.92 \cdot 10^{5}$	$-1.56 \cdot 10^{5}$	$-1.81 \cdot 10^{1}$	$2.71 \cdot 10^{-16}$	0.49
H13	$-2.21 \cdot 10^{4}$	$-3.02 \cdot 10^{4}$	$8.10 \cdot 10^{3}$	$5.25 \cdot 10^{1}$	$2.53 \cdot 10^{-17}$	0.05
H14	$-2.23 \cdot 10^{5}$	$-3.40 \cdot 10^{5}$	$1.17 \cdot 10^{5}$	$1.56 \cdot 10^{2}$	$2.55 \cdot 10^{-16}$	0.46
H15	$-2.12 \cdot 10^{6}$	$-2.52 \cdot 10^{6}$	$3.98 \cdot 10^{5}$	$-3.04 \cdot 10^{2}$	$2.43 \cdot 10^{-15}$	4.39
H16	$-6.72 \cdot 10^{5}$	$-1.14 \cdot 10^{6}$	$4.67 \cdot 10^{5}$	$-2.80 \cdot 10^{2}$	$7.69 \cdot 10^{-16}$	1.39
H17	$-5.08 \cdot 10^{5}$	$-5.19 \cdot 10^{5}$	$1.10 \cdot 10^{4}$	$-2.83 \cdot 10^{2}$	$5.82 \cdot 10^{-16}$	1.05
H18	$4.77 \cdot 10^{5}$	$6.52 \cdot 10^{5}$	$-1.74 \cdot 10^{5}$	$5.33 \cdot 10^{1}$	$5.47 \cdot 10^{-16}$	0.99
H19	$2.21 \cdot 10^{5}$	$3.29 \cdot 10^{5}$	$-1.08 \cdot 10^{5}$	9.77	$2.53 \cdot 10^{-16}$	0.46
H20	$1.89 \cdot 10^{5}$	$3.01 \cdot 10^{5}$	$-1.12 \cdot 10^{5}$	-6.24	$2.17 \cdot 10^{-16}$	0.39
H21	$4.91 \cdot 10^{5}$	$8.82 \cdot 10^{5}$	$-3.91 \cdot 10^{5}$	$-1.37 \cdot 10^{1}$	$5.62 \cdot 10^{-16}$	1.02
H22	$2.39 \cdot 10^{6}$	$3.35 \cdot 10^{6}$	$-9.57 \cdot 10^{5}$	$-5.71 \cdot 10^{1}$	$2.74 \cdot 10^{-15}$	4.95
H23	$2.90 \cdot 10^{5}$	$5.71 \cdot 10^{5}$	$-2.81 \cdot 10^{5}$	$3.63 \cdot 10^{2}$	$3.32 \cdot 10^{-16}$	0.60
H24	$6.64 \cdot 10^{5}$	$9.50 \cdot 10^{5}$	$-2.85 \cdot 10^{5}$	$-8.74 \cdot 10^{2}$	$7.60 \cdot 10^{-16}$	1.37

TABLE SI-XIX: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **6**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$-4.14 \cdot 10^{5}$	$-2.31 \cdot 10^{5}$	$-1.82 \cdot 10^{5}$	$4.95 \cdot 10^{1}$	$2.99 \cdot 10^{-17}$	0.05
C2	$-4.19 \cdot 10^{5}$	$-5.42 \cdot 10^{5}$	$1.23 \cdot 10^{5}$	$7.61 \cdot 10^{1}$	$3.03 \cdot 10^{-17}$	0.05
C3	$1.94 \cdot 10^{6}$	$3.50 \cdot 10^{6}$	$-1.56 \cdot 10^{6}$	$-8.89 \cdot 10^{1}$	$1.40 \cdot 10^{-16}$	0.25
C4	$1.28 \cdot 10^{6}$	$1.96 \cdot 10^{6}$	$-6.80 \cdot 10^{5}$	$-8.80 \cdot 10^{1}$	$9.29 \cdot 10^{-17}$	0.17
C5	$2.10 \cdot 10^{5}$	$3.62 \cdot 10^{5}$	$-1.53 \cdot 10^{5}$	$3.07 \cdot 10^{1}$	$1.52 \cdot 10^{-17}$	0.03
C6	$-7.70 \cdot 10^{5}$	$-1.18 \cdot 10^{6}$	$4.11 \cdot 10^{5}$	$2.37 \cdot 10^{2}$	$5.57 \cdot 10^{-17}$	0.10
C7	$-1.84 \cdot 10^{6}$	$-2.83 \cdot 10^{6}$	$9.86 \cdot 10^{5}$	$5.22 \cdot 10^{2}$	$1.33 \cdot 10^{-16}$	0.24
C8	$4.33 \cdot 10^{5}$	$7.55 \cdot 10^{5}$	$-3.23 \cdot 10^{5}$	$6.14 \cdot 10^{1}$	$3.13 \cdot 10^{-17}$	0.06
C9	$-4.57 \cdot 10^{5}$	$-6.82 \cdot 10^{5}$	$2.25 \cdot 10^{5}$	$1.48 \cdot 10^{2}$	$3.31 \cdot 10^{-17}$	0.06
C10	$9.51 \cdot 10^{4}$	$1.64 \cdot 10^{5}$	$-6.89 \cdot 10^{4}$	$3.75 \cdot 10^{1}$	$6.89 \cdot 10^{-18}$	0.01
C11	$7.59 \cdot 10^{5}$	$1.53 \cdot 10^{6}$	$-7.75 \cdot 10^{5}$	$-9.35 \cdot 10^{1}$	$5.50 \cdot 10^{-17}$	0.10
C12	$7.90 \cdot 10^{5}$	$1.23 \cdot 10^{6}$	$-4.36 \cdot 10^{5}$	$-4.84 \cdot 10^{1}$	$5.72 \cdot 10^{-17}$	0.10
C13	$3.60 \cdot 10^{5}$	$5.76 \cdot 10^{5}$	$-2.16 \cdot 10^{5}$	$-2.16 \cdot 10^{1}$	$2.61 \cdot 10^{-17}$	0.05
C14	$1.59 \cdot 10^{4}$	$3.43 \cdot 10^{4}$	$-1.85 \cdot 10^{4}$	$6.39 \cdot 10^{1}$	$1.15 \cdot 10^{-18}$	0.00
C15	$-4.60 \cdot 10^{4}$	$-5.61 \cdot 10^{4}$	$1.00 \cdot 10^{4}$	$1.30 \cdot 10^{2}$	$3.33 \cdot 10^{-18}$	0.01
C16	$-1.24 \cdot 10^{6}$	$-1.60 \cdot 10^{6}$	$3.56 \cdot 10^{5}$	$-4.66 \cdot 10^{2}$	$9.00 \cdot 10^{-17}$	0.16
C17	$6.02 \cdot 10^{5}$	$8.71 \cdot 10^{5}$	$-2.69 \cdot 10^{5}$	$1.86 \cdot 10^{1}$	$4.36 \cdot 10^{-17}$	0.08
C18	$3.28 \cdot 10^{5}$	$4.93 \cdot 10^{5}$	$-1.65 \cdot 10^{5}$	4.48	$2.37 \cdot 10^{-17}$	0.04
C19	$2.83 \cdot 10^{5}$	$4.43 \cdot 10^{5}$	$-1.60 \cdot 10^{5}$	-8.73	$2.05 \cdot 10^{-17}$	0.04

TABLE SI-XX: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **6**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$8.19 \cdot 10^{6}$	$1.18 \cdot 10^{7}$	$-3.57 \cdot 10^{6}$	$-6.27 \cdot 10^{2}$	$2.01 \cdot 10^{-15}$	3.63
O2	$5.53 \cdot 10^{6}$	$9.63 \cdot 10^{6}$	$-4.09 \cdot 10^{6}$	$2.38 \cdot 10^{2}$	$1.36 \cdot 10^{-15}$	2.45
O3	$-4.93 \cdot 10^{6}$	$-6.60 \cdot 10^{6}$	$1.67 \cdot 10^{6}$	$8.24 \cdot 10^{2}$	$1.21 \cdot 10^{-15}$	2.19
O4	$-4.09 \cdot 10^{5}$	$-7.47 \cdot 10^{5}$	$3.40 \cdot 10^{5}$	$-1.69 \cdot 10^{3}$	$1.00 \cdot 10^{-16}$	0.18
O5	$-9.42 \cdot 10^{5}$	$-3.54 \cdot 10^{5}$	$-5.89 \cdot 10^{5}$	$7.83 \cdot 10^{2}$	$2.31 \cdot 10^{-16}$	0.42
O6	$-5.84 \cdot 10^{6}$	$-8.96 \cdot 10^{6}$	$3.12 \cdot 10^{6}$	$1.98 \cdot 10^{3}$	$1.43 \cdot 10^{-15}$	2.59
O7	$-5.33 \cdot 10^{5}$	$-2.04 \cdot 10^{6}$	$1.50 \cdot 10^{6}$	$1.13 \cdot 10^{3}$	$1.31 \cdot 10^{-16}$	0.24
O8	$4.24 \cdot 10^{6}$	$3.82 \cdot 10^{6}$	$4.18 \cdot 10^{5}$	$-1.49 \cdot 10^{3}$	$1.04 \cdot 10^{-15}$	1.88
O9	$-5.47 \cdot 10^{6}$	$-6.33 \cdot 10^{6}$	$8.58 \cdot 10^{5}$	$-7.81 \cdot 10^{2}$	$1.34 \cdot 10^{-15}$	2.43
O10	$-3.69 \cdot 10^{5}$	$-5.90 \cdot 10^{5}$	$2.21 \cdot 10^{5}$	$-3.08 \cdot 10^{2}$	$9.05 \cdot 10^{-17}$	0.16
O11	$-4.47 \cdot 10^{5}$	$-6.58 \cdot 10^{5}$	$2.11 \cdot 10^{5}$	$3.56 \cdot 10^{2}$	$1.10 \cdot 10^{-16}$	0.20
N1	$7.30 \cdot 10^{5}$	$1.16 \cdot 10^{6}$	$-4.29 \cdot 10^{5}$	$-6.03 \cdot 10^{1}$	$1.16 \cdot 10^{-17}$	0.02
N2	$7.55 \cdot 10^{5}$	$1.35 \cdot 10^{6}$	$-5.92 \cdot 10^{5}$	1.75	$1.20 \cdot 10^{-17}$	0.02
N3	$2.34 \cdot 10^{5}$	$4.30 \cdot 10^{5}$	$-1.96 \cdot 10^{5}$	$1.79 \cdot 10^{2}$	$3.73 \cdot 10^{-18}$	0.01
N4	$-1.22 \cdot 10^{6}$	$-1.96 \cdot 10^{6}$	$7.49 \cdot 10^{5}$	$-8.48 \cdot 10^{2}$	$1.94 \cdot 10^{-17}$	0.04
N5	$-1.03 \cdot 10^{6}$	$-1.50 \cdot 10^{6}$	$4.61 \cdot 10^{5}$	$9.88 \cdot 10^{2}$	$1.65 \cdot 10^{-17}$	0.03
N6	$1.25 \cdot 10^{6}$	$1.84 \cdot 10^{6}$	$-5.88 \cdot 10^{5}$	$-2.80 \cdot 10^{1}$	$2.00 \cdot 10^{-17}$	0.04

TABLE SI-XXI: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **6**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert \mathrm{P}_y \rvert$	$\lvert \mathrm{V} \rvert$
H1	$-1.85 \cdot 10^{5}$	$-1.53 \cdot 10^{5}$	$-3.15 \cdot 10^{4}$	$-6.05 \cdot 10^{1}$	$2.11 \cdot 10^{-16}$	0.38
H2	$-4.42 \cdot 10^{3}$	$2.65 \cdot 10^{4}$	$-3.10 \cdot 10^{4}$	$6.31 \cdot 10^{1}$	$5.06 \cdot 10^{-18}$	0.01
H3	$-2.49 \cdot 10^{5}$	$-3.51 \cdot 10^{5}$	$1.02 \cdot 10^{5}$	$-1.50 \cdot 10^{2}$	$2.85 \cdot 10^{-16}$	0.52
H4	$5.88 \cdot 10^{4}$	$8.96 \cdot 10^{4}$	$-3.09 \cdot 10^{4}$	$1.29 \cdot 10^{2}$	$6.74 \cdot 10^{-17}$	0.12
H5	$-1.54 \cdot 10^{4}$	$-9.84 \cdot 10^{3}$	$-5.53 \cdot 10^{3}$	-3.88	$1.76 \cdot 10^{-17}$	0.03
H6	$-1.19 \cdot 10^{4}$	$-3.15 \cdot 10^{3}$	$-8.76 \cdot 10^{3}$	7.84	$1.36 \cdot 10^{-17}$	0.02
H7	$-3.69 \cdot 10^{4}$	$-2.53 \cdot 10^{4}$	$-1.16 \cdot 10^{4}$	$-1.76 \cdot 10^{1}$	$4.23 \cdot 10^{-17}$	0.08
H8	$2.19 \cdot 10^{5}$	$2.75 \cdot 10^{5}$	$-5.61 \cdot 10^{4}$	$-1.30 \cdot 10^{2}$	$2.50 \cdot 10^{-16}$	0.45
H9	$9.52 \cdot 10^{2}$	$1.58 \cdot 10^{4}$	$-1.49 \cdot 10^{4}$	1.85	$1.09 \cdot 10^{-18}$	0.00
H10	$1.71 \cdot 10^{5}$	$2.29 \cdot 10^{5}$	$-5.81 \cdot 10^{4}$	$-2.96 \cdot 10^{1}$	$1.96 \cdot 10^{-16}$	0.35
H11	$-1.04 \cdot 10^{4}$	$5.18 \cdot 10^{2}$	$-1.10 \cdot 10^{4}$	$1.34 \cdot 10^{2}$	$1.19 \cdot 10^{-17}$	0.02
H12	$5.48 \cdot 10^{5}$	$6.78 \cdot 10^{5}$	$-1.30 \cdot 10^{5}$	$8.05 \cdot 10^{1}$	$6.27 \cdot 10^{-16}$	1.13
H13	$-7.78 \cdot 10^{3}$	$-1.59 \cdot 10^{4}$	$8.17 \cdot 10^{3}$	$-7.05 \cdot 10^{1}$	$8.91 \cdot 10^{-18}$	0.02
H14	$-1.16 \cdot 10^{4}$	$5.75 \cdot 10^{3}$	$-1.73 \cdot 10^{4}$	$-2.11 \cdot 10^{1}$	$1.32 \cdot 10^{-17}$	0.02
H15	$3.19 \cdot 10^{5}$	$3.62 \cdot 10^{5}$	$-4.35 \cdot 10^{4}$	$5.29 \cdot 10^{2}$	$3.65 \cdot 10^{-16}$	0.66
H16	$-6.97 \cdot 10^{3}$	$6.32 \cdot 10^{3}$	$-1.33 \cdot 10^{4}$	-6.28	$7.99 \cdot 10^{-18}$	0.01
H17	$6.12 \cdot 10^{4}$	$8.08 \cdot 10^{4}$	$-1.97 \cdot 10^{4}$	-2.16	$7.00 \cdot 10^{-17}$	0.13
H18	$2.34 \cdot 10^{5}$	$3.08 \cdot 10^{5}$	$-7.36 \cdot 10^{4}$	$-1.09 \cdot 10^{1}$	$2.68 \cdot 10^{-16}$	0.48
H19	$5.92 \cdot 10^{4}$	$7.74 \cdot 10^{4}$	$-1.81 \cdot 10^{4}$	-2.39	$6.78 \cdot 10^{-17}$	0.12
H20	$7.42 \cdot 10^{4}$	$9.93 \cdot 10^{4}$	$-2.51 \cdot 10^{4}$	-9.74	$8.49 \cdot 10^{-17}$	0.15
H21	$-1.21 \cdot 10^{3}$	$2.12 \cdot 10^{4}$	$-2.25 \cdot 10^{4}$	$2.77 \cdot 10^{1}$	$1.39 \cdot 10^{-18}$	0.00
H22	$4.08 \cdot 10^{5}$	$5.75 \cdot 10^{5}$	$-1.67 \cdot 10^{5}$	$3.26 \cdot 10^{1}$	$4.68 \cdot 10^{-16}$	0.84
H23	$-9.24 \cdot 10^{3}$	$-4.36 \cdot 10^{3}$	$-4.88 \cdot 10^{3}$	2.24	$1.06 \cdot 10^{-17}$	0.02
H24	$-1.01 \cdot 10^{4}$	$-6.05 \cdot 10^{3}$	$-4.02 \cdot 10^{3}$	$-7.77 \cdot 10^{-1}$	$1.15 \cdot 10^{-17}$	0.02
H25	$8.32 \cdot 10^{4}$	$1.11 \cdot 10^{5}$	$-2.76 \cdot 10^{4}$	-7.06	$9.53 \cdot 10^{-17}$	0.17
H26	$2.60 \cdot 10^{4}$	$3.64 \cdot 10^{4}$	$-1.04 \cdot 10^{4}$	$-2.54 \cdot 10^{1}$	$2.98 \cdot 10^{-17}$	0.05
H27	$5.23 \cdot 10^{4}$	$7.47 \cdot 10^{4}$	$-2.24 \cdot 10^{4}$	-8.87	$5.99 \cdot 10^{-17}$	0.11
H28	$1.17 \cdot 10^{5}$	$1.64 \cdot 10^{5}$	$-4.71 \cdot 10^{4}$	8.58	$1.34 \cdot 10^{-16}$	0.24

TABLE SI-XXII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **7**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$-2.56 \cdot 10^{5}$	$-1.07 \cdot 10^{5}$	$-1.49 \cdot 10^{5}$	$-6.75 \cdot 10^{1}$	$1.85 \cdot 10^{-17}$	0.03
C2	$-9.04 \cdot 10^{4}$	$-4.16 \cdot 10^{4}$	$-4.88 \cdot 10^{4}$	$-3.64 \cdot 10^{1}$	$6.54 \cdot 10^{-18}$	0.01
C3	$-2.34 \cdot 10^{5}$	$-4.65 \cdot 10^{4}$	$-1.88 \cdot 10^{5}$	$1.67 \cdot 10^{2}$	$1.69 \cdot 10^{-17}$	0.03
C4	$-7.56 \cdot 10^{4}$	$-4.04 \cdot 10^{3}$	$-7.17 \cdot 10^{4}$	$8.26 \cdot 10^{1}$	$5.48 \cdot 10^{-18}$	0.01
C5	$9.20 \cdot 10^{4}$	$1.39 \cdot 10^{5}$	$-4.71 \cdot 10^{4}$	$-3.57 \cdot 10^{2}$	$6.66 \cdot 10^{-18}$	0.01
C6	$1.95 \cdot 10^{3}$	$-1.20 \cdot 10^{5}$	$1.21 \cdot 10^{5}$	$5.28 \cdot 10^{2}$	$1.41 \cdot 10^{-19}$	0.00
C7	$-5.99 \cdot 10^{4}$	$-2.34 \cdot 10^{4}$	$-3.65 \cdot 10^{4}$	$2.01 \cdot 10^{1}$	$4.34 \cdot 10^{-18}$	0.01
C8	$-8.53 \cdot 10^{4}$	$-3.84 \cdot 10^{4}$	$-4.68 \cdot 10^{4}$	$-3.03 \cdot 10^{1}$	$6.17 \cdot 10^{-18}$	0.01
C9	$-7.40 \cdot 10^{3}$	$4.21 \cdot 10^{4}$	$-4.96 \cdot 10^{4}$	$1.03 \cdot 10^{2}$	$5.35 \cdot 10^{-19}$	0.00
C10	$3.96 \cdot 10^{5}$	$5.27 \cdot 10^{5}$	$-1.31 \cdot 10^{5}$	$-3.34 \cdot 10^{1}$	$2.87 \cdot 10^{-17}$	0.05
C11	$-6.47 \cdot 10^{4}$	$-3.43 \cdot 10^{4}$	$-3.05 \cdot 10^{4}$	-6.60	$4.69 \cdot 10^{-18}$	0.01
C12	$-5.21 \cdot 10^{4}$	$2.11 \cdot 10^{4}$	$-7.32 \cdot 10^{4}$	$1.06 \cdot 10^{1}$	$3.77 \cdot 10^{-18}$	0.01
C13	$-4.58 \cdot 10^{5}$	$-6.60 \cdot 10^{5}$	$2.03 \cdot 10^{5}$	$-2.93 \cdot 10^{2}$	$3.31 \cdot 10^{-17}$	0.06
C14	$5.64 \cdot 10^{4}$	$1.11 \cdot 10^{5}$	$-5.43 \cdot 10^{4}$	$1.82 \cdot 10^{2}$	$4.08 \cdot 10^{-18}$	0.01
C15	$1.64 \cdot 10^{5}$	$2.39 \cdot 10^{5}$	$-7.44 \cdot 10^{4}$	$-9.93 \cdot 10^{1}$	$1.19 \cdot 10^{-17}$	0.02
C16	$-1.71 \cdot 10^{4}$	$-1.04 \cdot 10^{4}$	$-6.70 \cdot 10^{3}$	-2.38	$1.24 \cdot 10^{-18}$	0.00
C17	$-1.21 \cdot 10^{5}$	$5.53 \cdot 10^{4}$	$-1.77 \cdot 10^{5}$	$1.58 \cdot 10^{2}$	$8.78 \cdot 10^{-18}$	0.02
C18	$-1.49 \cdot 10^{4}$	$-6.03 \cdot 10^{3}$	$-8.84 \cdot 10^{3}$	5.45	$1.08 \cdot 10^{-18}$	0.00
C19	$-3.43 \cdot 10^{4}$	$-1.21 \cdot 10^{4}$	$-2.22 \cdot 10^{4}$	$-1.74 \cdot 10^{1}$	$2.48 \cdot 10^{-18}$	0.00
C20	$-2.63 \cdot 10^{4}$	$-1.49 \cdot 10^{4}$	$-1.14 \cdot 10^{4}$	-1.45	$1.90 \cdot 10^{-18}$	0.00
C21	$1.04 \cdot 10^{6}$	$1.38 \cdot 10^{6}$	$-3.44 \cdot 10^{5}$	$-1.64 \cdot 10^{2}$	$7.50 \cdot 10^{-17}$	0.14
C22	$4.29 \cdot 10^{5}$	$5.46 \cdot 10^{5}$	$-1.17 \cdot 10^{5}$	$-2.45 \cdot 10^{2}$	$3.11 \cdot 10^{-17}$	0.06
C23	$-3.23 \cdot 10^{3}$	$1.85 \cdot 10^{4}$	$-2.17 \cdot 10^{4}$	$2.67 \cdot 10^{-1}$	$2.34 \cdot 10^{-19}$	0.00
C24	$2.00 \cdot 10^{5}$	$2.66 \cdot 10^{5}$	$-6.66 \cdot 10^{4}$	$-2.23 \cdot 10^{1}$	$1.44 \cdot 10^{-17}$	0.03
C25	$-2.02 \cdot 10^{4}$	$1.09 \cdot 10^{4}$	$-3.14 \cdot 10^{4}$	$2.69 \cdot 10^{2}$	$1.47 \cdot 10^{-18}$	0.00
C26	$-1.00 \cdot 10^{6}$	$-1.54 \cdot 10^{6}$	$5.39 \cdot 10^{5}$	$-2.91 \cdot 10^{2}$	$7.27 \cdot 10^{-17}$	0.13
C27	$-2.46 \cdot 10^{4}$	$-1.13 \cdot 10^{4}$	$-1.33 \cdot 10^{4}$	5.68	$1.78 \cdot 10^{-18}$	0.00
C28	$-3.68 \cdot 10^{5}$	$-5.75 \cdot 10^{5}$	$2.07 \cdot 10^{5}$	$-6.06 \cdot 10^{1}$	$2.66 \cdot 10^{-17}$	0.05
C29	$2.94 \cdot 10^{5}$	$4.05 \cdot 10^{5}$	$-1.11 \cdot 10^{5}$	$-5.49 \cdot 10^{1}$	$2.13 \cdot 10^{-17}$	0.04
C30	$4.43 \cdot 10^{4}$	$6.21 \cdot 10^{4}$	$-1.78 \cdot 10^{4}$	$-6.46 \cdot 10^{1}$	$3.20 \cdot 10^{-18}$	0.01
C31	$-1.70 \cdot 10^{4}$	$1.17 \cdot 10^{4}$	$-2.86 \cdot 10^{4}$	$-3.42 \cdot 10^{1}$	$1.23 \cdot 10^{-18}$	0.00
C32	$1.94 \cdot 10^{5}$	$3.04 \cdot 10^{5}$	$-1.11 \cdot 10^{5}$	$5.08 \cdot 10^{2}$	$1.40 \cdot 10^{-17}$	0.03
C33	$-1.30 \cdot 10^{5}$	$-2.57 \cdot 10^{5}$	$1.28 \cdot 10^{5}$	$-4.46 \cdot 10^{2}$	$9.38 \cdot 10^{-18}$	0.02
C34	$-1.07 \cdot 10^{4}$	$8.59 \cdot 10^{3}$	$-1.92 \cdot 10^{4}$	-7.57	$7.72 \cdot 10^{-19}$	0.00
C35	$9.13 \cdot 10^{4}$	$1.21 \cdot 10^{5}$	$-2.95 \cdot 10^{4}$	-3.67	$6.61 \cdot 10^{-18}$	0.01
C36	$2.49 \cdot 10^{5}$	$3.29 \cdot 10^{5}$	$-7.99 \cdot 10^{4}$	-9.50	$1.80 \cdot 10^{-17}$	0.03
C37	$-1.94 \cdot 10^{5}$	$-3.08 \cdot 10^{5}$	$1.13 \cdot 10^{5}$	$-1.59 \cdot 10^{2}$	$1.41 \cdot 10^{-17}$	0.03
C38	$1.08 \cdot 10^{5}$	$1.42 \cdot 10^{5}$	$-3.41 \cdot 10^{4}$	-3.30	$7.79 \cdot 10^{-18}$	0.01
C39	$6.70 \cdot 10^{4}$	$1.05 \cdot 10^{5}$	$-3.78 \cdot 10^{4}$	$-3.20 \cdot 10^{1}$	$4.85 \cdot 10^{-18}$	0.01
C40	$-1.74 \cdot 10^{4}$	$-1.02 \cdot 10^{5}$	$8.39 \cdot 10^{4}$	$1.86 \cdot 10^{2}$	$1.26 \cdot 10^{-18}$	0.00
C41	$-6.75 \cdot 10^{3}$	$2.70 \cdot 10^{4}$	$-3.38 \cdot 10^{4}$	$1.44 \cdot 10^{1}$	$4.89 \cdot 10^{-19}$	0.00
C42	$2.54 \cdot 10^{5}$	$3.64 \cdot 10^{5}$	$-1.09 \cdot 10^{5}$	$-1.91 \cdot 10^{1}$	$1.84 \cdot 10^{-17}$	0.03
C43	$-1.19 \cdot 10^{4}$	$-5.92 \cdot 10^{3}$	$-6.00 \cdot 10^{3}$	2.13	$8.63 \cdot 10^{-19}$	0.00
C44	$-1.26 \cdot 10^{4}$	$-7.33 \cdot 10^{3}$	$-5.29 \cdot 10^{3}$	$-3.86 \cdot 10^{-1}$	$9.14 \cdot 10^{-19}$	0.00
C45	$1.14 \cdot 10^{5}$	$1.51 \cdot 10^{5}$	$-3.75 \cdot 10^{4}$	-8.35	$8.23 \cdot 10^{-18}$	0.01
C46	$4.67 \cdot 10^{4}$	$6.65 \cdot 10^{4}$	$-1.98 \cdot 10^{4}$	$-3.08 \cdot 10^{1}$	$3.38 \cdot 10^{-18}$	0.01
C47	$7.01 \cdot 10^{4}$	$1.00 \cdot 10^{5}$	$-3.02 \cdot 10^{4}$	$-1.51 \cdot 10^{1}$	$5.08 \cdot 10^{-18}$	0.01
C48	$1.28 \cdot 10^{5}$	$1.82 \cdot 10^{5}$	$-5.40 \cdot 10^{4}$	-5.20	$9.30 \cdot 10^{-18}$	0.02

TABLE SI-XXIII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **7**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$-9.10 \cdot 10^{5}$	$-3.46 \cdot 10^{5}$	$-5.64 \cdot 10^{5}$	$6.53 \cdot 10^{1}$	$2.23 \cdot 10^{-16}$	0.40
O2	$3.11 \cdot 10^{6}$	$4.13 \cdot 10^{6}$	$-1.02 \cdot 10^{6}$	$-2.18 \cdot 10^{1}$	$7.63 \cdot 10^{-16}$	1.38
O3	$1.80 \cdot 10^{6}$	$2.50 \cdot 10^{6}$	$-6.96 \cdot 10^{5}$	$-7.67 \cdot 10^{2}$	$4.42 \cdot 10^{-16}$	0.80
O4	$1.62 \cdot 10^{5}$	$-3.47 \cdot 10^{5}$	$5.08 \cdot 10^{5}$	$1.52 \cdot 10^{3}$	$3.98 \cdot 10^{-17}$	0.07
O5	$-2.42 \cdot 10^{6}$	$-4.07 \cdot 10^{6}$	$1.65 \cdot 10^{6}$	$-1.72 \cdot 10^{2}$	$5.95 \cdot 10^{-16}$	1.07
O6	$-1.93 \cdot 10^{6}$	$-2.79 \cdot 10^{6}$	$8.60 \cdot 10^{5}$	$-1.22 \cdot 10^{3}$	$4.74 \cdot 10^{-16}$	0.86
N1	$-6.94 \cdot 10^{4}$	$3.27 \cdot 10^{5}$	$-3.97 \cdot 10^{5}$	$9.52 \cdot 10^{2}$	$1.11 \cdot 10^{-18}$	0.00
N2	$1.15 \cdot 10^{4}$	$3.27 \cdot 10^{5}$	$-3.16 \cdot 10^{5}$	$-3.17 \cdot 10^{2}$	$1.84 \cdot 10^{-19}$	0.00
N3	$-3.12 \cdot 10^{4}$	$-9.83 \cdot 10^{3}$	$-2.14 \cdot 10^{4}$	$1.68 \cdot 10^{1}$	$4.98 \cdot 10^{-19}$	0.00
N4	$-3.67 \cdot 10^{4}$	$-2.12 \cdot 10^{4}$	$-1.55 \cdot 10^{4}$	-7.59	$5.85 \cdot 10^{-19}$	0.00
F1	$-2.13 \cdot 10^{5}$	$-3.17 \cdot 10^{5}$	$1.03 \cdot 10^{5}$	$-5.51 \cdot 10^{1}$	$2.16 \cdot 10^{-16}$	0.39
F2	$-2.11 \cdot 10^{5}$	$-3.67 \cdot 10^{5}$	$1.57 \cdot 10^{5}$	2.30	$2.14 \cdot 10^{-16}$	0.39
F3	$-2.79 \cdot 10^{5}$	$-4.15 \cdot 10^{5}$	$1.36 \cdot 10^{5}$	$-3.66 \cdot 10^{1}$	$2.83 \cdot 10^{-16}$	0.51
F4	$-4.90 \cdot 10^{4}$	$-9.70 \cdot 10^{4}$	$4.80 \cdot 10^{4}$	$-8.90 \cdot 10^{1}$	$4.98 \cdot 10^{-17}$	0.09
F5	$3.19 \cdot 10^{3}$	$-2.25 \cdot 10^{4}$	$2.56 \cdot 10^{4}$	$1.06 \cdot 10^{2}$	$3.24 \cdot 10^{-18}$	0.01
F6	$5.68 \cdot 10^{4}$	$2.16 \cdot 10^{4}$	$3.51 \cdot 10^{4}$	$1.55 \cdot 10^{2}$	$5.76 \cdot 10^{-17}$	0.10
F7	$-1.04 \cdot 10^{5}$	$-2.32 \cdot 10^{5}$	$1.27 \cdot 10^{5}$	$9.03 \cdot 10^{1}$	$1.06 \cdot 10^{-16}$	0.19
F8	$-2.61 \cdot 10^{5}$	$-4.30 \cdot 10^{5}$	$1.69 \cdot 10^{5}$	$-1.09 \cdot 10^{2}$	$2.65 \cdot 10^{-16}$	0.48
F9	$-1.76 \cdot 10^{5}$	$-2.35 \cdot 10^{5}$	$5.92 \cdot 10^{4}$	$-1.05 \cdot 10^{2}$	$1.78 \cdot 10^{-16}$	0.32

TABLE SI-XXIV: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **7**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
H1	$6.53 \cdot 10^{3}$	$-4.52 \cdot 10^{4}$	$5.18 \cdot 10^{4}$	$-6.38 \cdot 10^{1}$	$7.47 \cdot 10^{-18}$	0.01
H2	$-4.59 \cdot 10^{4}$	$-1.19 \cdot 10^{5}$	$7.31 \cdot 10^{4}$	$-1.06 \cdot 10^{2}$	$5.26 \cdot 10^{-17}$	0.09
H3	$-1.89 \cdot 10^{5}$	$-3.69 \cdot 10^{5}$	$1.81 \cdot 10^{5}$	$-2.45 \cdot 10^{2}$	$2.16 \cdot 10^{-16}$	0.39
H4	$-7.73 \cdot 10^{5}$	$-1.28 \cdot 10^{6}$	$5.07 \cdot 10^{5}$	$-4.59 \cdot 10^{2}$	$8.86 \cdot 10^{-16}$	1.60
H5	$-1.67 \cdot 10^{5}$	$-2.10 \cdot 10^{5}$	$4.27 \cdot 10^{4}$	$1.31 \cdot 10^{2}$	$1.91 \cdot 10^{-16}$	0.35
H6	$-1.24 \cdot 10^{5}$	$-1.40 \cdot 10^{5}$	$1.61 \cdot 10^{4}$	$4.99 \cdot 10^{1}$	$1.42 \cdot 10^{-16}$	0.26
H7	$-1.26 \cdot 10^{5}$	$-9.53 \cdot 10^{4}$	$-3.05 \cdot 10^{4}$	$-1.13 \cdot 10^{1}$	$1.44 \cdot 10^{-16}$	0.26
H8	$2.79 \cdot 10^{5}$	$5.52 \cdot 10^{5}$	$-2.73 \cdot 10^{5}$	$-3.32 \cdot 10^{2}$	$3.19 \cdot 10^{-16}$	0.58
H9	$-3.36 \cdot 10^{5}$	$-4.60 \cdot 10^{5}$	$1.21 \cdot 10^{5}$	$2.40 \cdot 10^{3}$	$3.85 \cdot 10^{-16}$	0.70
H10	$-1.37 \cdot 10^{4}$	$-1.01 \cdot 10^{4}$	$-4.12 \cdot 10^{3}$	$5.70 \cdot 10^{2}$	$1.56 \cdot 10^{-17}$	0.03
H11	$-3.32 \cdot 10^{4}$	$-3.59 \cdot 10^{4}$	$2.36 \cdot 10^{3}$	$2.98 \cdot 10^{2}$	$3.80 \cdot 10^{-17}$	0.07
H12	$-1.97 \cdot 10^{5}$	$-2.89 \cdot 10^{5}$	$9.17 \cdot 10^{4}$	$1.75 \cdot 10^{2}$	$2.25 \cdot 10^{-16}$	0.41
H13	$-3.64 \cdot 10^{5}$	$-5.80 \cdot 10^{5}$	$2.16 \cdot 10^{5}$	$-1.35 \cdot 10^{2}$	$4.17 \cdot 10^{-16}$	0.75
H14	$-3.05 \cdot 10^{5}$	$-5.09 \cdot 10^{5}$	$2.05 \cdot 10^{5}$	$-2.02 \cdot 10^{2}$	$3.49 \cdot 10^{-16}$	0.63
H15	$-3.84 \cdot 10^{5}$	$-6.92 \cdot 10^{5}$	$3.08 \cdot 10^{5}$	$-2.84 \cdot 10^{2}$	$4.40 \cdot 10^{-16}$	0.80
H16	$-9.93 \cdot 10^{5}$	$-2.06 \cdot 10^{6}$	$1.07 \cdot 10^{6}$	$-9.30 \cdot 10^{2}$	$1.14 \cdot 10^{-15}$	2.06
H17	$6.79 \cdot 10^{4}$	$1.06 \cdot 10^{5}$	$-3.82 \cdot 10^{4}$	$-7.15 \cdot 10^{1}$	$7.78 \cdot 10^{-17}$	0.14
H18	$1.47 \cdot 10^{4}$	$4.60 \cdot 10^{4}$	$-3.12 \cdot 10^{4}$	$-5.92 \cdot 10^{1}$	$1.69 \cdot 10^{-17}$	0.03
H19	$-7.13 \cdot 10^{4}$	$-3.35 \cdot 10^{4}$	$-3.78 \cdot 10^{4}$	$-3.81 \cdot 10^{1}$	$8.16 \cdot 10^{-17}$	0.15
H20	$-2.90 \cdot 10^{5}$	$-2.06 \cdot 10^{5}$	$-8.40 \cdot 10^{4}$	$2.32 \cdot 10^{2}$	$3.32 \cdot 10^{-16}$	0.60

TABLE SI-XXV: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **8**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$-1.14 \cdot 10^{4}$	$-9.59 \cdot 10^{4}$	$8.47 \cdot 10^{4}$	$-1.13 \cdot 10^{2}$	$8.22 \cdot 10^{-19}$	0.00
C2	$-5.92 \cdot 10^{4}$	$-1.61 \cdot 10^{5}$	$1.02 \cdot 10^{5}$	$-1.47 \cdot 10^{2}$	$4.28 \cdot 10^{-18}$	0.01
C3	$-1.64 \cdot 10^{5}$	$-3.55 \cdot 10^{5}$	$1.92 \cdot 10^{5}$	$-2.69 \cdot 10^{2}$	$1.19 \cdot 10^{-17}$	0.02
C4	$-2.54 \cdot 10^{5}$	$-6.20 \cdot 10^{5}$	$3.67 \cdot 10^{5}$	$-5.02 \cdot 10^{2}$	$1.84 \cdot 10^{-17}$	0.03
C5	$-1.07 \cdot 10^{6}$	$-2.21 \cdot 10^{6}$	$1.14 \cdot 10^{6}$	$-1.54 \cdot 10^{3}$	$7.74 \cdot 10^{-17}$	0.14
C6	$-1.42 \cdot 10^{6}$	$-2.39 \cdot 10^{6}$	$9.74 \cdot 10^{5}$	$-9.73 \cdot 10^{2}$	$1.03 \cdot 10^{-16}$	0.19
C7	$-2.04 \cdot 10^{6}$	$-3.20 \cdot 10^{6}$	$1.16 \cdot 10^{6}$	$-7.43 \cdot 10^{2}$	$1.48 \cdot 10^{-16}$	0.27
C8	$-6.82 \cdot 10^{5}$	$-1.02 \cdot 10^{6}$	$3.38 \cdot 10^{5}$	$-7.54 \cdot 10^{1}$	$4.93 \cdot 10^{-17}$	0.09
C9	$-2.24 \cdot 10^{5}$	$-2.71 \cdot 10^{5}$	$4.71 \cdot 10^{4}$	$1.65 \cdot 10^{2}$	$1.62 \cdot 10^{-17}$	0.03
C10	$-1.80 \cdot 10^{5}$	$-2.03 \cdot 10^{5}$	$2.27 \cdot 10^{4}$	$8.80 \cdot 10^{1}$	$1.30 \cdot 10^{-17}$	0.02
C11	$-2.14 \cdot 10^{5}$	$-2.06 \cdot 10^{5}$	$-8.30 \cdot 10^{3}$	$6.83 \cdot 10^{1}$	$1.55 \cdot 10^{-17}$	0.03
C12	$-4.43 \cdot 10^{5}$	$-4.17 \cdot 10^{5}$	$-2.68 \cdot 10^{4}$	$2.91 \cdot 10^{2}$	$3.21 \cdot 10^{-17}$	0.06
C13	$-2.74 \cdot 10^{5}$	$2.36 \cdot 10^{5}$	$-5.10 \cdot 10^{5}$	$2.23 \cdot 10^{2}$	$1.99 \cdot 10^{-17}$	0.04
C14	$6.48 \cdot 10^{5}$	$1.24 \cdot 10^{6}$	$-5.88 \cdot 10^{5}$	$-6.75 \cdot 10^{2}$	$4.69 \cdot 10^{-17}$	0.08
C15	$1.87 \cdot 10^{6}$	$2.75 \cdot 10^{6}$	$-8.71 \cdot 10^{5}$	$-1.65 \cdot 10^{3}$	$1.36 \cdot 10^{-16}$	0.24
C16	$6.60 \cdot 10^{5}$	$8.97 \cdot 10^{5}$	$-2.36 \cdot 10^{5}$	$-5.58 \cdot 10^{2}$	$4.78 \cdot 10^{-17}$	0.09
C17	$-6.21 \cdot 10^{4}$	$2.05 \cdot 10^{3}$	$-6.66 \cdot 10^{4}$	$2.42 \cdot 10^{3}$	$4.50 \cdot 10^{-18}$	0.01
C18	$-1.61 \cdot 10^{4}$	$4.99 \cdot 10^{3}$	$-2.20 \cdot 10^{4}$	$8.48 \cdot 10^{2}$	$1.17 \cdot 10^{-18}$	0.00
C19	$-5.30 \cdot 10^{4}$	$-5.54 \cdot 10^{4}$	$1.88 \cdot 10^{3}$	$4.95 \cdot 10^{2}$	$3.84 \cdot 10^{-18}$	0.01
C20	$-2.05 \cdot 10^{5}$	$-2.85 \cdot 10^{5}$	$7.96 \cdot 10^{4}$	$4.26 \cdot 10^{2}$	$1.48 \cdot 10^{-17}$	0.03
C21	$-6.41 \cdot 10^{5}$	$-9.31 \cdot 10^{5}$	$2.89 \cdot 10^{5}$	$8.20 \cdot 10^{2}$	$4.64 \cdot 10^{-17}$	0.08
C22	$-1.34 \cdot 10^{6}$	$-2.19 \cdot 10^{6}$	$8.46 \cdot 10^{5}$	$-6.38 \cdot 10^{2}$	$9.72 \cdot 10^{-17}$	0.18
C23	$-5.95 \cdot 10^{5}$	$-9.70 \cdot 10^{5}$	$3.76 \cdot 10^{5}$	$-3.26 \cdot 10^{2}$	$4.31 \cdot 10^{-17}$	0.08
C24	$-4.85 \cdot 10^{5}$	$-8.16 \cdot 10^{5}$	$3.32 \cdot 10^{5}$	$-3.40 \cdot 10^{2}$	$3.51 \cdot 10^{-17}$	0.06
C25	$-6.19 \cdot 10^{5}$	$-1.09 \cdot 10^{6}$	$4.76 \cdot 10^{5}$	$-4.94 \cdot 10^{2}$	$4.48 \cdot 10^{-17}$	0.08
C26	$-1.42 \cdot 10^{6}$	$-2.64 \cdot 10^{6}$	$1.22 \cdot 10^{6}$	$-1.38 \cdot 10^{3}$	$1.03 \cdot 10^{-16}$	0.19
C27	$8.00 \cdot 10^{4}$	$1.36 \cdot 10^{5}$	$-5.57 \cdot 10^{4}$	$-1.08 \cdot 10^{2}$	$5.79 \cdot 10^{-18}$	0.01
C28	$2.79 \cdot 10^{4}$	$7.48 \cdot 10^{4}$	$-4.68 \cdot 10^{4}$	$-8.90 \cdot 10^{1}$	$2.02 \cdot 10^{-18}$	0.00
C29	$-2.48 \cdot 10^{4}$	$3.66 \cdot 10^{4}$	$-6.13 \cdot 10^{4}$	$-9.50 \cdot 10^{1}$	$1.79 \cdot 10^{-18}$	0.00
C30	$9.25 \cdot 10^{4}$	$2.69 \cdot 10^{5}$	$-1.76 \cdot 10^{5}$	$-2.92 \cdot 10^{2}$	$6.70 \cdot 10^{-18}$	0.01
C31	$5.11 \cdot 10^{4}$	$5.56 \cdot 10^{5}$	$-5.04 \cdot 10^{5}$	$-4.96 \cdot 10^{2}$	$3.70 \cdot 10^{-18}$	0.01
C32	$-4.59 \cdot 10^{5}$	$-2.35 \cdot 10^{5}$	$-2.24 \cdot 10^{5}$	$4.50 \cdot 10^{2}$	$3.32 \cdot 10^{-17}$	0.06
C33	$-8.21 \cdot 10^{5}$	$-6.14 \cdot 10^{5}$	$-2.09 \cdot 10^{5}$	$1.92 \cdot 10^{3}$	$5.94 \cdot 10^{-17}$	0.11
C34	$-3.28 \cdot 10^{5}$	$-3.07 \cdot 10^{5}$	$-2.21 \cdot 10^{4}$	$8.98 \cdot 10^{2}$	$2.38 \cdot 10^{-17}$	0.04

TABLE SI-XXVI: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **8**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$-3.58 \cdot 10^{5}$	$-2.58 \cdot 10^{6}$	$2.23 \cdot 10^{6}$	$-4.46 \cdot 10^{3}$	$8.79 \cdot 10^{-17}$	0.16
O2	$-3.76 \cdot 10^{6}$	$-5.71 \cdot 10^{6}$	$1.95 \cdot 10^{6}$	$5.56 \cdot 10^{2}$	$9.23 \cdot 10^{-16}$	1.67
O3	$-1.36 \cdot 10^{6}$	$6.33 \cdot 10^{3}$	$-1.37 \cdot 10^{6}$	$3.76 \cdot 10^{3}$	$3.35 \cdot 10^{-16}$	0.61
O4	$5.62 \cdot 10^{6}$	$7.27 \cdot 10^{6}$	$-1.64 \cdot 10^{6}$	$-5.13 \cdot 10^{3}$	$1.38 \cdot 10^{-15}$	2.49
O5	$2.34 \cdot 10^{6}$	$4.32 \cdot 10^{6}$	$-1.97 \cdot 10^{6}$	$-2.99 \cdot 10^{3}$	$5.75 \cdot 10^{-16}$	1.04
O6	$-1.72 \cdot 10^{6}$	$-1.15 \cdot 10^{6}$	$-5.72 \cdot 10^{5}$	$7.75 \cdot 10^{3}$	$4.21 \cdot 10^{-16}$	0.76
N1	$-3.46 \cdot 10^{6}$	$-6.16 \cdot 10^{6}$	$2.70 \cdot 10^{6}$	$-3.52 \cdot 10^{3}$	$5.53 \cdot 10^{-17}$	0.10
N2	$-3.09 \cdot 10^{5}$	$-1.59 \cdot 10^{5}$	$-1.54 \cdot 10^{5}$	$4.74 \cdot 10^{3}$	$4.92 \cdot 10^{-18}$	0.01
F1	$-4.39 \cdot 10^{5}$	$-6.64 \cdot 10^{5}$	$2.26 \cdot 10^{5}$	$-1.14 \cdot 10^{2}$	$4.45 \cdot 10^{-16}$	0.80
F2	$-2.96 \cdot 10^{5}$	$-4.47 \cdot 10^{5}$	$1.51 \cdot 10^{5}$	$1.05 \cdot 10^{2}$	$3.01 \cdot 10^{-16}$	0.54
F3	$-4.76 \cdot 10^{5}$	$-6.64 \cdot 10^{5}$	$1.87 \cdot 10^{5}$	$-1.36 \cdot 10^{1}$	$4.83 \cdot 10^{-16}$	0.87
F4	$4.36 \cdot 10^{5}$	$6.20 \cdot 10^{5}$	$-1.84 \cdot 10^{5}$	$-3.83 \cdot 10^{2}$	$4.42 \cdot 10^{-16}$	0.80
F5	$2.83 \cdot 10^{5}$	$3.82 \cdot 10^{5}$	$-9.89 \cdot 10^{4}$	$-1.69 \cdot 10^{2}$	$2.87 \cdot 10^{-16}$	0.52
F6	$5.31 \cdot 10^{5}$	$6.34 \cdot 10^{5}$	$-1.02 \cdot 10^{5}$	$-4.97 \cdot 10^{2}$	$5.39 \cdot 10^{-16}$	0.97
F7	$-3.93 \cdot 10^{5}$	$-5.33 \cdot 10^{5}$	$1.39 \cdot 10^{5}$	$6.68 \cdot 10^{2}$	$3.99 \cdot 10^{-16}$	0.72
F8	$-3.84 \cdot 10^{4}$	$9.01 \cdot 10^{4}$	$-1.29 \cdot 10^{5}$	$8.04 \cdot 10^{2}$	$3.90 \cdot 10^{-17}$	0.07
F9	$-2.03 \cdot 10^{5}$	$-1.91 \cdot 10^{5}$	$-1.18 \cdot 10^{4}$	$3.98 \cdot 10^{2}$	$2.06 \cdot 10^{-16}$	0.37
S1	$2.69 \cdot 10^{4}$	$-1.27 \cdot 10^{5}$	$1.54 \cdot 10^{5}$	$-1.76 \cdot 10^{2}$	$9.09 \cdot 10^{-19}$	0.00
S2	$-4.71 \cdot 10^{5}$	$-5.66 \cdot 10^{5}$	$9.47 \cdot 10^{4}$	$4.84 \cdot 10^{2}$	$1.59 \cdot 10^{-17}$	0.03
S3	$2.27 \cdot 10^{5}$	$3.54 \cdot 10^{5}$	$-1.26 \cdot 10^{5}$	$-2.36 \cdot 10^{2}$	$7.68 \cdot 10^{-18}$	0.01

TABLE SI-XXVII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **8**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
H1	$6.91 \cdot 10^{4}$	$5.77 \cdot 10^{4}$	$1.15 \cdot 10^{4}$	$-1.16 \cdot 10^{2}$	$7.91 \cdot 10^{-17}$	0.14
H2	$4.67 \cdot 10^{4}$	$1.36 \cdot 10^{4}$	$3.31 \cdot 10^{4}$	$-7.54 \cdot 10^{1}$	$5.34 \cdot 10^{-17}$	0.10
H3	$4.33 \cdot 10^{4}$	$-6.55 \cdot 10^{4}$	$1.09 \cdot 10^{5}$	$-9.06 \cdot 10^{1}$	$4.96 \cdot 10^{-17}$	0.09
H4	$2.19 \cdot 10^{4}$	$-3.19 \cdot 10^{5}$	$3.41 \cdot 10^{5}$	$-9.53 \cdot 10^{1}$	$2.51 \cdot 10^{-17}$	0.05
H5	$8.10 \cdot 10^{4}$	$1.51 \cdot 10^{5}$	$-6.97 \cdot 10^{4}$	-9.82	$9.27 \cdot 10^{-17}$	0.17
H6	$-6.24 \cdot 10^{3}$	$3.62 \cdot 10^{4}$	$-4.25 \cdot 10^{4}$	$4.32 \cdot 10^{1}$	$7.14 \cdot 10^{-18}$	0.01
H7	$-1.65 \cdot 10^{5}$	$-1.36 \cdot 10^{5}$	$-2.96 \cdot 10^{4}$	$1.45 \cdot 10^{2}$	$1.89 \cdot 10^{-16}$	0.34
H8	$-7.44 \cdot 10^{5}$	$-8.68 \cdot 10^{5}$	$1.23 \cdot 10^{5}$	$3.55 \cdot 10^{2}$	$8.52 \cdot 10^{-16}$	1.54
H9	$-1.33 \cdot 10^{5}$	$-2.93 \cdot 10^{5}$	$1.59 \cdot 10^{5}$	-3.99	$1.53 \cdot 10^{-16}$	0.28
H10	$-5.65 \cdot 10^{4}$	$-1.68 \cdot 10^{5}$	$1.11 \cdot 10^{5}$	$-1.54 \cdot 10^{1}$	$6.47 \cdot 10^{-17}$	0.12
H11	$5.80 \cdot 10^{4}$	$-4.61 \cdot 10^{4}$	$1.04 \cdot 10^{5}$	$-5.91 \cdot 10^{1}$	$6.65 \cdot 10^{-17}$	0.12
H12	$6.11 \cdot 10^{5}$	$6.97 \cdot 10^{5}$	$-8.55 \cdot 10^{4}$	$-2.00 \cdot 10^{2}$	$7.00 \cdot 10^{-16}$	1.26
H13	$-1.80 \cdot 10^{5}$	$-5.67 \cdot 10^{5}$	$3.88 \cdot 10^{5}$	$-4.64 \cdot 10^{2}$	$2.06 \cdot 10^{-16}$	0.37
H14	$5.23 \cdot 10^{3}$	$-3.62 \cdot 10^{4}$	$4.15 \cdot 10^{4}$	$-1.07 \cdot 10^{2}$	$5.99 \cdot 10^{-18}$	0.01
H15	$1.57 \cdot 10^{4}$	$5.86 \cdot 10^{4}$	$-4.28 \cdot 10^{4}$	$-1.47 \cdot 10^{1}$	$1.80 \cdot 10^{-17}$	0.03
H16	$-1.93 \cdot 10^{4}$	$6.66 \cdot 10^{4}$	$-8.60 \cdot 10^{4}$	$6.64 \cdot 10^{1}$	$2.21 \cdot 10^{-17}$	0.04
H17	$-7.37 \cdot 10^{4}$	$2.17 \cdot 10^{4}$	$-9.55 \cdot 10^{4}$	$1.24 \cdot 10^{2}$	$8.44 \cdot 10^{-17}$	0.15
H18	$-1.77 \cdot 10^{5}$	$-1.10 \cdot 10^{5}$	$-6.69 \cdot 10^{4}$	$1.78 \cdot 10^{2}$	$2.02 \cdot 10^{-16}$	0.37
H19	$-3.20 \cdot 10^{5}$	$-3.40 \cdot 10^{5}$	$1.99 \cdot 10^{4}$	$2.03 \cdot 10^{2}$	$3.66 \cdot 10^{-16}$	0.66
H20	$-1.35 \cdot 10^{6}$	$-1.80 \cdot 10^{6}$	$4.48 \cdot 10^{5}$	$5.20 \cdot 10^{2}$	$1.55 \cdot 10^{-15}$	2.79

TABLE SI-XXVIII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **9**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$9.30 \cdot 10^{4}$	$6.69 \cdot 10^{4}$	$2.63 \cdot 10^{4}$	$-1.52 \cdot 10^{2}$	$6.73 \cdot 10^{-18}$	0.01
C2	$6.93 \cdot 10^{4}$	$2.36 \cdot 10^{4}$	$4.58 \cdot 10^{4}$	$-1.13 \cdot 10^{2}$	$5.02 \cdot 10^{-18}$	0.01
C3	$7.87 \cdot 10^{4}$	$-2.47 \cdot 10^{4}$	$1.04 \cdot 10^{5}$	$-1.36 \cdot 10^{2}$	$5.70 \cdot 10^{-18}$	0.01
C4	$2.32 \cdot 10^{5}$	$5.76 \cdot 10^{4}$	$1.75 \cdot 10^{5}$	$-3.51 \cdot 10^{2}$	$1.68 \cdot 10^{-17}$	0.03
C5	$4.47 \cdot 10^{5}$	$-2.12 \cdot 10^{5}$	$6.60 \cdot 10^{5}$	$-7.13 \cdot 10^{2}$	$3.24 \cdot 10^{-17}$	0.06
C6	$-6.81 \cdot 10^{2}$	$-6.93 \cdot 10^{5}$	$6.93 \cdot 10^{5}$	$-1.92 \cdot 10^{2}$	$4.93 \cdot 10^{-20}$	0.00
C7	$-4.59 \cdot 10^{5}$	$-1.64 \cdot 10^{6}$	$1.18 \cdot 10^{6}$	$-4.97 \cdot 10^{1}$	$3.33 \cdot 10^{-17}$	0.06
C8	$-2.21 \cdot 10^{5}$	$-6.31 \cdot 10^{5}$	$4.10 \cdot 10^{5}$	$-1.52 \cdot 10^{1}$	$1.60 \cdot 10^{-17}$	0.03
C9	$8.68 \cdot 10^{4}$	$1.80 \cdot 10^{5}$	$-9.36 \cdot 10^{4}$	9.45	$6.28 \cdot 10^{-18}$	0.01
C10	$6.24 \cdot 10^{3}$	$7.30 \cdot 10^{4}$	$-6.68 \cdot 10^{4}$	$5.52 \cdot 10^{1}$	$4.51 \cdot 10^{-19}$	0.00
C11	$-8.98 \cdot 10^{4}$	$-1.44 \cdot 10^{4}$	$-7.55 \cdot 10^{4}$	$1.36 \cdot 10^{2}$	$6.50 \cdot 10^{-18}$	0.01
C12	$-4.20 \cdot 10^{4}$	$1.66 \cdot 10^{5}$	$-2.08 \cdot 10^{5}$	$2.23 \cdot 10^{2}$	$3.04 \cdot 10^{-18}$	0.01
C13	$-7.17 \cdot 10^{5}$	$-3.47 \cdot 10^{5}$	$-3.70 \cdot 10^{5}$	$8.74 \cdot 10^{2}$	$5.19 \cdot 10^{-17}$	0.09
C14	$-1.32 \cdot 10^{6}$	$-1.43 \cdot 10^{6}$	$1.13 \cdot 10^{5}$	$7.28 \cdot 10^{2}$	$9.53 \cdot 10^{-17}$	0.17
C15	$-2.03 \cdot 10^{6}$	$-2.32 \cdot 10^{6}$	$2.84 \cdot 10^{5}$	$7.30 \cdot 10^{2}$	$1.47 \cdot 10^{-16}$	0.27
C16	$-6.91 \cdot 10^{5}$	$-8.28 \cdot 10^{5}$	$1.37 \cdot 10^{5}$	$1.31 \cdot 10^{2}$	$5.00 \cdot 10^{-17}$	0.09
C17	$-1.61 \cdot 10^{5}$	$-3.76 \cdot 10^{5}$	$2.15 \cdot 10^{5}$	-9.98	$1.16 \cdot 10^{-17}$	0.02
C18	$-8.51 \cdot 10^{4}$	$-2.49 \cdot 10^{5}$	$1.64 \cdot 10^{5}$	$-2.08 \cdot 10^{1}$	$6.16 \cdot 10^{-18}$	0.01
C19	$-1.05 \cdot 10^{4}$	$-1.89 \cdot 10^{5}$	$1.78 \cdot 10^{5}$	$-5.37 \cdot 10^{1}$	$7.60 \cdot 10^{-19}$	0.00
C20	$-1.44 \cdot 10^{5}$	$-6.10 \cdot 10^{5}$	$4.66 \cdot 10^{5}$	$-8.46 \cdot 10^{1}$	$1.04 \cdot 10^{-17}$	0.02
C21	$3.22 \cdot 10^{5}$	$-4.87 \cdot 10^{5}$	$8.09 \cdot 10^{5}$	$-3.46 \cdot 10^{2}$	$2.33 \cdot 10^{-17}$	0.04
C22	$1.17 \cdot 10^{6}$	$1.32 \cdot 10^{6}$	$-1.48 \cdot 10^{5}$	$-3.98 \cdot 10^{2}$	$8.49 \cdot 10^{-17}$	0.15
C23	$2.37 \cdot 10^{6}$	$3.35 \cdot 10^{6}$	$-9.76 \cdot 10^{5}$	$-7.08 \cdot 10^{2}$	$1.72 \cdot 10^{-16}$	0.31
C24	$8.65 \cdot 10^{5}$	$1.30 \cdot 10^{6}$	$-4.39 \cdot 10^{5}$	$-2.42 \cdot 10^{2}$	$6.26 \cdot 10^{-17}$	0.11
C25	$3.98 \cdot 10^{4}$	$-9.01 \cdot 10^{4}$	$1.30 \cdot 10^{5}$	$-4.32 \cdot 10^{2}$	$2.88 \cdot 10^{-18}$	0.01
C26	$2.90 \cdot 10^{4}$	$1.91 \cdot 10^{4}$	$1.00 \cdot 10^{4}$	$-1.33 \cdot 10^{2}$	$2.10 \cdot 10^{-18}$	0.00
C27	$2.42 \cdot 10^{4}$	$9.35 \cdot 10^{4}$	$-6.94 \cdot 10^{4}$	$-2.50 \cdot 10^{1}$	$1.75 \cdot 10^{-18}$	0.00
C28	$-1.96 \cdot 10^{4}$	$1.74 \cdot 10^{5}$	$-1.94 \cdot 10^{5}$	$1.03 \cdot 10^{2}$	$1.42 \cdot 10^{-18}$	0.00
C29	$-2.00 \cdot 10^{5}$	$3.50 \cdot 10^{5}$	$-5.51 \cdot 10^{5}$	$3.86 \cdot 10^{2}$	$1.45 \cdot 10^{-17}$	0.03
C30	$-4.48 \cdot 10^{4}$	$9.08 \cdot 10^{4}$	$-1.36 \cdot 10^{5}$	$1.17 \cdot 10^{2}$	$3.24 \cdot 10^{-18}$	0.01
C31	$-1.04 \cdot 10^{5}$	$3.95 \cdot 10^{4}$	$-1.44 \cdot 10^{5}$	$1.77 \cdot 10^{2}$	$7.54 \cdot 10^{-18}$	0.01
C32	$-3.01 \cdot 10^{5}$	$-8.23 \cdot 10^{4}$	$-2.20 \cdot 10^{5}$	$3.73 \cdot 10^{2}$	$2.18 \cdot 10^{-17}$	0.04
C33	$-7.74 \cdot 10^{5}$	$-1.94 \cdot 10^{5}$	$-5.81 \cdot 10^{5}$	$9.19 \cdot 10^{2}$	$5.60 \cdot 10^{-17}$	0.10
C34	$-2.96 \cdot 10^{5}$	$-1.93 \cdot 10^{5}$	$-1.04 \cdot 10^{5}$	$2.89 \cdot 10^{2}$	$2.15 \cdot 10^{-17}$	0.04
C35	$-4.78 \cdot 10^{5}$	$-4.53 \cdot 10^{5}$	$-2.45 \cdot 10^{4}$	$3.49 \cdot 10^{2}$	$3.46 \cdot 10^{-17}$	0.06
C36	$-1.37 \cdot 10^{6}$	$-1.48 \cdot 10^{6}$	$1.08 \cdot 10^{5}$	$8.41 \cdot 10^{2}$	$9.93 \cdot 10^{-17}$	0.18

TABLE SI-XXIX: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **9**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$1.85 \cdot 10^{6}$	$6.06 \cdot 10^{5}$	$1.25 \cdot 10^{6}$	$-2.98 \cdot 10^{3}$	$4.54 \cdot 10^{-16}$	0.82
O2	$-1.74 \cdot 10^{6}$	$-4.84 \cdot 10^{6}$	$3.10 \cdot 10^{6}$	$-1.81 \cdot 10^{2}$	$4.28 \cdot 10^{-16}$	0.77
O3	$8.70 \cdot 10^{5}$	$3.05 \cdot 10^{6}$	$-2.18 \cdot 10^{6}$	$1.36 \cdot 10^{3}$	$2.14 \cdot 10^{-16}$	0.39
O4	$-4.17 \cdot 10^{6}$	$-4.45 \cdot 10^{6}$	$2.79 \cdot 10^{5}$	$9.13 \cdot 10^{2}$	$1.02 \cdot 10^{-15}$	1.85
O5	$-1.81 \cdot 10^{6}$	$-5.94 \cdot 10^{6}$	$4.13 \cdot 10^{6}$	$-5.83 \cdot 10^{2}$	$4.45 \cdot 10^{-16}$	0.80
O6	$6.35 \cdot 10^{6}$	$9.60 \cdot 10^{6}$	$-3.25 \cdot 10^{6}$	$-2.08 \cdot 10^{3}$	$1.56 \cdot 10^{-15}$	2.82
N1	$-3.17 \cdot 10^{6}$	$-2.61 \cdot 10^{6}$	$-5.56 \cdot 10^{5}$	$2.51 \cdot 10^{3}$	$5.05 \cdot 10^{-17}$	0.09
N2	$7.85 \cdot 10^{4}$	$6.31 \cdot 10^{5}$	$-5.52 \cdot 10^{5}$	$-3.73 \cdot 10^{2}$	$1.25 \cdot 10^{-18}$	0.00
F1	$1.70 \cdot 10^{4}$	$-1.22 \cdot 10^{5}$	$1.39 \cdot 10^{5}$	-9.64	$1.73 \cdot 10^{-17}$	0.03
F2	$-9.80 \cdot 10^{4}$	$-3.28 \cdot 10^{5}$	$2.30 \cdot 10^{5}$	-7.22	$9.94 \cdot 10^{-17}$	0.18
F3	$-3.89 \cdot 10^{5}$	$-7.97 \cdot 10^{5}$	$4.07 \cdot 10^{5}$	$-1.60 \cdot 10^{1}$	$3.95 \cdot 10^{-16}$	0.71
F4	$-4.49 \cdot 10^{5}$	$-5.61 \cdot 10^{5}$	$1.13 \cdot 10^{5}$	$1.08 \cdot 10^{2}$	$4.55 \cdot 10^{-16}$	0.82
F5	$-2.54 \cdot 10^{5}$	$-1.65 \cdot 10^{5}$	$-8.95 \cdot 10^{4}$	$1.38 \cdot 10^{2}$	$2.58 \cdot 10^{-16}$	0.47
F6	$-5.54 \cdot 10^{5}$	$-7.96 \cdot 10^{5}$	$2.42 \cdot 10^{5}$	$-1.07 \cdot 10^{2}$	$5.63 \cdot 10^{-16}$	1.02
F7	$4.98 \cdot 10^{5}$	$7.31 \cdot 10^{5}$	$-2.33 \cdot 10^{5}$	$-1.17 \cdot 10^{2}$	$5.05 \cdot 10^{-16}$	0.91
F8	$4.52 \cdot 10^{5}$	$6.36 \cdot 10^{5}$	$-1.85 \cdot 10^{5}$	$-2.96 \cdot 10^{2}$	$4.58 \cdot 10^{-16}$	0.83
F9	$6.80 \cdot 10^{5}$	$1.16 \cdot 10^{6}$	$-4.75 \cdot 10^{5}$	$-3.68 \cdot 10^{1}$	$6.90 \cdot 10^{-16}$	1.25
S1	$2.21 \cdot 10^{5}$	$1.85 \cdot 10^{5}$	$3.64 \cdot 10^{4}$	$-3.58 \cdot 10^{2}$	$7.48 \cdot 10^{-18}$	0.01
S2	$2.72 \cdot 10^{5}$	$4.97 \cdot 10^{5}$	$-2.26 \cdot 10^{5}$	$-3.95 \cdot 10^{1}$	$9.18 \cdot 10^{-18}$	0.02
S3	$-3.87 \cdot 10^{5}$	$-8.75 \cdot 10^{5}$	$4.88 \cdot 10^{5}$	$-1.45 \cdot 10^{1}$	$1.31 \cdot 10^{-17}$	0.02

TABLE SI-XXX: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **9**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
H1	$1.71 \cdot 10^{5}$	$2.87 \cdot 10^{5}$	$-1.15 \cdot 10^{5}$	1.95	$1.96 \cdot 10^{-16}$	0.35
H2	$5.31 \cdot 10^{4}$	$1.12 \cdot 10^{5}$	$-5.85 \cdot 10^{4}$	1.87	$6.08 \cdot 10^{-17}$	0.11
H3	$-4.91 \cdot 10^{3}$	$5.05 \cdot 10^{4}$	$-5.55 \cdot 10^{4}$	3.51	$5.62 \cdot 10^{-18}$	0.01
H4	$6.60 \cdot 10^{5}$	$9.26 \cdot 10^{5}$	$-2.66 \cdot 10^{5}$	-3.64	$7.56 \cdot 10^{-16}$	1.37
H5	$5.52 \cdot 10^{4}$	$3.81 \cdot 10^{4}$	$1.71 \cdot 10^{4}$	$1.86 \cdot 10^{1}$	$6.32 \cdot 10^{-17}$	0.11
H6	$-2.98 \cdot 10^{4}$	$-4.66 \cdot 10^{4}$	$1.68 \cdot 10^{4}$	$1.60 \cdot 10^{1}$	$3.41 \cdot 10^{-17}$	0.06
H7	$-1.16 \cdot 10^{5}$	$-1.40 \cdot 10^{5}$	$2.42 \cdot 10^{4}$	$2.05 \cdot 10^{1}$	$1.33 \cdot 10^{-16}$	0.24
H8	$3.70 \cdot 10^{5}$	$3.41 \cdot 10^{5}$	$2.83 \cdot 10^{4}$	5.02	$4.23 \cdot 10^{-16}$	0.76
H9	$-6.10 \cdot 10^{4}$	$-1.73 \cdot 10^{5}$	$1.12 \cdot 10^{5}$	-6.58	$6.99 \cdot 10^{-17}$	0.13
H10	$5.10 \cdot 10^{4}$	$2.52 \cdot 10^{4}$	$2.58 \cdot 10^{4}$	-9.58	$5.84 \cdot 10^{-17}$	0.11
H11	$1.42 \cdot 10^{5}$	$1.58 \cdot 10^{5}$	$-1.62 \cdot 10^{4}$	$-1.56 \cdot 10^{1}$	$1.62 \cdot 10^{-16}$	0.29
H12	$-5.75 \cdot 10^{5}$	$-8.86 \cdot 10^{5}$	$3.11 \cdot 10^{5}$	$5.15 \cdot 10^{1}$	$6.58 \cdot 10^{-16}$	1.19
H13	$5.48 \cdot 10^{5}$	$8.46 \cdot 10^{5}$	$-2.98 \cdot 10^{5}$	$-1.91 \cdot 10^{2}$	$6.27 \cdot 10^{-16}$	1.13
H14	$2.66 \cdot 10^{4}$	$5.53 \cdot 10^{4}$	$-2.87 \cdot 10^{4}$	$-3.91 \cdot 10^{1}$	$3.05 \cdot 10^{-17}$	0.06
H15	$2.06 \cdot 10^{4}$	$1.78 \cdot 10^{4}$	$2.80 \cdot 10^{3}$	$-2.19 \cdot 10^{1}$	$2.35 \cdot 10^{-17}$	0.04
H16	$1.33 \cdot 10^{5}$	$1.49 \cdot 10^{5}$	$-1.56 \cdot 10^{4}$	$-2.21 \cdot 10^{1}$	$1.52 \cdot 10^{-16}$	0.28
H17	$2.68 \cdot 10^{5}$	$3.53 \cdot 10^{5}$	$-8.42 \cdot 10^{4}$	-9.81	$3.07 \cdot 10^{-16}$	0.56
H18	$9.92 \cdot 10^{5}$	$1.85 \cdot 10^{6}$	$-8.59 \cdot 10^{5}$	-8.34	$1.14 \cdot 10^{-15}$	2.05
H19	$1.06 \cdot 10^{5}$	$1.59 \cdot 10^{5}$	$-5.27 \cdot 10^{4}$	$-9.33 \cdot 10^{-1}$	$1.22 \cdot 10^{-16}$	0.22
H20	$1.69 \cdot 10^{5}$	$2.37 \cdot 10^{5}$	$-6.77 \cdot 10^{4}$	-1.08	$1.93 \cdot 10^{-16}$	0.35
H21	$9.38 \cdot 10^{4}$	$1.44 \cdot 10^{5}$	$-4.98 \cdot 10^{4}$	$-2.42 \cdot 10^{-1}$	$1.07 \cdot 10^{-16}$	0.19
H22	$1.97 \cdot 10^{5}$	$3.53 \cdot 10^{5}$	$-1.56 \cdot 10^{5}$	-2.87	$2.26 \cdot 10^{-16}$	0.41
H23	$5.29 \cdot 10^{4}$	$1.09 \cdot 10^{5}$	$-5.65 \cdot 10^{4}$	2.55	$6.06 \cdot 10^{-17}$	0.11
H24	$3.64 \cdot 10^{4}$	$9.82 \cdot 10^{4}$	$-6.18 \cdot 10^{4}$	5.82	$4.16 \cdot 10^{-17}$	0.08
H25	$2.76 \cdot 10^{5}$	$3.67 \cdot 10^{5}$	$-9.16 \cdot 10^{4}$	-8.12	$3.16 \cdot 10^{-16}$	0.57
H26	$3.62 \cdot 10^{5}$	$4.88 \cdot 10^{5}$	$-1.26 \cdot 10^{5}$	-3.32	$4.15 \cdot 10^{-16}$	0.75
H27	$1.85 \cdot 10^{5}$	$2.49 \cdot 10^{5}$	$-6.41 \cdot 10^{4}$	-2.34	$2.12 \cdot 10^{-16}$	0.38
H28	$1.00 \cdot 10^{5}$	$1.47 \cdot 10^{5}$	$-4.69 \cdot 10^{4}$	-2.53	$1.15 \cdot 10^{-16}$	0.21
H29	$9.48 \cdot 10^{4}$	$1.52 \cdot 10^{5}$	$-5.76 \cdot 10^{4}$	-2.37	$1.09 \cdot 10^{-16}$	0.20
H30	$1.40 \cdot 10^{5}$	$2.03 \cdot 10^{5}$	$-6.28 \cdot 10^{4}$	-6.01	$1.61 \cdot 10^{-16}$	0.29

TABLE SI-XXXI: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for hydrogen atoms of complex **10**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
C1	$9.81 \cdot 10^{5}$	$1.74 \cdot 10^{6}$	$-7.54 \cdot 10^{5}$	$1.74 \cdot 10^{1}$	$7.10 \cdot 10^{-17}$	0.13
C2	$2.45 \cdot 10^{5}$	$5.20 \cdot 10^{5}$	$-2.74 \cdot 10^{5}$	9.88	$1.78 \cdot 10^{-17}$	0.03
C3	$1.57 \cdot 10^{5}$	$2.93 \cdot 10^{5}$	$-1.36 \cdot 10^{5}$	3.85	$1.14 \cdot 10^{-17}$	0.02
C4	$6.60 \cdot 10^{4}$	$1.49 \cdot 10^{5}$	$-8.27 \cdot 10^{4}$	3.09	$4.78 \cdot 10^{-18}$	0.01
C5	$1.56 \cdot 10^{4}$	$9.80 \cdot 10^{4}$	$-8.24 \cdot 10^{4}$	4.58	$1.13 \cdot 10^{-18}$	0.00
C6	$1.17 \cdot 10^{6}$	$1.66 \cdot 10^{6}$	$-4.92 \cdot 10^{5}$	-7.62	$8.48 \cdot 10^{-17}$	0.15
C7	$1.38 \cdot 10^{6}$	$1.80 \cdot 10^{6}$	$-4.24 \cdot 10^{5}$	$-2.63 \cdot 10^{1}$	$9.98 \cdot 10^{-17}$	0.18
C8	$3.69 \cdot 10^{5}$	$4.63 \cdot 10^{5}$	$-9.40 \cdot 10^{4}$	-4.01	$2.67 \cdot 10^{-17}$	0.05
C9	$-3.65 \cdot 10^{5}$	$-7.53 \cdot 10^{5}$	$3.87 \cdot 10^{5}$	$1.79 \cdot 10^{2}$	$2.64 \cdot 10^{-17}$	0.05
C10	$-1.98 \cdot 10^{5}$	$-3.14 \cdot 10^{5}$	$1.16 \cdot 10^{5}$	$7.65 \cdot 10^{1}$	$1.44 \cdot 10^{-17}$	0.03
C11	$-5.13 \cdot 10^{3}$	$-3.93 \cdot 10^{4}$	$3.42 \cdot 10^{4}$	$2.92 \cdot 10^{1}$	$3.71 \cdot 10^{-19}$	0.00
C12	$-5.96 \cdot 10^{4}$	$-8.81 \cdot 10^{4}$	$2.84 \cdot 10^{4}$	$2.43 \cdot 10^{1}$	$4.32 \cdot 10^{-18}$	0.01
C13	$-1.44 \cdot 10^{5}$	$-1.81 \cdot 10^{5}$	$3.67 \cdot 10^{4}$	$2.96 \cdot 10^{1}$	$1.05 \cdot 10^{-17}$	0.02
C14	$5.79 \cdot 10^{5}$	$4.63 \cdot 10^{5}$	$1.16 \cdot 10^{5}$	$1.17 \cdot 10^{1}$	$4.19 \cdot 10^{-17}$	0.08
C15	$1.25 \cdot 10^{6}$	$1.23 \cdot 10^{6}$	$2.04 \cdot 10^{4}$	$-1.45 \cdot 10^{2}$	$9.07 \cdot 10^{-17}$	0.16
C16	$5.19 \cdot 10^{5}$	$5.68 \cdot 10^{5}$	$-4.83 \cdot 10^{4}$	$-7.66 \cdot 10^{1}$	$3.76 \cdot 10^{-17}$	0.07
C17	$-1.61 \cdot 10^{4}$	$-5.26 \cdot 10^{5}$	$5.10 \cdot 10^{5}$	-8.05	$1.16 \cdot 10^{-18}$	0.00
C18	$2.54 \cdot 10^{5}$	$1.36 \cdot 10^{5}$	$1.18 \cdot 10^{5}$	$-3.68 \cdot 10^{1}$	$1.84 \cdot 10^{-17}$	0.03
C19	$3.99 \cdot 10^{4}$	$-5.21 \cdot 10^{4}$	$9.21 \cdot 10^{4}$	$-1.54 \cdot 10^{1}$	$2.89 \cdot 10^{-18}$	0.01
C20	$8.84 \cdot 10^{4}$	$5.81 \cdot 10^{4}$	$3.03 \cdot 10^{4}$	$-1.44 \cdot 10^{1}$	$6.40 \cdot 10^{-18}$	0.01
C21	$1.73 \cdot 10^{5}$	$1.80 \cdot 10^{5}$	$-6.46 \cdot 10^{3}$	$-2.00 \cdot 10^{1}$	$1.26 \cdot 10^{-17}$	0.02
C22	$-1.07 \cdot 10^{6}$	$-1.66 \cdot 10^{6}$	$5.84 \cdot 10^{5}$	$1.06 \cdot 10^{2}$	$7.76 \cdot 10^{-17}$	0.14
C23	$-2.36 \cdot 10^{6}$	$-3.06 \cdot 10^{6}$	$7.03 \cdot 10^{5}$	$2.65 \cdot 10^{2}$	$1.71 \cdot 10^{-16}$	0.31
C24	$-9.17 \cdot 10^{5}$	$-1.10 \cdot 10^{6}$	$1.87 \cdot 10^{5}$	$1.04 \cdot 10^{2}$	$6.64 \cdot 10^{-17}$	0.12
C25	$2.30 \cdot 10^{5}$	$3.16 \cdot 10^{5}$	$-8.57 \cdot 10^{4}$	$-1.87 \cdot 10^{2}$	$1.67 \cdot 10^{-17}$	0.03
C26	$3.65 \cdot 10^{4}$	$5.24 \cdot 10^{4}$	$-1.59 \cdot 10^{4}$	$-5.98 \cdot 10^{1}$	$2.64 \cdot 10^{-18}$	0.00
C27	$3.84 \cdot 10^{4}$	$3.28 \cdot 10^{4}$	$5.61 \cdot 10^{3}$	$-3.69 \cdot 10^{1}$	$2.78 \cdot 10^{-18}$	0.01
C28	$1.42 \cdot 10^{5}$	$1.46 \cdot 10^{5}$	$-3.35 \cdot 10^{3}$	$-4.04 \cdot 10^{1}$	$1.03 \cdot 10^{-17}$	0.02
C29	$4.99 \cdot 10^{5}$	$5.31 \cdot 10^{5}$	$-3.21 \cdot 10^{4}$	$-1.07 \cdot 10^{2}$	$3.61 \cdot 10^{-17}$	0.07
C30	$9.68 \cdot 10^{5}$	$1.27 \cdot 10^{6}$	$-3.06 \cdot 10^{5}$	$-4.32 \cdot 10^{1}$	$7.01 \cdot 10^{-17}$	0.13
C31	$4.33 \cdot 10^{5}$	$5.91 \cdot 10^{5}$	$-1.58 \cdot 10^{5}$	$-1.07 \cdot 10^{1}$	$3.13 \cdot 10^{-17}$	0.06
C32	$3.37 \cdot 10^{5}$	$4.98 \cdot 10^{5}$	$-1.61 \cdot 10^{5}$	-1.88	$2.44 \cdot 10^{-17}$	0.04
C33	$4.71 \cdot 10^{5}$	$7.47 \cdot 10^{5}$	$-2.76 \cdot 10^{5}$	$3.39 \cdot 10^{-1}$	$3.41 \cdot 10^{-17}$	0.06
C34	$1.21 \cdot 10^{6}$	$1.99 \cdot 10^{6}$	$-7.81 \cdot 10^{5}$	3.67	$8.73 \cdot 10^{-17}$	0.16
C35	$1.68 \cdot 10^{5}$	$2.46 \cdot 10^{5}$	$-7.85 \cdot 10^{4}$	$-9.39 \cdot 10^{-1}$	$1.22 \cdot 10^{-17}$	0.02
C36	$1.34 \cdot 10^{5}$	$2.07 \cdot 10^{5}$	$-7.24 \cdot 10^{4}$	$-2.82 \cdot 10^{-1}$	$9.72 \cdot 10^{-18}$	0.02
C37	$2.30 \cdot 10^{5}$	$3.84 \cdot 10^{5}$	$-1.54 \cdot 10^{5}$	$-9.59 \cdot 10^{-1}$	$1.67 \cdot 10^{-17}$	0.03
C38	$2.03 \cdot 10^{5}$	$3.00 \cdot 10^{5}$	$-9.73 \cdot 10^{4}$	-3.47	$1.47 \cdot 10^{-17}$	0.03
C39	$8.43 \cdot 10^{4}$	$1.60 \cdot 10^{5}$	$-7.56 \cdot 10^{4}$	2.97	$6.11 \cdot 10^{-18}$	0.01
C40	$2.65 \cdot 10^{5}$	$3.62 \cdot 10^{5}$	$-9.62 \cdot 10^{4}$	-4.66	$1.92 \cdot 10^{-17}$	0.03
C41	$1.26 \cdot 10^{5}$	$1.89 \cdot 10^{5}$	$-6.26 \cdot 10^{4}$	-3.65	$9.13 \cdot 10^{-18}$	0.02

TABLE SI-XXXII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for carbon atoms of complex **10**.

Atom	$\bar{\Phi}^{p}$	$\bar{\Phi}^{p(2)}$	$\bar{\Phi}^{p(1)}$	$\bar{\Phi}^{p(0)}$	$\lvert P_y \rvert$	$\lvert V \rvert$
O1	$-6.63 \cdot 10^{4}$	$1.64 \cdot 10^{6}$	$-1.70 \cdot 10^{6}$	$2.09 \cdot 10^{2}$	$1.63 \cdot 10^{-17}$	0.03
O2	$2.11 \cdot 10^{6}$	$2.51 \cdot 10^{6}$	$-4.01 \cdot 10^{5}$	$-1.95 \cdot 10^{2}$	$5.18 \cdot 10^{-16}$	0.94
O3	$-4.16 \cdot 10^{6}$	$-5.69 \cdot 10^{6}$	$1.54 \cdot 10^{6}$	$7.43 \cdot 10^{2}$	$1.02 \cdot 10^{-15}$	1.84
O4	$3.37 \cdot 10^{6}$	$3.52 \cdot 10^{6}$	$-1.52 \cdot 10^{5}$	$-6.63 \cdot 10^{2}$	$8.27 \cdot 10^{-16}$	1.49
O5	$2.95 \cdot 10^{6}$	$2.61 \cdot 10^{6}$	$3.46 \cdot 10^{5}$	$-2.71 \cdot 10^{2}$	$7.25 \cdot 10^{-16}$	1.31
O6	$-6.73 \cdot 10^{6}$	$-7.89 \cdot 10^{6}$	$1.16 \cdot 10^{6}$	$7.81 \cdot 10^{2}$	$1.65 \cdot 10^{-15}$	2.98
N1	$5.82 \cdot 10^{5}$	$4.40 \cdot 10^{5}$	$1.42 \cdot 10^{5}$	$-4.10 \cdot 10^{2}$	$9.28 \cdot 10^{-18}$	0.02
N2	$2.81 \cdot 10^{6}$	$4.16 \cdot 10^{6}$	$-1.35 \cdot 10^{6}$	$-1.93 \cdot 10^{1}$	$4.48 \cdot 10^{-17}$	0.08
F1	$2.79 \cdot 10^{5}$	$3.59 \cdot 10^{5}$	$-8.02 \cdot 10^{4}$	2.05	$2.83 \cdot 10^{-16}$	0.51
F2	$1.90 \cdot 10^{5}$	$2.21 \cdot 10^{5}$	$-3.04 \cdot 10^{4}$	$-2.36 \cdot 10^{1}$	$1.93 \cdot 10^{-16}$	0.35
F3	$1.01 \cdot 10^{5}$	$1.24 \cdot 10^{5}$	$-2.27 \cdot 10^{4}$	$2.41 \cdot 10^{1}$	$1.02 \cdot 10^{-16}$	0.19
F4	$-6.24 \cdot 10^{5}$	$-7.28 \cdot 10^{5}$	$1.04 \cdot 10^{5}$	$7.64 \cdot 10^{1}$	$6.33 \cdot 10^{-16}$	1.14
F5	$-4.96 \cdot 10^{5}$	$-6.29 \cdot 10^{5}$	$1.33 \cdot 10^{5}$	$5.35 \cdot 10^{1}$	$5.04 \cdot 10^{-16}$	0.91
F6	$-6.57 \cdot 10^{5}$	$-7.07 \cdot 10^{5}$	$4.98 \cdot 10^{4}$	$7.41 \cdot 10^{1}$	$6.67 \cdot 10^{-16}$	1.20
F7	$2.97 \cdot 10^{5}$	$2.83 \cdot 10^{5}$	$1.36 \cdot 10^{4}$	$-7.74 \cdot 10^{1}$	$3.01 \cdot 10^{-16}$	0.54
F8	$2.78 \cdot 10^{5}$	$2.91 \cdot 10^{5}$	$-1.33 \cdot 10^{4}$	$-3.21 \cdot 10^{1}$	$2.82 \cdot 10^{-16}$	0.51
F9	$4.87 \cdot 10^{5}$	$6.36 \cdot 10^{5}$	$-1.50 \cdot 10^{5}$	$-5.92 \cdot 10^{1}$	$4.94 \cdot 10^{-16}$	0.89
S1	$-2.42 \cdot 10^{4}$	$1.42 \cdot 10^{5}$	$-1.66 \cdot 10^{5}$	$1.07 \cdot 10^{1}$	$8.19 \cdot 10^{-19}$	0.00
S2	$-4.13 \cdot 10^{5}$	$-5.05 \cdot 10^{5}$	$9.17 \cdot 10^{4}$	$7.05 \cdot 10^{1}$	$1.40 \cdot 10^{-17}$	0.03
S3	$4.66 \cdot 10^{5}$	$5.36 \cdot 10^{5}$	$-6.97 \cdot 10^{4}$	$-4.21 \cdot 10^{1}$	$1.58 \cdot 10^{-17}$	0.03

TABLE SI-XXXIII: Values of $\bar{\Phi}$ (expressed in ppm au), of its temperature–dependent components, of the induced rotating chiral polarization (expressed in $\mathrm{C\,m^{-2}}$) and of the induced rf–voltage (expressed in µV) for the other atoms of complex **10**.

KD–DEPENDENT COMPONENTS OF $\bar{\Phi}$

$\bar{\Phi}^{p(2)}$

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
H1	$-1.25 \cdot 10^6$	$-5.93 \cdot 10^5$
H2	$-3.08 \cdot 10^5$	$1.57 \cdot 10^4$
H3	$-1.25 \cdot 10^6$	$-5.82 \cdot 10^5$
H4	$1.37 \cdot 10^6$	$1.14 \cdot 10^6$
H5	$1.64 \cdot 10^6$	$9.58 \cdot 10^5$
H6	$1.53 \cdot 10^6$	$9.83 \cdot 10^5$
H7	$1.90 \cdot 10^6$	$1.04 \cdot 10^6$
H8	$6.39 \cdot 10^4$	$-1.48 \cdot 10^5$
H9	$7.52 \cdot 10^5$	$3.89 \cdot 10^5$
H10	$1.27 \cdot 10^6$	$5.80 \cdot 10^5$
H11	$8.36 \cdot 10^5$	$5.66 \cdot 10^5$
H12	$-1.95 \cdot 10^5$	$-1.15 \cdot 10^5$
H13	$1.48 \cdot 10^5$	$1.43 \cdot 10^5$
H14	$4.59 \cdot 10^3$	$1.11 \cdot 10^4$
H15	$2.04 \cdot 10^6$	$1.47 \cdot 10^6$
H16	$7.78 \cdot 10^5$	$7.03 \cdot 10^5$
H17	$1.27 \cdot 10^6$	$1.01 \cdot 10^6$
H18	$-7.46 \cdot 10^5$	$-1.81 \cdot 10^5$
H19	$-1.77 \cdot 10^6$	$-1.18 \cdot 10^6$
H20	$-1.25 \cdot 10^6$	$-7.63 \cdot 10^5$
H21	$-1.63 \cdot 10^6$	$-1.17 \cdot 10^6$
H22	$-1.54 \cdot 10^6$	$-1.46 \cdot 10^6$
H23	$9.89 \cdot 10^5$	$3.09 \cdot 10^5$
H24	$2.23 \cdot 10^6$	$2.88 \cdot 10^5$
H25	$-4.03 \cdot 10^5$	$-1.69 \cdot 10^5$

TABLE SI-XXXIV: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
C1	$-1.03 \cdot 10^6$	$-3.64 \cdot 10^5$
C2	$-5.89 \cdot 10^5$	$5.19 \cdot 10^5$
C3	$2.60 \cdot 10^6$	$2.18 \cdot 10^6$
C4	$5.99 \cdot 10^6$	$3.98 \cdot 10^6$
C5	$2.24 \cdot 10^6$	$1.35 \cdot 10^6$
C6	$8.53 \cdot 10^5$	$3.41 \cdot 10^5$
C7	$1.86 \cdot 10^6$	$8.35 \cdot 10^5$
C8	$1.36 \cdot 10^6$	$9.08 \cdot 10^5$
C9	$6.22 \cdot 10^5$	$5.49 \cdot 10^5$
C10	$4.59 \cdot 10^4$	$6.69 \cdot 10^4$
C11	$1.59 \cdot 10^6$	$1.29 \cdot 10^6$
C12	$2.12 \cdot 10^6$	$2.27 \cdot 10^6$
C13	$-1.60 \cdot 10^6$	$-4.45 \cdot 10^5$
C14	$-5.27 \cdot 10^6$	$-3.11 \cdot 10^6$
C15	$-2.03 \cdot 10^6$	$-1.33 \cdot 10^6$

TABLE SI-XXXV: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
O1	$-1.05 \cdot 10^7$	$-4.60 \cdot 10^6$
O2	$1.70 \cdot 10^7$	$9.91 \cdot 10^6$
O3	$-5.26 \cdot 10^5$	$-2.12 \cdot 10^6$
O4	$-4.22 \cdot 10^4$	$7.29 \cdot 10^3$
O5	$1.26 \cdot 10^7$	$1.00 \cdot 10^7$
O6	$-1.64 \cdot 10^7$	$-1.11 \cdot 10^7$
O7	$2.22 \cdot 10^5$	$-1.31 \cdot 10^6$
O8	$3.10 \cdot 10^5$	$1.25 \cdot 10^5$

TABLE SI-XXXVI: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
H1	$2.98 \cdot 10^4$	$2.19 \cdot 10^4$
H2	$-5.31 \cdot 10^3$	$-4.16 \cdot 10^3$
H3	$2.22 \cdot 10^6$	$1.47 \cdot 10^6$
H4	$7.70 \cdot 10^5$	$5.31 \cdot 10^5$
H5	$1.36 \cdot 10^6$	$9.05 \cdot 10^5$
H6	$-1.19 \cdot 10^4$	$-1.06 \cdot 10^4$
H7	$5.77 \cdot 10^4$	$1.27 \cdot 10^4$
H8	$2.52 \cdot 10^5$	$1.78 \cdot 10^5$
H9	$9.93 \cdot 10^5$	$6.81 \cdot 10^5$
H10	$4.35 \cdot 10^5$	$2.32 \cdot 10^5$
H11	$3.30 \cdot 10^6$	$1.95 \cdot 10^6$
H12	$5.62 \cdot 10^3$	$4.38 \cdot 10^3$
H13	$6.94 \cdot 10^5$	$4.85 \cdot 10^5$
H14	$6.08 \cdot 10^5$	$4.06 \cdot 10^5$
H15	$-3.84 \cdot 10^4$	$-3.68 \cdot 10^4$
H16	$1.13 \cdot 10^5$	$8.44 \cdot 10^4$
H17	$-1.30 \cdot 10^4$	$3.72 \cdot 10^3$
H18	$-1.62 \cdot 10^6$	$-1.03 \cdot 10^6$
H19	$-4.57 \cdot 10^5$	$-2.66 \cdot 10^5$
H20	$-1.45 \cdot 10^6$	$-9.10 \cdot 10^5$
H21	$1.69 \cdot 10^6$	$1.06 \cdot 10^6$
H22	$1.41 \cdot 10^6$	$9.08 \cdot 10^5$
H23	$2.01 \cdot 10^6$	$1.27 \cdot 10^6$
H24	$2.52 \cdot 10^6$	$1.63 \cdot 10^6$
H25	$-2.21 \cdot 10^6$	$-1.46 \cdot 10^6$
H26	$-1.78 \cdot 10^6$	$-1.15 \cdot 10^6$
H27	$-1.76 \cdot 10^6$	$-1.16 \cdot 10^6$
H28	$-1.18 \cdot 10^6$	$-7.25 \cdot 10^5$
H29	$-3.15 \cdot 10^5$	$-2.23 \cdot 10^5$
H30	$2.59 \cdot 10^5$	$1.71 \cdot 10^5$
H31	$1.12 \cdot 10^6$	$7.08 \cdot 10^5$

TABLE SI-XXXVII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
C1	$3.84 \cdot 10^5$	$2.98 \cdot 10^5$
C2	$1.61 \cdot 10^4$	$1.23 \cdot 10^4$
C3	$1.19 \cdot 10^4$	$9.46 \cdot 10^3$
C4	$2.65 \cdot 10^5$	$1.96 \cdot 10^5$
C5	$-5.19 \cdot 10^3$	$-3.92 \cdot 10^3$
C6	$1.67 \cdot 10^6$	$1.12 \cdot 10^6$
C7	$-1.53 \cdot 10^6$	$-8.59 \cdot 10^5$
C8	$6.19 \cdot 10^6$	$4.01 \cdot 10^6$
C9	$9.62 \cdot 10^5$	$6.53 \cdot 10^5$
C10	$-1.10 \cdot 10^4$	$-8.89 \cdot 10^3$
C11	$-3.42 \cdot 10^4$	$-2.79 \cdot 10^4$
C12	$-4.81 \cdot 10^4$	$-6.12 \cdot 10^4$
C13	$9.67 \cdot 10^4$	$2.28 \cdot 10^4$
C14	$3.99 \cdot 10^5$	$2.81 \cdot 10^5$
C15	$-6.76 \cdot 10^6$	$-4.36 \cdot 10^6$
C16	$4.80 \cdot 10^4$	$3.75 \cdot 10^4$
C17	$-1.02 \cdot 10^5$	$-1.21 \cdot 10^5$
C18	$2.02 \cdot 10^6$	$1.38 \cdot 10^6$
C19	$-1.30 \cdot 10^4$	$-1.01 \cdot 10^4$
C20	$4.71 \cdot 10^5$	$2.35 \cdot 10^5$
C21	$2.04 \cdot 10^6$	$1.45 \cdot 10^6$
C22	$5.34 \cdot 10^5$	$4.17 \cdot 10^5$
C23	$1.82 \cdot 10^6$	$9.89 \cdot 10^5$
C24	$3.83 \cdot 10^3$	$3.13 \cdot 10^3$
C25	$1.05 \cdot 10^6$	$7.45 \cdot 10^5$
C26	$7.93 \cdot 10^5$	$5.40 \cdot 10^5$
C27	$5.23 \cdot 10^4$	$4.42 \cdot 10^4$
C28	$-1.35 \cdot 10^6$	$-8.35 \cdot 10^5$
C29	$2.26 \cdot 10^6$	$1.44 \cdot 10^6$
C30	$2.11 \cdot 10^6$	$1.42 \cdot 10^6$
C31	$-2.53 \cdot 10^6$	$-1.65 \cdot 10^6$
C32	$-2.40 \cdot 10^6$	$-1.47 \cdot 10^6$
C33	$4.46 \cdot 10^5$	$2.80 \cdot 10^5$

TABLE SI-XXXVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
O1	$-4.22 \cdot 10^4$	$-3.52 \cdot 10^4$
O2	$1.89 \cdot 10^7$	$1.19 \cdot 10^7$
O3	$-1.21 \cdot 10^7$	$-7.58 \cdot 10^6$
O4	$1.47 \cdot 10^7$	$9.77 \cdot 10^6$
O5	$-2.70 \cdot 10^6$	$-1.85 \cdot 10^6$
O6	$-2.03 \cdot 10^7$	$-1.33 \cdot 10^7$
N1	$2.96 \cdot 10^6$	$2.12 \cdot 10^6$
N2	$1.59 \cdot 10^6$	$6.92 \cdot 10^5$
N3	$5.26 \cdot 10^4$	$3.94 \cdot 10^4$
N4	$-2.71 \cdot 10^4$	$-2.34 \cdot 10^4$

TABLE SI-XXXIX: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
H1	$-8.78 \cdot 10^5$	$7.89 \cdot 10^4$	$1.17 \cdot 10^6$
H2	$-2.91 \cdot 10^5$	$-1.01 \cdot 10^5$	$1.70 \cdot 10^5$
H3	$-1.28 \cdot 10^5$	$-8.13 \cdot 10^4$	$2.71 \cdot 10^4$
H4	$-4.34 \cdot 10^3$	$-5.36 \cdot 10^3$	$-2.08 \cdot 10^3$
H5	$3.11 \cdot 10^3$	$8.51 \cdot 10^3$	$4.27 \cdot 10^3$
H6	$4.66 \cdot 10^4$	$1.28 \cdot 10^5$	$1.15 \cdot 10^5$
H7	$7.76 \cdot 10^4$	$2.95 \cdot 10^5$	$3.34 \cdot 10^5$
H8	$-3.27 \cdot 10^5$	$9.20 \cdot 10^5$	$1.53 \cdot 10^6$
H9	$-2.58 \cdot 10^6$	$-1.76 \cdot 10^6$	$-6.94 \cdot 10^5$
H10	$-1.19 \cdot 10^6$	$-9.76 \cdot 10^5$	$-5.90 \cdot 10^5$
H11	$-1.74 \cdot 10^6$	$-1.33 \cdot 10^6$	$-6.64 \cdot 10^5$
H12	$6.89 \cdot 10^5$	$3.38 \cdot 10^4$	$-5.37 \cdot 10^5$
H13	$2.50 \cdot 10^6$	$1.60 \cdot 10^6$	$4.76 \cdot 10^5$
H14	$1.71 \cdot 10^6$	$9.57 \cdot 10^5$	$1.12 \cdot 10^5$
H15	$2.57 \cdot 10^6$	$1.63 \cdot 10^6$	$5.09 \cdot 10^5$
H16	$-1.88 \cdot 10^6$	$-9.56 \cdot 10^5$	$2.64 \cdot 10^4$
H17	$-1.84 \cdot 10^6$	$-1.11 \cdot 10^6$	$-2.82 \cdot 10^5$
H18	$-1.82 \cdot 10^6$	$-8.99 \cdot 10^5$	$-1.36 \cdot 10^4$
H19	$-2.50 \cdot 10^6$	$-1.84 \cdot 10^6$	$-8.49 \cdot 10^5$
H20	$7.11 \cdot 10^5$	$4.24 \cdot 10^5$	$1.74 \cdot 10^5$
H21	$8.08 \cdot 10^5$	$1.90 \cdot 10^5$	$-3.68 \cdot 10^5$
H22	$-4.74 \cdot 10^5$	$-5.64 \cdot 10^5$	$-4.91 \cdot 10^5$
H23	$1.41 \cdot 10^5$	$-1.98 \cdot 10^5$	$-4.09 \cdot 10^5$
H24	$1.12 \cdot 10^6$	$1.00 \cdot 10^6$	$7.41 \cdot 10^5$
H25	$7.71 \cdot 10^5$	$5.97 \cdot 10^5$	$3.88 \cdot 10^5$
H26	$1.93 \cdot 10^6$	$1.32 \cdot 10^6$	$5.60 \cdot 10^5$
H27	$1.55 \cdot 10^4$	$-3.18 \cdot 10^3$	$-3.58 \cdot 10^4$
H28	$-6.50 \cdot 10^4$	$-5.66 \cdot 10^4$	$-1.66 \cdot 10^4$
H29	$7.78 \cdot 10^4$	$1.19 \cdot 10^5$	$6.55 \cdot 10^4$

TABLE SI-XL: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
C1	$-9.09 \cdot 10^5$	$-2.89 \cdot 10^5$	$6.48 \cdot 10^5$
C2	$-3.71 \cdot 10^5$	$-1.62 \cdot 10^5$	$1.83 \cdot 10^5$
C3	$-1.96 \cdot 10^5$	$-1.24 \cdot 10^5$	$4.52 \cdot 10^4$
C4	$-1.20 \cdot 10^5$	$-1.05 \cdot 10^5$	$-6.28 \cdot 10^3$
C5	$-1.94 \cdot 10^4$	$-2.09 \cdot 10^4$	$-7.52 \cdot 10^3$
C6	$-3.94 \cdot 10^3$	$-4.71 \cdot 10^3$	$-2.43 \cdot 10^3$
C7	$3.66 \cdot 10^3$	$8.50 \cdot 10^3$	$3.55 \cdot 10^3$
C8	$1.77 \cdot 10^4$	$3.29 \cdot 10^4$	$1.62 \cdot 10^4$
C9	$7.56 \cdot 10^4$	$1.55 \cdot 10^5$	$1.07 \cdot 10^5$
C10	$7.59 \cdot 10^4$	$2.06 \cdot 10^5$	$1.85 \cdot 10^5$
C11	$1.00 \cdot 10^5$	$3.85 \cdot 10^5$	$4.13 \cdot 10^5$
C12	$5.88 \cdot 10^4$	$9.51 \cdot 10^5$	$1.17 \cdot 10^6$
C13	$1.54 \cdot 10^5$	$2.91 \cdot 10^5$	$1.77 \cdot 10^5$
C14	$-2.12 \cdot 10^5$	$-2.03 \cdot 10^5$	$-4.03 \cdot 10^4$
C15	$-2.22 \cdot 10^6$	$-1.68 \cdot 10^6$	$-8.64 \cdot 10^5$
C16	$-3.87 \cdot 10^6$	$-3.45 \cdot 10^6$	$-2.34 \cdot 10^6$
C17	$1.30 \cdot 10^6$	$4.10 \cdot 10^4$	$-1.05 \cdot 10^6$
C18	$6.67 \cdot 10^6$	$3.58 \cdot 10^6$	$1.74 \cdot 10^5$
C19	$2.89 \cdot 10^6$	$1.74 \cdot 10^6$	$3.97 \cdot 10^5$
C20	$-2.55 \cdot 10^6$	$-1.42 \cdot 10^6$	$-1.98 \cdot 10^5$
C21	$-7.79 \cdot 10^6$	$-4.82 \cdot 10^6$	$-1.31 \cdot 10^6$
C22	$-4.86 \cdot 10^6$	$-3.57 \cdot 10^6$	$-1.66 \cdot 10^6$
C23	$-2.63 \cdot 10^6$	$-2.77 \cdot 10^6$	$-2.19 \cdot 10^6$
C24	$1.10 \cdot 10^5$	$-1.70 \cdot 10^4$	$-1.51 \cdot 10^4$
C25	$1.20 \cdot 10^6$	$7.33 \cdot 10^5$	$3.55 \cdot 10^5$
C26	$3.40 \cdot 10^6$	$2.48 \cdot 10^6$	$1.43 \cdot 10^6$
C27	$-3.07 \cdot 10^4$	$-4.10 \cdot 10^5$	$-6.10 \cdot 10^5$
C28	$1.60 \cdot 10^6$	$1.21 \cdot 10^6$	$6.96 \cdot 10^5$
C29	$-1.15 \cdot 10^3$	$5.62 \cdot 10^2$	$-9.17 \cdot 10^3$

captionValues of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
O1	$4.32 \cdot 10^6$	$-3.01 \cdot 10^5$	$-4.00 \cdot 10^6$
O2	$-1.84 \cdot 10^7$	$-9.67 \cdot 10^6$	$-6.58 \cdot 10^5$
O3	$7.95 \cdot 10^4$	$8.59 \cdot 10^4$	$3.64 \cdot 10^4$
O4	$1.11 \cdot 10^7$	$9.09 \cdot 10^6$	$5.97 \cdot 10^6$
O5	$-1.94 \cdot 10^7$	$-1.41 \cdot 10^7$	$-6.43 \cdot 10^6$
O6	$2.41 \cdot 10^7$	$1.51 \cdot 10^7$	$4.18 \cdot 10^6$
N1	$-1.42 \cdot 10^6$	$-9.09 \cdot 10^5$	$4.23 \cdot 10^5$
N2	$3.44 \cdot 10^5$	$1.63 \cdot 10^6$	$1.57 \cdot 10^6$
N3	$-1.79 \cdot 10^4$	$-1.90 \cdot 10^4$	$-3.98 \cdot 10^3$
N4	$1.20 \cdot 10^4$	$2.81 \cdot 10^4$	$1.70 \cdot 10^4$

TABLE SI-XLI: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
H1	$-3.30 \cdot 10^6$	$1.13 \cdot 10^5$
H2	$-3.58 \cdot 10^5$	$1.89 \cdot 10^5$
H3	$6.53 \cdot 10^3$	$1.24 \cdot 10^5$
H4	$3.66 \cdot 10^4$	$2.45 \cdot 10^4$
H5	$-5.43 \cdot 10^4$	$-3.49 \cdot 10^4$
H6	$-2.43 \cdot 10^5$	$-4.12 \cdot 10^4$
H7	$-4.66 \cdot 10^5$	$1.09 \cdot 10^5$
H8	$-1.66 \cdot 10^6$	$1.14 \cdot 10^6$
H9	$-1.60 \cdot 10^6$	$-1.51 \cdot 10^6$
H10	$-1.16 \cdot 10^6$	$-1.30 \cdot 10^6$
H11	$-2.95 \cdot 10^6$	$-2.15 \cdot 10^6$
H12	$1.31 \cdot 10^6$	$-2.23 \cdot 10^5$
H13	$2.91 \cdot 10^6$	$1.95 \cdot 10^6$
H14	$2.10 \cdot 10^6$	$1.02 \cdot 10^6$
H15	$2.75 \cdot 10^6$	$1.66 \cdot 10^6$
H16	$-9.92 \cdot 10^5$	$2.56 \cdot 10^5$
H17	$5.77 \cdot 10^4$	$6.01 \cdot 10^5$
H18	$9.12 \cdot 10^5$	$1.46 \cdot 10^6$
H19	$-8.93 \cdot 10^5$	$-1.58 \cdot 10^5$
H20	$-4.70 \cdot 10^3$	$-3.10 \cdot 10^4$
H21	$-3.27 \cdot 10^5$	$-2.50 \cdot 10^5$
H22	$1.14 \cdot 10^5$	$-1.66 \cdot 10^5$
H23	$1.12 \cdot 10^6$	$-7.03 \cdot 10^4$
H24	$-2.11 \cdot 10^5$	$-7.48 \cdot 10^5$
H25	$8.21 \cdot 10^5$	$-2.36 \cdot 10^5$
H26	$-2.37 \cdot 10^6$	$-2.10 \cdot 10^6$
H27	$-2.50 \cdot 10^6$	$-1.06 \cdot 10^6$
H28	$-2.05 \cdot 10^6$	$-1.27 \cdot 10^6$
H29	$-2.38 \cdot 10^6$	$-1.22 \cdot 10^6$

TABLE SI-XLII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
C1	$-1.72 \cdot 10^6$	$4.50 \cdot 10^5$
C2	$-3.65 \cdot 10^5$	$2.67 \cdot 10^5$
C3	$-1.71 \cdot 10^4$	$1.82 \cdot 10^5$
C4	$8.61 \cdot 10^4$	$1.24 \cdot 10^5$
C5	$3.74 \cdot 10^4$	$1.80 \cdot 10^4$
C6	$-5.21 \cdot 10^4$	$-4.02 \cdot 10^4$
C7	$-2.65 \cdot 10^5$	$-1.05 \cdot 10^5$
C8	$-3.75 \cdot 10^5$	$-5.33 \cdot 10^4$
C9	$-6.41 \cdot 10^5$	$7.72 \cdot 10^4$
C10	$-1.62 \cdot 10^6$	$5.06 \cdot 10^5$
C11	$-4.26 \cdot 10^5$	$-1.88 \cdot 10^5$
C12	$1.40 \cdot 10^5$	$1.65 \cdot 10^5$
C13	$-2.22 \cdot 10^6$	$-2.08 \cdot 10^6$
C14	$-3.11 \cdot 10^6$	$-4.52 \cdot 10^6$
C15	$2.55 \cdot 10^6$	$-4.35 \cdot 10^5$
C16	$8.28 \cdot 10^6$	$3.58 \cdot 10^6$
C17	$3.36 \cdot 10^6$	$1.90 \cdot 10^6$
C18	$-5.03 \cdot 10^4$	$9.49 \cdot 10^5$
C19	$-3.88 \cdot 10^5$	$1.95 \cdot 10^6$
C20	$-1.44 \cdot 10^6$	$-1.15 \cdot 10^5$
C21	$-1.21 \cdot 10^6$	$-6.91 \cdot 10^5$
C22	$-1.90 \cdot 10^5$	$-2.23 \cdot 10^5$
C23	$5.36 \cdot 10^5$	$-6.20 \cdot 10^5$
C24	$-9.46 \cdot 10^5$	$-3.25 \cdot 10^6$
C25	$-4.49 \cdot 10^6$	$-4.06 \cdot 10^6$
C26	$-8.52 \cdot 10^6$	$-5.48 \cdot 10^6$
C27	$-3.07 \cdot 10^6$	$-1.66 \cdot 10^6$

TABLE SI-XLIII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$
O1	$-2.06 \cdot 10^7$	$-1.74 \cdot 10^7$
O2	$2.72 \cdot 10^7$	$1.67 \cdot 10^7$
O3	$8.96 \cdot 10^6$	$1.24 \cdot 10^7$
O4	$-2.92 \cdot 10^3$	$-4.29 \cdot 10^5$
O5	$1.04 \cdot 10^7$	$-1.12 \cdot 10^6$
O6	$-2.34 \cdot 10^7$	$-1.19 \cdot 10^7$
N1	$-1.55 \cdot 10^6$	$7.10 \cdot 10^5$
N2	$-2.48 \cdot 10^6$	$2.09 \cdot 10^5$

TABLE SI-XLIV: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$	$\bar{\Phi}_3^{p(2)}$
H1	$-2.10 \cdot 10^6$	$-3.70 \cdot 10^6$	$-5.90 \cdot 10^5$	$7.76 \cdot 10^5$
H2	$7.25 \cdot 10^6$	$1.57 \cdot 10^6$	$3.29 \cdot 10^5$	$1.08 \cdot 10^6$
H3	$1.89 \cdot 10^6$	$-1.02 \cdot 10^5$	$3.05 \cdot 10^5$	$5.18 \cdot 10^5$
H4	$-3.64 \cdot 10^6$	$-2.14 \cdot 10^6$	$-1.93 \cdot 10^5$	$2.75 \cdot 10^5$
H5	$-4.36 \cdot 10^5$	$-7.34 \cdot 10^5$	$1.46 \cdot 10^5$	$2.65 \cdot 10^5$
H6	$5.34 \cdot 10^5$	$4.63 \cdot 10^5$	$-2.20 \cdot 10^5$	$-3.99 \cdot 10^4$
H7	$-3.83 \cdot 10^5$	$-1.13 \cdot 10^5$	$1.65 \cdot 10^4$	$-1.86 \cdot 10^5$
H8	$-3.18 \cdot 10^6$	$-2.56 \cdot 10^6$	$-1.19 \cdot 10^6$	$-3.11 \cdot 10^5$
H9	$1.28 \cdot 10^6$	$-1.47 \cdot 10^6$	$-1.78 \cdot 10^6$	$2.34 \cdot 10^5$
H10	$1.22 \cdot 10^6$	$2.56 \cdot 10^5$	$-7.15 \cdot 10^5$	$-3.62 \cdot 10^4$
H11	$-1.80 \cdot 10^6$	$1.10 \cdot 10^5$	$2.70 \cdot 10^5$	$-2.83 \cdot 10^5$
H12	$1.29 \cdot 10^6$	$6.38 \cdot 10^5$	$-4.08 \cdot 10^5$	$-3.41 \cdot 10^4$
H13	$3.55 \cdot 10^6$	$3.07 \cdot 10^6$	$6.79 \cdot 10^5$	$-8.91 \cdot 10^4$

TABLE SI-XLV: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$	$\bar{\Phi}_3^{p(2)}$
C1	$2.68 \cdot 10^6$	$-1.24 \cdot 10^6$	$1.56 \cdot 10^5$	$1.08 \cdot 10^6$
C2	$-1.53 \cdot 10^6$	$-1.53 \cdot 10^6$	$1.18 \cdot 10^5$	$4.36 \cdot 10^5$
C3	$2.19 \cdot 10^5$	$2.39 \cdot 10^5$	$-2.44 \cdot 10^5$	$-8.98 \cdot 10^4$
C4	$7.80 \cdot 10^4$	$-1.17 \cdot 10^6$	$-1.59 \cdot 10^6$	$-1.22 \cdot 10^5$
C5	$-1.28 \cdot 10^7$	$-6.02 \cdot 10^6$	$-5.49 \cdot 10^5$	$-7.17 \cdot 10^5$
C6	$-3.48 \cdot 10^6$	$2.53 \cdot 10^5$	$5.54 \cdot 10^5$	$-5.69 \cdot 10^5$
C7	$5.22 \cdot 10^6$	$6.64 \cdot 10^6$	$1.72 \cdot 10^6$	$-5.59 \cdot 10^5$
C8	$-5.32 \cdot 10^6$	$-3.12 \cdot 10^6$	$-4.79 \cdot 10^5$	$-1.68 \cdot 10^5$
C9	$3.63 \cdot 10^6$	$3.20 \cdot 10^6$	$6.39 \cdot 10^5$	$-9.51 \cdot 10^4$
C10	$1.57 \cdot 10^6$	$1.33 \cdot 10^6$	$-4.80 \cdot 10^5$	$-7.48 \cdot 10^4$
C11	$2.09 \cdot 10^6$	$9.68 \cdot 10^5$	$-8.21 \cdot 10^5$	$-8.88 \cdot 10^4$
C12	$2.99 \cdot 10^5$	$-1.66 \cdot 10^6$	$-1.98 \cdot 10^6$	$-1.27 \cdot 10^4$
C13	$6.52 \cdot 10^4$	$2.33 \cdot 10^5$	$-8.71 \cdot 10^4$	$1.98 \cdot 10^4$
C14	$-3.69 \cdot 10^5$	$-1.18 \cdot 10^6$	$-8.03 \cdot 10^5$	$7.04 \cdot 10^4$
C15	$1.41 \cdot 10^7$	$8.81 \cdot 10^6$	$1.74 \cdot 10^6$	$4.20 \cdot 10^5$
C16	$6.87 \cdot 10^6$	$5.99 \cdot 10^6$	$1.35 \cdot 10^6$	$-1.82 \cdot 10^5$
C17	$1.16 \cdot 10^6$	$4.40 \cdot 10^6$	$1.41 \cdot 10^6$	$-7.03 \cdot 10^5$
C18	$4.97 \cdot 10^6$	$2.56 \cdot 10^6$	$4.37 \cdot 10^5$	$2.84 \cdot 10^5$
C19	$-1.43 \cdot 10^6$	$3.98 \cdot 10^5$	$2.96 \cdot 10^5$	$-2.66 \cdot 10^5$

TABLE SI-XLVI: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$	$\bar{\Phi}_3^{p(2)}$
O1	$3.96 \cdot 10^6$	$-2.46 \cdot 10^6$	$1.66 \cdot 10^6$	$2.21 \cdot 10^6$
O2	$4.49 \cdot 10^6$	$2.07 \cdot 10^6$	$-2.69 \cdot 10^6$	$-4.99 \cdot 10^5$
O3	$-4.22 \cdot 10^7$	$-2.58 \cdot 10^7$	$-4.37 \cdot 10^6$	$-1.34 \cdot 10^6$
O4	$3.26 \cdot 10^7$	$2.64 \cdot 10^7$	$5.59 \cdot 10^6$	$-4.26 \cdot 10^5$
O5	$-1.54 \cdot 10^6$	$-6.34 \cdot 10^5$	$-2.76 \cdot 10^5$	$4.24 \cdot 10^5$
O6	$-1.36 \cdot 10^7$	$-1.53 \cdot 10^7$	$-6.73 \cdot 10^6$	$5.16 \cdot 10^4$
O7	$3.72 \cdot 10^7$	$1.80 \cdot 10^7$	$3.71 \cdot 10^6$	$2.52 \cdot 10^6$
O8	$-1.80 \cdot 10^7$	$-1.51 \cdot 10^6$	$1.68 \cdot 10^6$	$-2.23 \cdot 10^6$
F1	$-3.97 \cdot 10^6$	$-2.83 \cdot 10^6$	$-4.99 \cdot 10^5$	$4.73 \cdot 10^4$
F2	$-2.67 \cdot 10^6$	$-1.35 \cdot 10^6$	$-1.52 \cdot 10^5$	$-1.25 \cdot 10^5$
F3	$-4.01 \cdot 10^6$	$-2.53 \cdot 10^6$	$-4.94 \cdot 10^5$	$-1.56 \cdot 10^5$
F4	$3.68 \cdot 10^6$	$2.70 \cdot 10^6$	$5.86 \cdot 10^5$	$1.45 \cdot 10^4$
F5	$3.43 \cdot 10^6$	$2.58 \cdot 10^6$	$2.83 \cdot 10^5$	$-6.64 \cdot 10^2$
F6	$1.26 \cdot 10^6$	$1.42 \cdot 10^6$	$3.35 \cdot 10^5$	$-9.51 \cdot 10^4$
F7	$-6.00 \cdot 10^5$	$-1.63 \cdot 10^4$	$-4.07 \cdot 10^4$	$1.57 \cdot 10^4$
F8	$3.42 \cdot 10^5$	$3.16 \cdot 10^5$	$-8.22 \cdot 10^4$	$-9.43 \cdot 10^3$
F9	$-1.99 \cdot 10^5$	$-1.66 \cdot 10^5$	$1.25 \cdot 10^4$	$6.33 \cdot 10^4$
F10	$8.89 \cdot 10^3$	$-1.17 \cdot 10^6$	$-6.66 \cdot 10^5$	$2.13 \cdot 10^5$
F11	$-1.68 \cdot 10^6$	$-1.54 \cdot 10^6$	$-5.98 \cdot 10^5$	$-4.59 \cdot 10^4$
F12	$5.04 \cdot 10^5$	$-1.49 \cdot 10^5$	$-3.83 \cdot 10^5$	$4.38 \cdot 10^4$
F13	$3.18 \cdot 10^6$	$9.48 \cdot 10^5$	$3.40 \cdot 10^4$	$3.59 \cdot 10^5$
F14	$3.19 \cdot 10^6$	$1.71 \cdot 10^6$	$4.85 \cdot 10^5$	$1.81 \cdot 10^5$
F15	$2.91 \cdot 10^6$	$1.67 \cdot 10^6$	$2.46 \cdot 10^5$	$1.17 \cdot 10^5$
F16	$-2.41 \cdot 10^6$	$-5.93 \cdot 10^5$	$1.15 \cdot 10^5$	$-2.58 \cdot 10^5$
F17	$-1.94 \cdot 10^6$	$-4.04 \cdot 10^5$	$4.70 \cdot 10^4$	$-1.29 \cdot 10^5$
F18	$3.79 \cdot 10^4$	$7.43 \cdot 10^5$	$2.39 \cdot 10^5$	$-1.34 \cdot 10^5$

TABLE SI-XLVII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
H1	$2.64 \cdot 10^6$	$1.05 \cdot 10^6$	$-5.79 \cdot 10^5$
H2	$-2.92 \cdot 10^6$	$-2.64 \cdot 10^6$	$-1.67 \cdot 10^6$
H3	$3.26 \cdot 10^5$	$-4.74 \cdot 10^5$	$-1.02 \cdot 10^6$
H4	$-2.73 \cdot 10^6$	$-2.66 \cdot 10^6$	$-1.82 \cdot 10^6$
H5	$1.33 \cdot 10^6$	$7.81 \cdot 10^5$	$1.82 \cdot 10^5$
H6	$-3.17 \cdot 10^6$	$-2.41 \cdot 10^6$	$-9.35 \cdot 10^5$
H7	$-2.84 \cdot 10^6$	$-2.26 \cdot 10^6$	$-1.07 \cdot 10^6$
H8	$-5.32 \cdot 10^6$	$-3.75 \cdot 10^6$	$-1.21 \cdot 10^6$
H9	$-1.06 \cdot 10^6$	$-1.61 \cdot 10^6$	$-1.62 \cdot 10^6$
H10	$4.36 \cdot 10^5$	$2.74 \cdot 10^5$	$1.22 \cdot 10^5$
H11	$3.47 \cdot 10^6$	$1.34 \cdot 10^6$	$-7.85 \cdot 10^5$
H12	$1.74 \cdot 10^6$	$8.95 \cdot 10^5$	$-4.30 \cdot 10^4$
H13	$-2.17 \cdot 10^5$	$-1.34 \cdot 10^5$	$5.27 \cdot 10^4$
H14	$-1.63 \cdot 10^6$	$-1.07 \cdot 10^6$	$-1.05 \cdot 10^5$
H15	$-1.20 \cdot 10^7$	$-7.50 \cdot 10^6$	$-2.11 \cdot 10^6$
H16	$-5.24 \cdot 10^6$	$-1.74 \cdot 10^6$	$1.17 \cdot 10^6$
H17	$-2.92 \cdot 10^6$	$-1.16 \cdot 10^6$	$2.91 \cdot 10^5$
H18	$2.69 \cdot 10^6$	$1.90 \cdot 10^6$	$8.66 \cdot 10^5$
H19	$1.37 \cdot 10^6$	$8.82 \cdot 10^5$	$2.86 \cdot 10^5$
H20	$1.29 \cdot 10^6$	$7.49 \cdot 10^5$	$1.19 \cdot 10^5$
H21	$3.60 \cdot 10^6$	$1.97 \cdot 10^6$	$1.68 \cdot 10^5$
H22	$1.47 \cdot 10^7$	$9.55 \cdot 10^6$	$2.86 \cdot 10^6$
H23	$1.54 \cdot 10^6$	$9.39 \cdot 10^5$	$8.71 \cdot 10^5$
H24	$3.38 \cdot 10^6$	$4.98 \cdot 10^6$	$3.84 \cdot 10^6$

TABLE SI-XLVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
C1	$1.21 \cdot 10^5$	$-2.85 \cdot 10^6$	$-4.56 \cdot 10^6$
C2	$-1.84 \cdot 10^6$	$-2.22 \cdot 10^6$	$-1.92 \cdot 10^6$
C3	$1.45 \cdot 10^7$	$7.71 \cdot 10^6$	$3.28 \cdot 10^5$
C4	$1.01 \cdot 10^7$	$4.06 \cdot 10^6$	$-2.15 \cdot 10^6$
C5	$1.39 \cdot 10^6$	$8.39 \cdot 10^5$	$2.51 \cdot 10^5$
C6	$-4.83 \cdot 10^6$	$-3.65 \cdot 10^6$	$-1.48 \cdot 10^6$
C7	$-1.10 \cdot 10^7$	$-9.00 \cdot 10^6$	$-4.51 \cdot 10^6$
C8	$2.90 \cdot 10^6$	$1.73 \cdot 10^6$	$5.02 \cdot 10^5$
C9	$-1.75 \cdot 10^6$	$-2.92 \cdot 10^6$	$-3.08 \cdot 10^6$
C10	$5.83 \cdot 10^5$	$3.66 \cdot 10^5$	$1.70 \cdot 10^5$
C11	$6.85 \cdot 10^6$	$2.66 \cdot 10^6$	$-1.51 \cdot 10^6$
C12	$5.43 \cdot 10^6$	$3.06 \cdot 10^6$	$2.86 \cdot 10^5$
C13	$2.52 \cdot 10^6$	$1.40 \cdot 10^6$	$1.02 \cdot 10^5$
C14	$1.64 \cdot 10^4$	$1.68 \cdot 10^4$	$1.22 \cdot 10^5$
C15	$-4.67 \cdot 10^5$	$-2.95 \cdot 10^5$	$1.34 \cdot 10^5$
C16	$-7.87 \cdot 10^6$	$-3.49 \cdot 10^6$	$4.66 \cdot 10^5$
C17	$3.67 \cdot 10^6$	$2.41 \cdot 10^6$	$8.06 \cdot 10^5$
C18	$2.08 \cdot 10^6$	$1.31 \cdot 10^6$	$3.70 \cdot 10^5$
C19	$1.90 \cdot 10^6$	$1.12 \cdot 10^6$	$1.97 \cdot 10^5$

TABLE SI-XLIX: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
O1	$5.48 \cdot 10^7$	$3.09 \cdot 10^7$	$2.28 \cdot 10^6$
O2	$3.83 \cdot 10^7$	$2.23 \cdot 10^7$	$4.59 \cdot 10^6$
O3	$-2.47 \cdot 10^7$	$-2.44 \cdot 10^7$	$-1.72 \cdot 10^7$
O4	$-4.93 \cdot 10^6$	$3.13 \cdot 10^6$	$6.70 \cdot 10^6$
O5	$-4.42 \cdot 10^6$	$-4.07 \cdot 10^6$	$-1.18 \cdot 10^6$
O6	$-3.73 \cdot 10^7$	$-2.76 \cdot 10^7$	$-1.03 \cdot 10^7$
O7	$-9.66 \cdot 10^6$	$-2.75 \cdot 10^6$	$5.13 \cdot 10^6$
O8	$1.86 \cdot 10^7$	$2.03 \cdot 10^7$	$1.39 \cdot 10^7$
O9	$-3.04 \cdot 10^7$	$-1.94 \cdot 10^7$	$-5.98 \cdot 10^6$
O10	$-2.91 \cdot 10^6$	$-5.44 \cdot 10^5$	$1.12 \cdot 10^6$
O11	$-3.26 \cdot 10^6$	$-2.18 \cdot 10^6$	$-1.88 \cdot 10^5$
N1	$5.44 \cdot 10^6$	$2.61 \cdot 10^6$	$-4.72 \cdot 10^5$
N2	$5.42 \cdot 10^6$	$3.04 \cdot 10^6$	$4.25 \cdot 10^5$
N3	$1.35 \cdot 10^6$	$8.40 \cdot 10^5$	$5.42 \cdot 10^5$
N4	$-9.47 \cdot 10^6$	$-2.25 \cdot 10^6$	$3.11 \cdot 10^6$
N5	$-7.78 \cdot 10^6$	$-5.16 \cdot 10^6$	$-1.60 \cdot 10^5$
N6	$7.97 \cdot 10^6$	$4.99 \cdot 10^6$	$1.26 \cdot 10^6$

TABLE SI-L: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
H1	$-7.81 \cdot 10^5$	$-8.30 \cdot 10^5$	$-5.60 \cdot 10^5$
H2	$4.90 \cdot 10^4$	$5.70 \cdot 10^4$	$1.89 \cdot 10^5$
H3	$-2.15 \cdot 10^6$	$-1.03 \cdot 10^6$	$3.39 \cdot 10^4$
H4	$4.01 \cdot 10^5$	$2.83 \cdot 10^5$	$4.28 \cdot 10^5$
H5	$-5.30 \cdot 10^4$	$-6.08 \cdot 10^4$	$-4.90 \cdot 10^4$
H6	$-4.15 \cdot 10^4$	$-2.77 \cdot 10^4$	$1.16 \cdot 10^4$
H7	$-1.02 \cdot 10^5$	$-1.74 \cdot 10^5$	$-1.82 \cdot 10^5$
H8	$1.56 \cdot 10^6$	$1.20 \cdot 10^6$	$-1.98 \cdot 10^5$
H9	$1.02 \cdot 10^5$	$2.65 \cdot 10^4$	$-8.93 \cdot 10^4$
H10	$1.33 \cdot 10^6$	$8.59 \cdot 10^5$	$-7.85 \cdot 10^4$
H11	$-7.46 \cdot 10^4$	$-2.98 \cdot 10^4$	$2.27 \cdot 10^5$
H12	$4.51 \cdot 10^6$	$1.95 \cdot 10^6$	$-5.00 \cdot 10^5$
H13	$-1.58 \cdot 10^5$	$6.95 \cdot 10^4$	$-2.63 \cdot 10^3$
H14	$1.14 \cdot 10^5$	$-7.99 \cdot 10^4$	$-2.42 \cdot 10^5$
H15	$1.89 \cdot 10^6$	$1.13 \cdot 10^6$	$1.70 \cdot 10^6$
H16	$5.54 \cdot 10^4$	$-1.90 \cdot 10^4$	$-1.06 \cdot 10^5$
H17	$5.09 \cdot 10^5$	$2.62 \cdot 10^5$	$-6.90 \cdot 10^4$
H18	$2.11 \cdot 10^6$	$8.42 \cdot 10^5$	$-5.13 \cdot 10^5$
H19	$5.40 \cdot 10^5$	$2.04 \cdot 10^5$	$-1.39 \cdot 10^5$
H20	$7.41 \cdot 10^5$	$2.16 \cdot 10^5$	$-2.72 \cdot 10^5$
H21	$1.17 \cdot 10^5$	$3.66 \cdot 10^4$	$-8.24 \cdot 10^4$
H22	$3.18 \cdot 10^6$	$2.10 \cdot 10^6$	$3.04 \cdot 10^5$
H23	$-3.55 \cdot 10^4$	$-2.74 \cdot 10^4$	$-5.01 \cdot 10^3$
H24	$-3.81 \cdot 10^4$	$-3.58 \cdot 10^4$	$-2.08 \cdot 10^4$
H25	$6.64 \cdot 10^5$	$3.93 \cdot 10^5$	$-5.27 \cdot 10^4$
H26	$1.77 \cdot 10^5$	$1.78 \cdot 10^5$	$5.90 \cdot 10^3$
H27	$4.02 \cdot 10^5$	$2.91 \cdot 10^5$	$2.60 \cdot 10^4$
H28	$9.11 \cdot 10^5$	$5.98 \cdot 10^5$	$7.93 \cdot 10^4$

TABLE SI-LI: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
C1	$-5.21 \cdot 10^5$	$-9.37 \cdot 10^5$	$-1.13 \cdot 10^6$
C2	$-1.65 \cdot 10^5$	$-3.64 \cdot 10^5$	$-4.68 \cdot 10^5$
C3	$-6.83 \cdot 10^5$	$-5.43 \cdot 10^5$	$6.27 \cdot 10^4$
C4	$-2.15 \cdot 10^5$	$-1.39 \cdot 10^5$	$1.43 \cdot 10^5$
C5	$3.34 \cdot 10^5$	$1.15 \cdot 10^6$	$1.27 \cdot 10^5$
C6	$-8.22 \cdot 10^5$	$-4.34 \cdot 10^5$	$1.50 \cdot 10^6$
C7	$-2.07 \cdot 10^5$	$-1.69 \cdot 10^5$	$-3.58 \cdot 10^4$
C8	$-1.65 \cdot 10^5$	$-3.32 \cdot 10^5$	$-4.16 \cdot 10^5$
C9	$7.64 \cdot 10^4$	$8.93 \cdot 10^4$	$3.04 \cdot 10^5$
C10	$3.19 \cdot 10^6$	$1.84 \cdot 10^6$	$-3.09 \cdot 10^5$
C11	$-2.09 \cdot 10^5$	$-2.28 \cdot 10^5$	$-1.74 \cdot 10^5$
C12	$1.21 \cdot 10^5$	$-1.04 \cdot 10^5$	$-3.61 \cdot 10^5$
C13	$-4.03 \cdot 10^6$	$-1.90 \cdot 10^6$	$4.49 \cdot 10^4$
C14	$4.34 \cdot 10^5$	$3.34 \cdot 10^5$	$5.95 \cdot 10^5$
C15	$1.20 \cdot 10^6$	$1.05 \cdot 10^6$	$8.55 \cdot 10^4$
C16	$-6.24 \cdot 10^4$	$-6.31 \cdot 10^4$	$-4.26 \cdot 10^4$
C17	$1.30 \cdot 10^5$	$-1.62 \cdot 10^5$	$-3.48 \cdot 10^5$
C18	$-5.51 \cdot 10^4$	$-4.11 \cdot 10^4$	$-2.02 \cdot 10^3$
C19	$-2.83 \cdot 10^4$	$-1.40 \cdot 10^5$	$-2.21 \cdot 10^5$
C20	$-9.54 \cdot 10^4$	$-9.18 \cdot 10^4$	$-5.57 \cdot 10^4$
C21	$8.15 \cdot 10^6$	$5.08 \cdot 10^6$	$-6.49 \cdot 10^5$
C22	$3.08 \cdot 10^6$	$2.37 \cdot 10^6$	$-3.40 \cdot 10^5$
C23	$1.21 \cdot 10^5$	$1.74 \cdot 10^4$	$-1.31 \cdot 10^5$
C24	$1.58 \cdot 10^6$	$9.58 \cdot 10^5$	$-1.21 \cdot 10^5$
C25	$-1.13 \cdot 10^5$	$-3.69 \cdot 10^4$	$4.81 \cdot 10^5$
C26	$-8.81 \cdot 10^6$	$-5.08 \cdot 10^6$	$6.72 \cdot 10^4$
C27	$-9.14 \cdot 10^4$	$-7.34 \cdot 10^4$	$-1.87 \cdot 10^4$
C28	$-3.21 \cdot 10^6$	$-1.99 \cdot 10^6$	$3.76 \cdot 10^4$
C29	$3.01 \cdot 10^6$	$8.93 \cdot 10^5$	$-1.17 \cdot 10^6$
C30	$2.76 \cdot 10^5$	$3.42 \cdot 10^5$	$1.52 \cdot 10^4$
C31	$1.98 \cdot 10^5$	$-1.21 \cdot 10^5$	$-3.94 \cdot 10^5$
C32	$1.30 \cdot 10^6$	$9.43 \cdot 10^5$	$1.65 \cdot 10^6$
C33	$-1.76 \cdot 10^6$	$-1.06 \cdot 10^5$	$-1.46 \cdot 10^5$
C34	$7.26 \cdot 10^4$	$-2.71 \cdot 10^4$	$-1.45 \cdot 10^5$
C35	$7.55 \cdot 10^5$	$3.98 \cdot 10^5$	$-9.56 \cdot 10^4$
C36	$2.10 \cdot 10^6$	$1.04 \cdot 10^6$	$-3.35 \cdot 10^5$
C37	$-1.85 \cdot 10^6$	$-8.15 \cdot 10^5$	$-2.26 \cdot 10^4$
C38	$9.22 \cdot 10^5$	$4.33 \cdot 10^5$	$-1.62 \cdot 10^5$
C39	$8.48 \cdot 10^5$	$1.56 \cdot 10^5$	$-4.91 \cdot 10^5$
C40	$-5.65 \cdot 10^5$	$-3.61 \cdot 10^5$	$5.60 \cdot 10^5$
C41	$1.60 \cdot 10^5$	$2.83 \cdot 10^4$	$-1.61 \cdot 10^5$
C42	$1.97 \cdot 10^6$	$1.38 \cdot 10^6$	$1.56 \cdot 10^5$
C43	$-4.57 \cdot 10^4$	$-3.66 \cdot 10^4$	$-1.02 \cdot 10^4$
C44	$-4.79 \cdot 10^4$	$-4.37 \cdot 10^4$	$-2.33 \cdot 10^4$
C45	$9.14 \cdot 10^5$	$5.27 \cdot 10^5$	$-8.24 \cdot 10^4$
C46	$3.36 \cdot 10^5$	$2.98 \cdot 10^5$	$1.57 \cdot 10^4$
C47	$5.37 \cdot 10^5$	$3.96 \cdot 10^5$	$3.36 \cdot 10^4$
C48	$9.97 \cdot 10^5$	$6.86 \cdot 10^5$	$7.59 \cdot 10^4$

TABLE SI-LII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
O1	$-2.44 \cdot 10^6$	$-2.84 \cdot 10^6$	$-2.28 \cdot 10^6$
O2	$2.48 \cdot 10^7$	$1.43 \cdot 10^7$	$-1.37 \cdot 10^6$
O3	$1.34 \cdot 10^7$	$1.04 \cdot 10^7$	$1.32 \cdot 10^5$
O4	$-1.83 \cdot 10^6$	$-1.47 \cdot 10^6$	$4.61 \cdot 10^6$
O5	$-2.25 \cdot 10^7$	$-1.39 \cdot 10^7$	$9.34 \cdot 10^5$
O6	$-1.70 \cdot 10^7$	$-8.08 \cdot 10^6$	$1.82 \cdot 10^5$
N1	$5.31 \cdot 10^5$	$6.29 \cdot 10^5$	$2.58 \cdot 10^6$
N2	$3.15 \cdot 10^6$	$-3.08 \cdot 10^5$	$-3.78 \cdot 10^6$
N3	$-1.09 \cdot 10^5$	$-7.86 \cdot 10^4$	$1.11 \cdot 10^4$
N4	$-1.18 \cdot 10^5$	$-1.38 \cdot 10^5$	$-1.16 \cdot 10^5$
F1	$-1.81 \cdot 10^6$	$-1.08 \cdot 10^6$	$2.23 \cdot 10^3$
F2	$-2.01 \cdot 10^6$	$-1.25 \cdot 10^6$	$1.23 \cdot 10^5$
F3	$-2.25 \cdot 10^6$	$-1.56 \cdot 10^6$	$-8.17 \cdot 10^4$
F4	$-5.83 \cdot 10^5$	$-1.75 \cdot 10^5$	$-5.48 \cdot 10^4$
F5	$-1.52 \cdot 10^5$	$-8.37 \cdot 10^4$	$3.09 \cdot 10^5$
F6	$1.57 \cdot 10^5$	$2.46 \cdot 10^4$	$4.67 \cdot 10^5$
F7	$-1.25 \cdot 10^6$	$-7.73 \cdot 10^5$	$3.08 \cdot 10^5$
F8	$-2.46 \cdot 10^6$	$-1.31 \cdot 10^6$	$4.52 \cdot 10^3$
F9	$-1.47 \cdot 10^6$	$-6.93 \cdot 10^5$	$4.41 \cdot 10^4$

TABLE SI-LIII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
H1	$1.02 \cdot 10^5$	$-1.92 \cdot 10^4$	$-2.04 \cdot 10^5$
H2	$-1.65 \cdot 10^5$	$-3.02 \cdot 10^5$	$-3.75 \cdot 10^5$
H3	$-8.64 \cdot 10^5$	$-1.07 \cdot 10^6$	$-1.01 \cdot 10^6$
H4	$-4.56 \cdot 10^6$	$-3.17 \cdot 10^6$	$-2.56 \cdot 10^6$
H5	$-1.66 \cdot 10^6$	$8.56 \cdot 10^4$	$1.37 \cdot 10^5$
H6	$-1.37 \cdot 10^6$	$2.65 \cdot 10^5$	$2.88 \cdot 10^5$
H7	$-1.91 \cdot 10^6$	$9.96 \cdot 10^5$	$9.18 \cdot 10^5$
H8	$1.11 \cdot 10^5$	$3.37 \cdot 10^6$	$2.68 \cdot 10^6$
H9	$-3.70 \cdot 10^6$	$9.97 \cdot 10^4$	$-2.25 \cdot 10^4$
H10	$-1.75 \cdot 10^5$	$-5.37 \cdot 10^4$	$-2.10 \cdot 10^4$
H11	$4.79 \cdot 10^2$	$-4.32 \cdot 10^5$	$-2.26 \cdot 10^5$
H12	$-6.52 \cdot 10^5$	$-1.48 \cdot 10^6$	$-9.24 \cdot 10^5$
H13	$-1.68 \cdot 10^6$	$-2.08 \cdot 10^6$	$-1.48 \cdot 10^6$
H14	$-1.68 \cdot 10^6$	$-1.40 \cdot 10^6$	$-1.12 \cdot 10^6$
H15	$-2.30 \cdot 10^6$	$-1.53 \cdot 10^6$	$-1.45 \cdot 10^6$
H16	$-5.87 \cdot 10^6$	$-3.96 \cdot 10^6$	$-4.75 \cdot 10^6$
H17	$1.51 \cdot 10^5$	$7.06 \cdot 10^5$	$4.89 \cdot 10^5$
H18	$-2.76 \cdot 10^5$	$5.90 \cdot 10^5$	$4.65 \cdot 10^5$
H19	$-1.34 \cdot 10^6$	$9.24 \cdot 10^5$	$8.21 \cdot 10^5$
H20	$-4.22 \cdot 10^6$	$1.86 \cdot 10^6$	$1.86 \cdot 10^6$

TABLE SI-LIV: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
C1	$4.26 \cdot 10^4$	$-1.42 \cdot 10^5$	$-3.69 \cdot 10^5$
C2	$-2.05 \cdot 10^5$	$-3.95 \cdot 10^5$	$-5.16 \cdot 10^5$
C3	$-7.05 \cdot 10^5$	$-9.73 \cdot 10^5$	$-1.03 \cdot 10^6$
C4	$-1.04 \cdot 10^6$	$-1.53 \cdot 10^6$	$-1.85 \cdot 10^6$
C5	$-4.86 \cdot 10^6$	$-6.05 \cdot 10^6$	$-6.13 \cdot 10^6$
C6	$-7.90 \cdot 10^6$	$-6.41 \cdot 10^6$	$-5.21 \cdot 10^6$
C7	$-1.13 \cdot 10^7$	$-9.23 \cdot 10^6$	$-6.60 \cdot 10^6$
C8	$-4.17 \cdot 10^6$	$-2.54 \cdot 10^6$	$-1.68 \cdot 10^6$
C9	$-2.29 \cdot 10^6$	$2.11 \cdot 10^5$	$2.80 \cdot 10^5$
C10	$-1.98 \cdot 10^6$	$3.72 \cdot 10^5$	$4.10 \cdot 10^5$
C11	$-2.71 \cdot 10^6$	$9.27 \cdot 10^5$	$9.19 \cdot 10^5$
C12	$-5.58 \cdot 10^6$	$1.77 \cdot 10^6$	$1.82 \cdot 10^6$
C13	$-8.13 \cdot 10^6$	$7.04 \cdot 10^6$	$6.53 \cdot 10^6$
C14	$1.00 \cdot 10^6$	$6.78 \cdot 10^6$	$5.38 \cdot 10^6$
C15	$1.04 \cdot 10^7$	$9.75 \cdot 10^6$	$6.47 \cdot 10^6$
C16	$4.00 \cdot 10^6$	$3.05 \cdot 10^6$	$1.80 \cdot 10^6$
C17	$-4.63 \cdot 10^5$	$-7.19 \cdot 10^5$	$-2.23 \cdot 10^5$
C18	$4.02 \cdot 10^3$	$-3.63 \cdot 10^5$	$-1.49 \cdot 10^5$
C19	$3.10 \cdot 10^4$	$-7.38 \cdot 10^5$	$-3.85 \cdot 10^5$
C20	$-4.41 \cdot 10^5$	$-1.88 \cdot 10^6$	$-1.12 \cdot 10^6$
C21	$-1.19 \cdot 10^6$	$-6.12 \cdot 10^6$	$-3.79 \cdot 10^6$
C22	$-5.32 \cdot 10^6$	$-8.82 \cdot 10^6$	$-6.33 \cdot 10^6$
C23	$-2.82 \cdot 10^6$	$-3.30 \cdot 10^6$	$-2.44 \cdot 10^6$
C24	$-2.59 \cdot 10^6$	$-2.32 \cdot 10^6$	$-1.86 \cdot 10^6$
C25	$-3.49 \cdot 10^6$	$-2.72 \cdot 10^6$	$-2.42 \cdot 10^6$
C26	$-7.62 \cdot 10^6$	$-6.69 \cdot 10^6$	$-6.29 \cdot 10^6$
C27	$5.30 \cdot 10^4$	$1.01 \cdot 10^6$	$7.26 \cdot 10^5$
C28	$-3.48 \cdot 10^5$	$8.70 \cdot 10^5$	$6.81 \cdot 10^5$
C29	$-1.12 \cdot 10^6$	$1.23 \cdot 10^6$	$1.04 \cdot 10^6$
C30	$-1.28 \cdot 10^6$	$3.01 \cdot 10^6$	$2.40 \cdot 10^6$
C31	$-5.29 \cdot 10^6$	$7.79 \cdot 10^6$	$6.60 \cdot 10^6$
C32	$-7.46 \cdot 10^6$	$3.88 \cdot 10^6$	$3.82 \cdot 10^6$
C33	$-1.07 \cdot 10^7$	$3.02 \cdot 10^6$	$3.61 \cdot 10^6$
C34	$-3.80 \cdot 10^6$	$5.69 \cdot 10^5$	$8.27 \cdot 10^5$

TABLE SI-LV: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
O1	$3.89 \cdot 10^6$	$-7.87 \cdot 10^6$	$-1.21 \cdot 10^7$
O2	$-1.63 \cdot 10^7$	$-2.29 \cdot 10^7$	$-1.50 \cdot 10^7$
O3	$-2.60 \cdot 10^7$	$1.50 \cdot 10^7$	$1.57 \cdot 10^7$
O4	$3.79 \cdot 10^7$	$2.08 \cdot 10^7$	$1.06 \cdot 10^7$
O5	$2.57 \cdot 10^6$	$2.68 \cdot 10^7$	$2.05 \cdot 10^7$
O6	$-2.15 \cdot 10^7$	$3.68 \cdot 10^6$	$6.09 \cdot 10^6$
N1	$-1.43 \cdot 10^7$	$-2.19 \cdot 10^7$	$-1.77 \cdot 10^7$
N2	$2.78 \cdot 10^6$	$-8.31 \cdot 10^6$	$-4.23 \cdot 10^6$
F1	$-2.81 \cdot 10^6$	$-1.48 \cdot 10^6$	$-1.02 \cdot 10^6$
F2	$-1.12 \cdot 10^6$	$-2.04 \cdot 10^6$	$-1.32 \cdot 10^6$
F3	$-3.82 \cdot 10^6$	$-4.91 \cdot 10^5$	$-1.82 \cdot 10^5$
F4	$2.69 \cdot 10^6$	$1.90 \cdot 10^6$	$1.20 \cdot 10^6$
F5	$1.39 \cdot 10^6$	$1.82 \cdot 10^6$	$1.10 \cdot 10^6$
F6	$3.72 \cdot 10^6$	$1.80 \cdot 10^6$	$7.21 \cdot 10^5$
F7	$-3.78 \cdot 10^6$	$-6.11 \cdot 10^4$	$-9.14 \cdot 10^3$
F8	$-8.76 \cdot 10^5$	$2.82 \cdot 10^5$	$6.10 \cdot 10^5$
F9	$-2.39 \cdot 10^6$	$4.68 \cdot 10^5$	$5.90 \cdot 10^5$
S1	$3.29 \cdot 10^5$	$4.83 \cdot 10^2$	$-5.82 \cdot 10^5$
S2	$-4.84 \cdot 10^6$	$4.00 \cdot 10^5$	$5.63 \cdot 10^5$
S3	$5.78 \cdot 10^5$	$2.24 \cdot 10^6$	$1.55 \cdot 10^6$

TABLE SI-LVI: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
H1	$4.13 \cdot 10^5$	$1.63 \cdot 10^5$	$-2.75 \cdot 10^4$
H2	$1.70 \cdot 10^5$	$-3.68 \cdot 10^4$	$-1.24 \cdot 10^5$
H3	$-1.82 \cdot 10^5$	$-4.23 \cdot 10^5$	$-3.78 \cdot 10^5$
H4	$-1.48 \cdot 10^6$	$-1.59 \cdot 10^6$	$-1.05 \cdot 10^6$
H5	$6.61 \cdot 10^5$	$7.34 \cdot 10^5$	$4.50 \cdot 10^5$
H6	$1.16 \cdot 10^5$	$3.48 \cdot 10^5$	$3.03 \cdot 10^5$
H7	$-7.15 \cdot 10^5$	$-1.45 \cdot 10^4$	$3.09 \cdot 10^5$
H8	$-4.03 \cdot 10^6$	$-2.13 \cdot 10^6$	$-3.52 \cdot 10^5$
H9	$-1.44 \cdot 10^6$	$-8.80 \cdot 10^5$	$-2.98 \cdot 10^5$
H10	$-7.96 \cdot 10^5$	$-6.02 \cdot 10^5$	$-2.86 \cdot 10^5$
H11	$-1.60 \cdot 10^5$	$-4.01 \cdot 10^5$	$-3.64 \cdot 10^5$
H12	$3.48 \cdot 10^6$	$1.51 \cdot 10^6$	$-1.49 \cdot 10^4$
H13	$-3.43 \cdot 10^6$	$-1.70 \cdot 10^5$	$1.13 \cdot 10^6$
H14	$-3.19 \cdot 10^5$	$-1.49 \cdot 10^4$	$1.03 \cdot 10^5$
H15	$2.23 \cdot 10^5$	$6.92 \cdot 10^3$	$-6.93 \cdot 10^4$
H16	$3.05 \cdot 10^5$	$-4.27 \cdot 10^3$	$-9.46 \cdot 10^4$
H17	$1.06 \cdot 10^5$	$-5.16 \cdot 10^4$	$-4.91 \cdot 10^4$
H18	$-5.29 \cdot 10^5$	$-2.13 \cdot 10^5$	$5.66 \cdot 10^4$
H19	$-1.69 \cdot 10^6$	$-4.81 \cdot 10^5$	$2.58 \cdot 10^5$
H20	$-9.03 \cdot 10^6$	$-2.60 \cdot 10^6$	$1.19 \cdot 10^6$

TABLE SI-LVII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
C1	$5.11 \cdot 10^5$	$1.51 \cdot 10^5$	$-8.83 \cdot 10^4$
C2	$2.69 \cdot 10^5$	$-3.58 \cdot 10^4$	$-1.72 \cdot 10^5$
C3	$8.00 \cdot 10^4$	$-3.06 \cdot 10^5$	$-3.77 \cdot 10^5$
C4	$7.67 \cdot 10^5$	$-2.58 \cdot 10^5$	$-6.60 \cdot 10^5$
C5	$1.00 \cdot 10^3$	$-2.16 \cdot 10^6$	$-2.38 \cdot 10^6$
C6	$-3.20 \cdot 10^6$	$-3.29 \cdot 10^6$	$-2.10 \cdot 10^6$
C7	$-8.44 \cdot 10^6$	$-6.03 \cdot 10^6$	$-2.70 \cdot 10^6$
C8	$-3.35 \cdot 10^6$	$-2.04 \cdot 10^6$	$-7.08 \cdot 10^5$
C9	$7.71 \cdot 10^5$	$9.40 \cdot 10^5$	$6.11 \cdot 10^5$
C10	$2.63 \cdot 10^5$	$5.71 \cdot 10^5$	$4.64 \cdot 10^5$
C11	$-1.86 \cdot 10^5$	$4.82 \cdot 10^5$	$5.77 \cdot 10^5$
C12	$5.17 \cdot 10^5$	$1.65 \cdot 10^6$	$1.45 \cdot 10^6$
C13	$-2.20 \cdot 10^6$	$1.56 \cdot 10^6$	$2.62 \cdot 10^6$
C14	$-6.67 \cdot 10^6$	$-3.40 \cdot 10^6$	$-4.29 \cdot 10^5$
C15	$-1.02 \cdot 10^7$	$-7.15 \cdot 10^6$	$-2.59 \cdot 10^6$
C16	$-3.51 \cdot 10^6$	$-2.73 \cdot 10^6$	$-1.16 \cdot 10^6$
C17	$-1.83 \cdot 10^6$	$-1.19 \cdot 10^6$	$-4.50 \cdot 10^5$
C18	$-1.19 \cdot 10^6$	$-8.86 \cdot 10^5$	$-4.15 \cdot 10^5$
C19	$-8.55 \cdot 10^5$	$-8.61 \cdot 10^5$	$-5.40 \cdot 10^5$
C20	$-2.88 \cdot 10^6$	$-2.41 \cdot 10^6$	$-1.28 \cdot 10^6$
C21	$-2.06 \cdot 10^6$	$-3.37 \cdot 10^6$	$-2.72 \cdot 10^6$
C22	$6.63 \cdot 10^6$	$2.83 \cdot 10^6$	$-7.83 \cdot 10^4$
C23	$1.64 \cdot 10^7$	$9.89 \cdot 10^6$	$2.87 \cdot 10^6$
C24	$6.27 \cdot 10^6$	$4.24 \cdot 10^6$	$1.56 \cdot 10^6$
C25	$-9.83 \cdot 10^5$	$-7.38 \cdot 10^3$	$3.54 \cdot 10^5$
C26	$-9.57 \cdot 10^4$	$-3.66 \cdot 10^3$	$3.26 \cdot 10^4$
C27	$3.57 \cdot 10^5$	$6.57 \cdot 10^3$	$-1.15 \cdot 10^5$
C28	$7.77 \cdot 10^5$	$-2.87 \cdot 10^4$	$-2.70 \cdot 10^5$
C29	$1.65 \cdot 10^6$	$-4.31 \cdot 10^5$	$-8.59 \cdot 10^5$
C30	$4.22 \cdot 10^5$	$-2.99 \cdot 10^4$	$-1.46 \cdot 10^5$
C31	$1.95 \cdot 10^5$	$-9.13 \cdot 10^4$	$-1.02 \cdot 10^5$
C32	$-3.65 \cdot 10^5$	$-3.86 \cdot 10^5$	$-1.07 \cdot 10^5$
C33	$-7.93 \cdot 10^5$	$-1.27 \cdot 10^6$	$-5.91 \cdot 10^5$
C34	$-9.22 \cdot 10^5$	$-3.87 \cdot 10^5$	$7.79 \cdot 10^4$
C35	$-2.22 \cdot 10^6$	$-7.16 \cdot 10^5$	$2.85 \cdot 10^5$
C36	$-7.26 \cdot 10^6$	$-2.41 \cdot 10^6$	$7.76 \cdot 10^5$

TABLE SI-LVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$
O1	$7.04 \cdot 10^6$	$-1.10 \cdot 10^6$	$-4.68 \cdot 10^6$
O2	$-2.61 \cdot 10^7$	$-1.50 \cdot 10^7$	$-4.62 \cdot 10^6$
O3	$1.23 \cdot 10^7$	$1.83 \cdot 10^7$	$1.32 \cdot 10^7$
O4	$-1.85 \cdot 10^7$	$-1.61 \cdot 10^7$	$-7.55 \cdot 10^6$
O5	$-2.83 \cdot 10^7$	$-2.19 \cdot 10^7$	$-1.07 \cdot 10^7$
O6	$4.62 \cdot 10^7$	$3.25 \cdot 10^7$	$1.27 \cdot 10^7$
N1	$-1.22 \cdot 10^7$	$-6.08 \cdot 10^6$	$-2.64 \cdot 10^5$
N2	$2.44 \cdot 10^6$	$-3.98 \cdot 10^5$	$-1.17 \cdot 10^6$
F1	$-9.37 \cdot 10^5$	$-6.06 \cdot 10^5$	$-2.43 \cdot 10^5$
F2	$-1.71 \cdot 10^6$	$-1.17 \cdot 10^6$	$-4.95 \cdot 10^5$
F3	$-4.05 \cdot 10^6$	$-2.03 \cdot 10^6$	$-3.87 \cdot 10^5$
F4	$-2.45 \cdot 10^6$	$-1.73 \cdot 10^6$	$-6.54 \cdot 10^5$
F5	$-6.49 \cdot 10^5$	$-8.32 \cdot 10^5$	$-4.72 \cdot 10^5$
F6	$-3.25 \cdot 10^6$	$-2.62 \cdot 10^6$	$-1.22 \cdot 10^6$
F7	$3.52 \cdot 10^6$	$2.21 \cdot 10^6$	$7.08 \cdot 10^5$
F8	$3.18 \cdot 10^6$	$2.29 \cdot 10^6$	$9.08 \cdot 10^5$
F9	$5.36 \cdot 10^6$	$4.07 \cdot 10^6$	$1.81 \cdot 10^6$
S1	$1.31 \cdot 10^6$	$5.10 \cdot 10^5$	$-9.35 \cdot 10^4$
S2	$2.19 \cdot 10^6$	$2.38 \cdot 10^6$	$1.44 \cdot 10^6$
S3	$-4.31 \cdot 10^6$	$-2.67 \cdot 10^6$	$-9.29 \cdot 10^5$

TABLE SI-LIX: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$	$\bar{\Phi}_3^{p(2)}$
H1	$9.23 \cdot 10^5$	$1.69 \cdot 10^5$	$7.43 \cdot 10^5$	$1.09 \cdot 10^6$
H2	$2.74 \cdot 10^5$	$8.59 \cdot 10^4$	$1.80 \cdot 10^5$	$5.09 \cdot 10^5$
H3	$-1.05 \cdot 10^5$	$7.80 \cdot 10^4$	$-1.14 \cdot 10^5$	$4.48 \cdot 10^5$
H4	$5.22 \cdot 10^6$	$-1.33 \cdot 10^6$	$3.14 \cdot 10^6$	$2.20 \cdot 10^6$
H5	$1.57 \cdot 10^6$	$-1.71 \cdot 10^6$	$4.62 \cdot 10^5$	$-4.83 \cdot 10^5$
H6	$3.83 \cdot 10^5$	$-1.03 \cdot 10^6$	$6.50 \cdot 10^4$	$-2.67 \cdot 10^5$
H7	$-3.46 \cdot 10^5$	$-9.68 \cdot 10^5$	$-2.86 \cdot 10^5$	$-2.72 \cdot 10^5$
H8	$5.65 \cdot 10^6$	$-3.33 \cdot 10^6$	$1.61 \cdot 10^6$	$-1.42 \cdot 10^6$
H9	$-3.71 \cdot 10^5$	$3.99 \cdot 10^5$	$-3.89 \cdot 10^5$	$-1.04 \cdot 10^6$
H10	$6.40 \cdot 10^5$	$-2.55 \cdot 10^4$	$1.03 \cdot 10^5$	$-3.94 \cdot 10^5$
H11	$1.53 \cdot 10^6$	$-2.47 \cdot 10^5$	$4.25 \cdot 10^5$	$-1.73 \cdot 10^5$
H12	$-4.41 \cdot 10^6$	$4.00 \cdot 10^5$	$-2.25 \cdot 10^6$	$-2.38 \cdot 10^6$
H13	$5.22 \cdot 10^6$	$1.80 \cdot 10^6$	$8.72 \cdot 10^4$	$7.39 \cdot 10^5$
H14	$2.61 \cdot 10^5$	$4.28 \cdot 10^5$	$-2.28 \cdot 10^5$	$2.50 \cdot 10^4$
H15	$1.33 \cdot 10^4$	$2.41 \cdot 10^5$	$5.72 \cdot 10^4$	$1.02 \cdot 10^4$
H16	$5.63 \cdot 10^5$	$2.01 \cdot 10^5$	$7.75 \cdot 10^5$	$3.90 \cdot 10^5$
H17	$1.50 \cdot 10^6$	$1.35 \cdot 10^4$	$1.44 \cdot 10^6$	$1.02 \cdot 10^6$
H18	$7.33 \cdot 10^6$	$-1.50 \cdot 10^5$	$3.20 \cdot 10^6$	$6.57 \cdot 10^6$
H19	$4.28 \cdot 10^5$	$2.24 \cdot 10^5$	$5.26 \cdot 10^5$	$6.10 \cdot 10^5$
H20	$1.27 \cdot 10^6$	$-2.88 \cdot 10^5$	$8.17 \cdot 10^5$	$5.91 \cdot 10^5$
H21	$6.48 \cdot 10^5$	$-5.47 \cdot 10^4$	$4.14 \cdot 10^5$	$4.33 \cdot 10^5$
H22	$1.51 \cdot 10^6$	$-8.52 \cdot 10^4$	$6.55 \cdot 10^5$	$1.17 \cdot 10^6$
H23	$2.03 \cdot 10^5$	$1.41 \cdot 10^5$	$2.01 \cdot 10^5$	$5.31 \cdot 10^5$
H24	$-2.73 \cdot 10^5$	$4.82 \cdot 10^5$	$1.69 \cdot 10^5$	$7.39 \cdot 10^5$
H25	$2.81 \cdot 10^6$	$-9.23 \cdot 10^5$	$1.10 \cdot 10^6$	$3.91 \cdot 10^5$
H26	$3.57 \cdot 10^6$	$-1.34 \cdot 10^6$	$1.61 \cdot 10^6$	$6.94 \cdot 10^5$
H27	$1.84 \cdot 10^6$	$-6.72 \cdot 10^5$	$8.06 \cdot 10^5$	$3.39 \cdot 10^5$
H28	$8.95 \cdot 10^5$	$-2.04 \cdot 10^5$	$3.92 \cdot 10^5$	$3.02 \cdot 10^5$
H29	$7.90 \cdot 10^5$	$-1.12 \cdot 10^5$	$3.41 \cdot 10^5$	$4.03 \cdot 10^5$
H30	$1.32 \cdot 10^6$	$-2.89 \cdot 10^5$	$5.07 \cdot 10^5$	$3.50 \cdot 10^5$

TABLE SI-LX: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for hydrogen atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$	$\bar{\Phi}_3^{p(2)}$
C1	$5.24 \cdot 10^6$	$1.13 \cdot 10^6$	$4.03 \cdot 10^6$	$6.95 \cdot 10^6$
C2	$1.19 \cdot 10^6$	$4.62 \cdot 10^5$	$8.45 \cdot 10^5$	$2.43 \cdot 10^6$
C3	$8.10 \cdot 10^5$	$2.21 \cdot 10^5$	$6.19 \cdot 10^5$	$1.24 \cdot 10^6$
C4	$3.15 \cdot 10^5$	$1.34 \cdot 10^5$	$2.09 \cdot 10^5$	$7.19 \cdot 10^5$
C5	$-1.29 \cdot 10^4$	$1.30 \cdot 10^5$	$-5.30 \cdot 10^4$	$6.81 \cdot 10^5$
C6	$8.50 \cdot 10^6$	$-1.56 \cdot 10^6$	$5.61 \cdot 10^6$	$4.39 \cdot 10^6$
C7	$1.01 \cdot 10^7$	$-2.92 \cdot 10^6$	$7.47 \cdot 10^6$	$4.31 \cdot 10^6$
C8	$3.30 \cdot 10^6$	$-1.89 \cdot 10^6$	$2.25 \cdot 10^6$	$8.84 \cdot 10^5$
C9	$4.65 \cdot 10^6$	$-1.09 \cdot 10^7$	$1.09 \cdot 10^5$	$-5.19 \cdot 10^6$
C10	$1.22 \cdot 10^6$	$-4.39 \cdot 10^6$	$-5.14 \cdot 10^4$	$-1.56 \cdot 10^6$
C11	$1.31 \cdot 10^6$	$-2.11 \cdot 10^6$	$3.17 \cdot 10^5$	$-6.29 \cdot 10^5$
C12	$4.21 \cdot 10^5$	$-1.47 \cdot 10^6$	$2.56 \cdot 10^4$	$-4.15 \cdot 10^5$
C13	$-2.79 \cdot 10^5$	$-1.46 \cdot 10^6$	$-3.08 \cdot 10^5$	$-4.27 \cdot 10^5$
C14	$9.60 \cdot 10^6$	$-5.88 \cdot 10^6$	$2.51 \cdot 10^6$	$-3.14 \cdot 10^6$
C15	$1.43 \cdot 10^7$	$-2.52 \cdot 10^6$	$3.67 \cdot 10^6$	$-3.27 \cdot 10^6$
C16	$5.30 \cdot 10^6$	$-1.74 \cdot 10^5$	$1.35 \cdot 10^6$	$-7.22 \cdot 10^5$
C17	$3.25 \cdot 10^6$	$-1.93 \cdot 10^6$	$-5.12 \cdot 10^5$	$-5.89 \cdot 10^6$
C18	$3.44 \cdot 10^6$	$-6.47 \cdot 10^5$	$6.17 \cdot 10^5$	$-1.91 \cdot 10^6$
C19	$7.43 \cdot 10^5$	$8.89 \cdot 10^4$	$-3.88 \cdot 10^4$	$-1.08 \cdot 10^6$
C20	$1.08 \cdot 10^6$	$-9.51 \cdot 10^4$	$2.06 \cdot 10^5$	$-5.33 \cdot 10^5$
C21	$1.92 \cdot 10^6$	$-3.15 \cdot 10^5$	$5.10 \cdot 10^5$	$-3.51 \cdot 10^5$
C22	$-7.68 \cdot 10^6$	$-5.28 \cdot 10^4$	$-4.10 \cdot 10^6$	$-4.63 \cdot 10^6$
C23	$-1.86 \cdot 10^7$	$-2.08 \cdot 10^5$	$-8.73 \cdot 10^6$	$-4.40 \cdot 10^6$
C24	$-7.49 \cdot 10^6$	$9.82 \cdot 10^4$	$-3.45 \cdot 10^6$	$-9.03 \cdot 10^5$
C25	$1.55 \cdot 10^6$	$2.67 \cdot 10^6$	$-5.68 \cdot 10^5$	$-1.06 \cdot 10^5$
C26	$1.60 \cdot 10^5$	$7.65 \cdot 10^5$	$-2.35 \cdot 10^5$	$-4.45 \cdot 10^4$
C27	$1.77 \cdot 10^4$	$4.61 \cdot 10^5$	$1.05 \cdot 10^5$	$1.79 \cdot 10^4$
C28	$4.31 \cdot 10^5$	$5.10 \cdot 10^5$	$8.01 \cdot 10^5$	$3.56 \cdot 10^5$
C29	$1.37 \cdot 10^6$	$1.95 \cdot 10^6$	$2.77 \cdot 10^6$	$1.46 \cdot 10^6$
C30	$4.52 \cdot 10^6$	$1.16 \cdot 10^6$	$5.17 \cdot 10^6$	$4.05 \cdot 10^6$
C31	$2.38 \cdot 10^6$	$1.41 \cdot 10^5$	$2.24 \cdot 10^6$	$1.81 \cdot 10^6$
C32	$1.98 \cdot 10^6$	$7.06 \cdot 10^4$	$1.61 \cdot 10^6$	$1.61 \cdot 10^6$
C33	$3.11 \cdot 10^6$	$-8.57 \cdot 10^4$	$2.03 \cdot 10^6$	$2.43 \cdot 10^6$
C34	$7.89 \cdot 10^6$	$-4.95 \cdot 10^2$	$4.99 \cdot 10^6$	$6.75 \cdot 10^6$
C35	$1.05 \cdot 10^6$	$-3.31 \cdot 10^4$	$8.00 \cdot 10^5$	$7.60 \cdot 10^5$
C36	$9.20 \cdot 10^5$	$-6.89 \cdot 10^4$	$5.90 \cdot 10^5$	$6.31 \cdot 10^5$
C37	$1.66 \cdot 10^6$	$-9.77 \cdot 10^4$	$8.90 \cdot 10^5$	$1.24 \cdot 10^6$
C38	$1.73 \cdot 10^6$	$-3.78 \cdot 10^5$	$8.26 \cdot 10^5$	$6.81 \cdot 10^5$
C39	$3.36 \cdot 10^5$	$2.04 \cdot 10^5$	$3.48 \cdot 10^5$	$7.34 \cdot 10^5$
C40	$2.59 \cdot 10^6$	$-8.70 \cdot 10^5$	$1.12 \cdot 10^6$	$5.22 \cdot 10^5$
C41	$1.12 \cdot 10^6$	$-2.30 \cdot 10^5$	$4.77 \cdot 10^5$	$4.04 \cdot 10^5$

TABLE SI-LXI: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for carbon atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_0^{p(2)}$	$\bar{\Phi}_1^{p(2)}$	$\bar{\Phi}_2^{p(2)}$	$\bar{\Phi}_3^{p(2)}$
O1	$-9.41 \cdot 10^6$	$7.94 \cdot 10^6$	$-1.46 \cdot 10^6$	$1.73 \cdot 10^7$
O2	$1.26 \cdot 10^7$	$-2.18 \cdot 10^6$	$1.26 \cdot 10^7$	$6.22 \cdot 10^6$
O3	$-1.57 \cdot 10^7$	$-2.62 \cdot 10^7$	$-1.18 \cdot 10^7$	$-1.50 \cdot 10^7$
O4	$3.20 \cdot 10^7$	$4.84 \cdot 10^6$	$7.21 \cdot 10^6$	$-5.97 \cdot 10^6$
O5	$3.74 \cdot 10^7$	$-1.07 \cdot 10^7$	$9.27 \cdot 10^6$	$-1.14 \cdot 10^7$
O6	$-5.27 \cdot 10^7$	$-2.86 \cdot 10^6$	$-2.52 \cdot 10^7$	$-5.71 \cdot 10^6$
N1	$-7.33 \cdot 10^5$	$8.85 \cdot 10^6$	$1.31 \cdot 10^6$	$1.91 \cdot 10^4$
N2	$1.49 \cdot 10^7$	$2.13 \cdot 10^6$	$1.36 \cdot 10^7$	$1.42 \cdot 10^7$
F1	$2.63 \cdot 10^6$	$-1.40 \cdot 10^6$	$1.58 \cdot 10^6$	$6.29 \cdot 10^5$
F2	$9.04 \cdot 10^5$	$1.44 \cdot 10^5$	$1.11 \cdot 10^6$	$5.86 \cdot 10^5$
F3	$2.30 \cdot 10^6$	$-3.12 \cdot 10^6$	$1.17 \cdot 10^6$	$-2.52 \cdot 10^4$
F4	$-4.31 \cdot 10^6$	$-1.10 \cdot 10^6$	$-2.26 \cdot 10^6$	$-6.74 \cdot 10^5$
F5	$-4.17 \cdot 10^6$	$2.94 \cdot 10^5$	$-1.87 \cdot 10^6$	$-7.12 \cdot 10^5$
F6	$-6.10 \cdot 10^6$	$9.34 \cdot 10^5$	$-2.60 \cdot 10^6$	$2.84 \cdot 10^5$
F7	$2.53 \cdot 10^6$	$1.12 \cdot 10^6$	$4.80 \cdot 10^5$	$-7.28 \cdot 10^5$
F8	$3.06 \cdot 10^6$	$-4.88 \cdot 10^5$	$8.15 \cdot 10^5$	$-5.30 \cdot 10^5$
F9	$4.82 \cdot 10^6$	$-3.94 \cdot 10^5$	$1.33 \cdot 10^6$	$3.00 \cdot 10^5$
S1	$-3.74 \cdot 10^5$	$2.25 \cdot 10^5$	$-3.87 \cdot 10^5$	$1.33 \cdot 10^6$
S2	$-1.48 \cdot 10^6$	$-2.99 \cdot 10^6$	$-1.10 \cdot 10^6$	$-9.66 \cdot 10^5$
S3	$5.08 \cdot 10^6$	$-1.11 \cdot 10^6$	$1.50 \cdot 10^6$	$-3.97 \cdot 10^5$

TABLE SI-LXII: Values of the KD–dependent components of $\bar{\Phi}^{p(2)}$ (expressed in ppm au) for the other atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

$\bar{\Phi}^{p(1)}$

Atom	$\bar{\Phi}^{p(1)}_{01}$
H1	$3.96 \cdot 10^5$
H2	$9.00 \cdot 10^4$
H3	$3.61 \cdot 10^5$
H4	$-4.28 \cdot 10^5$
H5	$-5.03 \cdot 10^5$
H6	$-4.68 \cdot 10^5$
H7	$-5.71 \cdot 10^5$
H8	$-2.29 \cdot 10^4$
H9	$-2.26 \cdot 10^5$
H10	$-3.79 \cdot 10^5$
H11	$-2.42 \cdot 10^5$
H12	$1.04 \cdot 10^5$
H13	$-2.29 \cdot 10^4$
H14	$7.72 \cdot 10^3$
H15	$-6.16 \cdot 10^5$
H16	$-2.35 \cdot 10^5$
H17	$-4.04 \cdot 10^5$
H18	$2.46 \cdot 10^5$
H19	$5.52 \cdot 10^5$
H20	$4.05 \cdot 10^5$
H21	$5.40 \cdot 10^5$
H22	$6.37 \cdot 10^5$
H23	$-3.40 \cdot 10^5$
H24	$-5.76 \cdot 10^5$
H25	$5.97 \cdot 10^4$

TABLE SI-LXIII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$
C1	$3.07 \cdot 10^5$
C2	$1.52 \cdot 10^5$
C3	$-8.19 \cdot 10^5$
C4	$-1.85 \cdot 10^6$
C5	$-6.82 \cdot 10^5$
C6	$-2.57 \cdot 10^5$
C7	$-5.71 \cdot 10^5$
C8	$-4.00 \cdot 10^5$
C9	$-1.38 \cdot 10^5$
C10	$1.59 \cdot 10^4$
C11	$-4.89 \cdot 10^5$
C12	$-6.60 \cdot 10^5$
C13	$5.13 \cdot 10^5$
C14	$1.67 \cdot 10^6$
C15	$6.53 \cdot 10^5$

TABLE SI-LXIV: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$
O1	$3.18 \cdot 10^6$
O2	$-5.20 \cdot 10^6$
O3	$1.15 \cdot 10^5$
O4	$1.54 \cdot 10^5$
O5	$-4.00 \cdot 10^6$
O6	$5.13 \cdot 10^6$
O7	$1.76 \cdot 10^5$
O8	$-2.06 \cdot 10^5$

TABLE SI-LXV: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$
H1	$-1.03 \cdot 10^4$
H2	$2.29 \cdot 10^3$
H3	$-7.65 \cdot 10^5$
H4	$-2.83 \cdot 10^5$
H5	$-4.82 \cdot 10^5$
H6	$5.46 \cdot 10^3$
H7	$-7.98 \cdot 10^3$
H8	$-8.53 \cdot 10^4$
H9	$-3.76 \cdot 10^5$
H10	$-1.21 \cdot 10^5$
H11	$-1.00 \cdot 10^6$
H12	$-1.85 \cdot 10^3$
H13	$-2.32 \cdot 10^5$
H14	$-1.97 \cdot 10^5$
H15	$1.97 \cdot 10^4$
H16	$-3.82 \cdot 10^4$
H17	$1.34 \cdot 10^3$
H18	$5.25 \cdot 10^5$
H19	$1.27 \cdot 10^5$
H20	$4.60 \cdot 10^5$
H21	$-5.61 \cdot 10^5$
H22	$-4.83 \cdot 10^5$
H23	$-6.65 \cdot 10^5$
H24	$-7.88 \cdot 10^5$
H25	$7.66 \cdot 10^5$
H26	$5.94 \cdot 10^5$
H27	$6.01 \cdot 10^5$
H28	$3.63 \cdot 10^5$
H29	$1.35 \cdot 10^5$
H30	$-7.32 \cdot 10^4$
H31	$-3.49 \cdot 10^5$

TABLE SI-LXVI: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$
C1	$-1.35 \cdot 10^5$
C2	$-5.49 \cdot 10^3$
C3	$-3.84 \cdot 10^3$
C4	$-9.18 \cdot 10^4$
C5	$2.26 \cdot 10^3$
C6	$-5.95 \cdot 10^5$
C7	$3.97 \cdot 10^5$
C8	$-2.13 \cdot 10^6$
C9	$-2.76 \cdot 10^5$
C10	$4.75 \cdot 10^3$
C11	$1.52 \cdot 10^4$
C12	$3.01 \cdot 10^4$
C13	$-1.42 \cdot 10^4$
C14	$-1.35 \cdot 10^5$
C15	$2.25 \cdot 10^6$
C16	$-1.63 \cdot 10^4$
C17	$6.03 \cdot 10^4$
C18	$-7.59 \cdot 10^5$
C19	$5.62 \cdot 10^3$
C20	$-1.24 \cdot 10^5$
C21	$-8.00 \cdot 10^5$
C22	$-1.89 \cdot 10^5$
C23	$-5.18 \cdot 10^5$
C24	$-1.16 \cdot 10^3$
C25	$-3.48 \cdot 10^5$
C26	$-2.61 \cdot 10^5$
C27	$-1.77 \cdot 10^4$
C28	$4.19 \cdot 10^5$
C29	$-7.60 \cdot 10^5$
C30	$-6.85 \cdot 10^5$
C31	$8.58 \cdot 10^5$
C32	$7.38 \cdot 10^5$
C33	$-1.22 \cdot 10^5$

TABLE SI-LXVII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$
O1	$3.64 \cdot 10^4$
O2	$-6.26 \cdot 10^6$
O3	$3.84 \cdot 10^6$
O4	$-5.20 \cdot 10^6$
O5	$1.13 \cdot 10^6$
O6	$6.92 \cdot 10^6$
N1	$-1.00 \cdot 10^6$
N2	$-3.88 \cdot 10^5$
N3	$-1.81 \cdot 10^4$
N4	$1.22 \cdot 10^4$

TABLE SI-LXVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$
H1	$-1.32 \cdot 10^5$	$3.37 \cdot 10^4$	$-1.60 \cdot 10^6$
H2	$-1.59 \cdot 10^4$	$7.04 \cdot 10^3$	$-3.10 \cdot 10^5$
H3	$-2.60 \cdot 10^4$	$2.52 \cdot 10^3$	$-1.76 \cdot 10^5$
H4	$-7.47 \cdot 10^3$	-3.88	$-4.36 \cdot 10^4$
H5	$3.31 \cdot 10^3$	$-2.22 \cdot 10^2$	$-1.68 \cdot 10^4$
H6	$4.36 \cdot 10^4$	$1.26 \cdot 10^2$	$2.39 \cdot 10^4$
H7	$6.09 \cdot 10^4$	$3.16 \cdot 10^3$	$-4.30 \cdot 10^4$
H8	$4.03 \cdot 10^5$	$2.16 \cdot 10^4$	$-1.67 \cdot 10^5$
H9	$1.21 \cdot 10^6$	$-3.56 \cdot 10^1$	$2.47 \cdot 10^6$
H10	$5.83 \cdot 10^5$	$-5.06 \cdot 10^3$	$1.36 \cdot 10^6$
H11	$8.24 \cdot 10^5$	$-1.68 \cdot 10^3$	$2.04 \cdot 10^6$
H12	$-2.64 \cdot 10^5$	$-1.34 \cdot 10^4$	$-2.97 \cdot 10^4$
H13	$-1.12 \cdot 10^6$	$-3.94 \cdot 10^3$	$-2.04 \cdot 10^6$
H14	$-7.93 \cdot 10^5$	$-6.66 \cdot 10^3$	$-1.46 \cdot 10^6$
H15	$-1.28 \cdot 10^6$	$-3.45 \cdot 10^3$	$-2.75 \cdot 10^6$
H16	$8.55 \cdot 10^5$	$9.48 \cdot 10^3$	$1.36 \cdot 10^6$
H17	$8.69 \cdot 10^5$	$3.02 \cdot 10^3$	$1.57 \cdot 10^6$
H18	$9.11 \cdot 10^5$	$5.53 \cdot 10^3$	$1.39 \cdot 10^6$
H19	$1.18 \cdot 10^6$	$-1.39 \cdot 10^3$	$2.72 \cdot 10^6$
H20	$-5.54 \cdot 10^5$	$7.05 \cdot 10^2$	$-1.69 \cdot 10^6$
H21	$-2.68 \cdot 10^5$	$-9.27 \cdot 10^3$	$2.72 \cdot 10^5$
H22	$2.75 \cdot 10^5$	$-4.69 \cdot 10^3$	$1.15 \cdot 10^6$
H23	$4.63 \cdot 10^4$	$-5.21 \cdot 10^3$	$1.05 \cdot 10^6$
H24	$-6.56 \cdot 10^5$	$9.13 \cdot 10^3$	$-1.80 \cdot 10^6$
H25	$-5.07 \cdot 10^5$	$4.62 \cdot 10^3$	$-1.40 \cdot 10^6$
H26	$-1.01 \cdot 10^6$	$1.16 \cdot 10^3$	$-2.34 \cdot 10^6$
H27	$-4.57 \cdot 10^4$	$-2.19 \cdot 10^3$	$-3.90 \cdot 10^5$
H28	$-6.11 \cdot 10^3$	$5.26 \cdot 10^2$	$-6.32 \cdot 10^4$
H29	$2.65 \cdot 10^4$	$-1.42 \cdot 10^3$	$-5.60 \cdot 10^4$

TABLE SI-LXIX: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$
C1	$-1.77 \cdot 10^5$	$2.60 \cdot 10^4$	$-1.45 \cdot 10^6$
C2	$-5.18 \cdot 10^4$	$8.87 \cdot 10^3$	$-4.77 \cdot 10^5$
C3	$-4.76 \cdot 10^4$	$4.01 \cdot 10^3$	$-2.99 \cdot 10^5$
C4	$-6.30 \cdot 10^4$	$1.98 \cdot 10^3$	$-3.26 \cdot 10^5$
C5	$-2.17 \cdot 10^4$	$2.48 \cdot 10^1$	$-1.33 \cdot 10^5$
C6	$-7.76 \cdot 10^3$	$-6.83 \cdot 10^1$	$-5.17 \cdot 10^4$
C7	$1.78 \cdot 10^3$	$-2.68 \cdot 10^2$	$-2.76 \cdot 10^4$
C8	$8.35 \cdot 10^3$	$-6.90 \cdot 10^2$	$-5.25 \cdot 10^4$
C9	$5.52 \cdot 10^4$	$-1.22 \cdot 10^3$	$-2.42 \cdot 10^3$
C10	$6.99 \cdot 10^4$	$1.96 \cdot 10^2$	$3.81 \cdot 10^4$
C11	$1.09 \cdot 10^5$	$3.00 \cdot 10^3$	$1.15 \cdot 10^4$
C12	$3.59 \cdot 10^5$	$1.06 \cdot 10^4$	$6.85 \cdot 10^4$
C13	$9.76 \cdot 10^4$	$-3.55 \cdot 10^3$	$-1.07 \cdot 10^5$
C14	$-1.32 \cdot 10^5$	$2.59 \cdot 10^3$	$-7.23 \cdot 10^5$
C15	$1.06 \cdot 10^6$	$-4.14 \cdot 10^3$	$2.44 \cdot 10^6$
C16	$1.93 \cdot 10^6$	$-2.20 \cdot 10^4$	$5.10 \cdot 10^6$
C17	$-4.88 \cdot 10^5$	$-2.56 \cdot 10^4$	$3.66 \cdot 10^4$
C18	$-2.99 \cdot 10^6$	$-3.04 \cdot 10^4$	$-4.99 \cdot 10^6$
C19	$-1.35 \cdot 10^6$	$-7.32 \cdot 10^3$	$-2.57 \cdot 10^6$
C20	$1.21 \cdot 10^6$	$7.32 \cdot 10^3$	$2.04 \cdot 10^6$
C21	$3.64 \cdot 10^6$	$1.29 \cdot 10^4$	$6.77 \cdot 10^6$
C22	$2.29 \cdot 10^6$	$-3.02 \cdot 10^3$	$5.27 \cdot 10^6$
C23	$1.42 \cdot 10^6$	$-1.95 \cdot 10^4$	$5.18 \cdot 10^6$
C24	$-3.71 \cdot 10^5$	$-1.06 \cdot 10^2$	$-1.67 \cdot 10^6$
C25	$-1.00 \cdot 10^6$	$3.21 \cdot 10^3$	$-3.12 \cdot 10^6$
C26	$-2.21 \cdot 10^6$	$1.44 \cdot 10^4$	$-6.03 \cdot 10^6$
C27	$1.25 \cdot 10^5$	$-8.19 \cdot 10^3$	$1.25 \cdot 10^6$
C28	$-9.30 \cdot 10^5$	$6.25 \cdot 10^3$	$-2.40 \cdot 10^6$
C29	$-3.00 \cdot 10^4$	$-1.17 \cdot 10^3$	$-2.88 \cdot 10^5$

TABLE SI-LXX: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
O1	$-9.82 \cdot 10^5$	$-7.57 \cdot 10^4$	$6.21 \cdot 10^6$
O2	$8.84 \cdot 10^6$	$6.13 \cdot 10^4$	$1.43 \cdot 10^7$
O3	$-2.27 \cdot 10^4$	$-1.56 \cdot 10^3$	$-2.41 \cdot 10^5$
O4	$-6.50 \cdot 10^6$	$6.54 \cdot 10^4$	$-1.72 \cdot 10^7$
O5	$9.15 \cdot 10^6$	$-1.20 \cdot 10^4$	$2.06 \cdot 10^7$
O6	$-1.09 \cdot 10^7$	$-4.51 \cdot 10^4$	$-2.01 \cdot 10^7$
N1	$-5.57 \cdot 10^5$	$3.33 \cdot 10^4$	$-2.99 \cdot 10^6$
N2	$7.67 \cdot 10^5$	$1.26 \cdot 10^3$	$4.92 \cdot 10^5$
N3	$-1.83 \cdot 10^4$	$2.28 \cdot 10^2$	$-9.56 \cdot 10^4$
N4	$1.18 \cdot 10^4$	$-4.40 \cdot 10^2$	$-1.72 \cdot 10^4$

TABLE SI-LXXI: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$
H1	$7.76 \cdot 10^5$
H2	$4.42 \cdot 10^4$
H3	$-3.09 \cdot 10^4$
H4	$-1.28 \cdot 10^4$
H5	$2.85 \cdot 10^4$
H6	$8.77 \cdot 10^4$
H7	$1.29 \cdot 10^5$
H8	$3.26 \cdot 10^5$
H9	$6.49 \cdot 10^5$
H10	$5.18 \cdot 10^5$
H11	$1.12 \cdot 10^6$
H12	$-3.13 \cdot 10^5$
H13	$-1.08 \cdot 10^6$
H14	$-7.18 \cdot 10^5$
H15	$-9.88 \cdot 10^5$
H16	$2.38 \cdot 10^5$
H17	$-9.13 \cdot 10^4$
H18	$-4.58 \cdot 10^5$
H19	$3.06 \cdot 10^5$
H20	$1.89 \cdot 10^4$
H21	$1.52 \cdot 10^5$
H22	$2.41 \cdot 10^4$
H23	$-2.78 \cdot 10^5$
H24	$1.88 \cdot 10^5$
H25	$-1.55 \cdot 10^5$
H26	$9.60 \cdot 10^5$
H27	$8.12 \cdot 10^5$
H28	$7.25 \cdot 10^5$
H29	$7.86 \cdot 10^5$

TABLE SI-LXXII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$
C1	$2.97 \cdot 10^5$
C2	$2.41 \cdot 10^4$
C3	$-4.03 \cdot 10^4$
C4	$-5.02 \cdot 10^4$
C5	$-9.80 \cdot 10^3$
C6	$3.13 \cdot 10^4$
C7	$1.16 \cdot 10^5$
C8	$1.35 \cdot 10^5$
C9	$1.94 \cdot 10^5$
C10	$4.39 \cdot 10^5$
C11	$2.09 \cdot 10^5$
C12	$-7.12 \cdot 10^4$
C13	$9.13 \cdot 10^5$
C14	$1.52 \cdot 10^6$
C15	$-6.11 \cdot 10^5$
C16	$-2.76 \cdot 10^6$
C17	$-1.19 \cdot 10^6$
C18	$-1.13 \cdot 10^5$
C19	$-1.16 \cdot 10^5$
C20	$4.84 \cdot 10^5$
C21	$5.32 \cdot 10^5$
C22	$1.16 \cdot 10^5$
C23	$-2.43 \cdot 10^4$
C24	$7.98 \cdot 10^5$
C25	$1.83 \cdot 10^6$
C26	$3.06 \cdot 10^6$
C27	$1.05 \cdot 10^6$

TABLE SI-LXXIII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$
O1	$8.11 \cdot 10^6$
O2	$-9.80 \cdot 10^6$
O3	$-4.17 \cdot 10^6$
O4	$2.14 \cdot 10^5$
O5	$-2.48 \cdot 10^6$
O6	$7.79 \cdot 10^6$
N1	$1.29 \cdot 10^5$
N2	$8.54 \cdot 10^5$

TABLE SI-LXXIV: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{03}$	$\bar{\Phi}^{p(1)}_{12}$	$\bar{\Phi}^{p(1)}_{13}$	$\bar{\Phi}^{p(1)}_{23}$
H1	$7.76 \cdot 10^5$	$3.20 \cdot 10^4$	$-2.72 \cdot 10^4$	$3.56 \cdot 10^6$	$-2.96 \cdot 10^5$	$-4.79 \cdot 10^6$
H2	$-2.36 \cdot 10^6$	$-1.39 \cdot 10^5$	$-1.00 \cdot 10^5$	$-2.80 \cdot 10^6$	$-2.44 \cdot 10^6$	$5.47 \cdot 10^6$
H3	$-6.55 \cdot 10^5$	$-3.90 \cdot 10^4$	$-3.70 \cdot 10^4$	$-5.19 \cdot 10^5$	$-8.73 \cdot 10^5$	$4.48 \cdot 10^5$
H4	$8.57 \cdot 10^5$	$1.06 \cdot 10^5$	$4.92 \cdot 10^4$	$-3.09 \cdot 10^6$	$9.67 \cdot 10^5$	$-1.40 \cdot 10^7$
H5	$5.24 \cdot 10^4$	$1.26 \cdot 10^4$	$-2.72 \cdot 10^3$	$-4.58 \cdot 10^5$	$-8.38 \cdot 10^4$	$-3.09 \cdot 10^6$
H6	$-1.93 \cdot 10^5$	$2.02 \cdot 10^2$	$5.25 \cdot 10^3$	$-1.35 \cdot 10^6$	$4.58 \cdot 10^4$	$-6.61 \cdot 10^5$
H7	$2.70 \cdot 10^5$	$-1.17 \cdot 10^4$	$-6.24 \cdot 10^3$	$2.66 \cdot 10^6$	$1.58 \cdot 10^4$	$4.03 \cdot 10^6$
H8	$1.53 \cdot 10^6$	$2.23 \cdot 10^4$	$-4.97 \cdot 10^3$	$8.44 \cdot 10^6$	$5.02 \cdot 10^5$	$5.86 \cdot 10^6$
H9	$1.24 \cdot 10^5$	$-4.53 \cdot 10^4$	$-5.12 \cdot 10^4$	$5.44 \cdot 10^6$	$-6.79 \cdot 10^5$	$7.54 \cdot 10^6$
H10	$-2.03 \cdot 10^5$	$-2.58 \cdot 10^4$	$-1.54 \cdot 10^4$	$9.61 \cdot 10^5$	$-2.43 \cdot 10^5$	$3.65 \cdot 10^6$
H11	$4.26 \cdot 10^5$	$4.57 \cdot 10^4$	$3.81 \cdot 10^4$	$-1.47 \cdot 10^6$	$7.43 \cdot 10^5$	$-4.00 \cdot 10^6$
H12	$-3.43 \cdot 10^5$	$-1.98 \cdot 10^4$	$-7.33 \cdot 10^3$	$-5.84 \cdot 10^5$	$-1.80 \cdot 10^5$	$1.87 \cdot 10^6$
H13	$-1.37 \cdot 10^6$	$-4.76 \cdot 10^4$	$-1.40 \cdot 10^3$	$-5.49 \cdot 10^6$	$-4.48 \cdot 10^5$	$1.09 \cdot 10^6$

TABLE SI-LXXV: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{03}$	$\bar{\Phi}^{p(1)}_{12}$	$\bar{\Phi}^{p(1)}_{13}$	$\bar{\Phi}^{p(1)}_{23}$
C1	$-8.79 \cdot 10^5$	$-5.71 \cdot 10^4$	$-7.04 \cdot 10^4$	$2.17 \cdot 10^5$	$-1.54 \cdot 10^6$	$-3.60 \cdot 10^5$
C2	$2.78 \cdot 10^5$	$4.73 \cdot 10^4$	$1.10 \cdot 10^4$	$-1.74 \cdot 10^6$	$1.63 \cdot 10^5$	$-8.33 \cdot 10^6$
C3	$-2.91 \cdot 10^4$	$-1.63 \cdot 10^3$	$2.57 \cdot 10^3$	$-1.18 \cdot 10^5$	$6.31 \cdot 10^4$	$6.65 \cdot 10^5$
C4	$4.95 \cdot 10^5$	$-2.49 \cdot 10^4$	$-2.79 \cdot 10^4$	$5.74 \cdot 10^6$	$-1.60 \cdot 10^5$	$7.68 \cdot 10^6$
C5	$4.17 \cdot 10^6$	$2.31 \cdot 10^5$	$1.15 \cdot 10^5$	$7.71 \cdot 10^6$	$3.14 \cdot 10^6$	$-1.30 \cdot 10^7$
C6	$8.33 \cdot 10^5$	$8.67 \cdot 10^4$	$7.34 \cdot 10^4$	$-2.66 \cdot 10^6$	$1.44 \cdot 10^6$	$-7.34 \cdot 10^6$
C7	$-2.35 \cdot 10^6$	$-4.25 \cdot 10^4$	$4.57 \cdot 10^4$	$-1.34 \cdot 10^7$	$8.60 \cdot 10^3$	$-2.68 \cdot 10^6$
C8	$1.83 \cdot 10^6$	$9.00 \cdot 10^4$	$3.52 \cdot 10^4$	$4.54 \cdot 10^6$	$1.13 \cdot 10^6$	$-4.54 \cdot 10^6$
C9	$-1.42 \cdot 10^6$	$-4.49 \cdot 10^4$	$1.84 \cdot 10^3$	$-6.08 \cdot 10^6$	$-4.10 \cdot 10^5$	$4.60 \cdot 10^5$
C10	$-5.94 \cdot 10^5$	$-9.19 \cdot 10^2$	$1.35 \cdot 10^4$	$-4.00 \cdot 10^6$	$7.85 \cdot 10^4$	$-2.11 \cdot 10^6$
C11	$-5.03 \cdot 10^5$	$-3.42 \cdot 10^4$	$-1.35 \cdot 10^4$	$-4.09 \cdot 10^5$	$-2.85 \cdot 10^5$	$3.85 \cdot 10^6$
C12	$5.34 \cdot 10^5$	$-3.34 \cdot 10^4$	$-4.08 \cdot 10^4$	$6.96 \cdot 10^6$	$-3.42 \cdot 10^5$	$8.89 \cdot 10^6$
C13	$-1.18 \cdot 10^5$	$1.40 \cdot 10^4$	$1.18 \cdot 10^4$	$-2.01 \cdot 10^6$	$1.49 \cdot 10^5$	$-2.85 \cdot 10^6$
C14	$3.76 \cdot 10^5$	$-6.13 \cdot 10^3$	$-1.76 \cdot 10^4$	$3.36 \cdot 10^6$	$-1.22 \cdot 10^5$	$2.83 \cdot 10^6$
C15	$-5.00 \cdot 10^6$	$-2.32 \cdot 10^5$	$-8.25 \cdot 10^4$	$-1.39 \cdot 10^7$	$-2.91 \cdot 10^6$	$1.00 \cdot 10^7$
C16	$-2.66 \cdot 10^6$	$-9.30 \cdot 10^4$	$-2.67 \cdot 10^3$	$-1.06 \cdot 10^7$	$-8.69 \cdot 10^5$	$2.25 \cdot 10^6$
C17	$-9.94 \cdot 10^5$	$2.94 \cdot 10^4$	$7.66 \cdot 10^4$	$-1.05 \cdot 10^7$	$9.24 \cdot 10^5$	$-6.77 \cdot 10^6$
C18	$-1.70 \cdot 10^6$	$-8.55 \cdot 10^4$	$-3.95 \cdot 10^4$	$-3.96 \cdot 10^6$	$-1.18 \cdot 10^6$	$3.87 \cdot 10^6$
C19	$2.67 \cdot 10^5$	$4.37 \cdot 10^4$	$3.93 \cdot 10^4$	$-2.38 \cdot 10^6$	$7.11 \cdot 10^5$	$-4.55 \cdot 10^6$

TABLE SI-LXXVI: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{03}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$	$\bar{\Phi}_{13}^{p(1)}$	$\bar{\Phi}_{23}^{p(1)}$
O1	$-1.63 \cdot 10^6$	$-8.62 \cdot 10^4$	$-1.21 \cdot 10^5$	$-1.33 \cdot 10^6$	$-2.84 \cdot 10^6$	$-5.43 \cdot 10^6$
O2	$-7.97 \cdot 10^5$	$-8.23 \cdot 10^4$	$-3.07 \cdot 10^4$	$1.65 \cdot 10^6$	$-4.41 \cdot 10^5$	$1.30 \cdot 10^7$
O3	$1.49 \cdot 10^7$	$6.83 \cdot 10^5$	$2.48 \cdot 10^5$	$4.14 \cdot 10^7$	$8.65 \cdot 10^6$	$-2.90 \cdot 10^7$
O4	$-1.23 \cdot 10^7$	$-4.58 \cdot 10^5$	$-5.25 \cdot 10^4$	$-4.62 \cdot 10^7$	$-4.68 \cdot 10^6$	$1.30 \cdot 10^7$
O5	$-6.45 \cdot 10^4$	$1.04 \cdot 10^5$	$6.00 \cdot 10^4$	$-9.05 \cdot 10^6$	$8.43 \cdot 10^5$	$-1.88 \cdot 10^7$
O6	$6.70 \cdot 10^6$	$1.10 \cdot 10^5$	$-7.73 \cdot 10^4$	$3.78 \cdot 10^7$	$1.19 \cdot 10^6$	$1.77 \cdot 10^7$
O7	$-1.27 \cdot 10^7$	$-6.60 \cdot 10^5$	$-3.27 \cdot 10^5$	$-2.71 \cdot 10^7$	$-9.42 \cdot 10^6$	$3.03 \cdot 10^7$
O8	$4.60 \cdot 10^6$	$4.40 \cdot 10^5$	$3.33 \cdot 10^5$	$-9.93 \cdot 10^6$	$6.75 \cdot 10^6$	$-3.80 \cdot 10^7$
F1	$1.37 \cdot 10^6$	$6.86 \cdot 10^4$	$1.94 \cdot 10^4$	$3.54 \cdot 10^6$	$7.19 \cdot 10^5$	$-4.33 \cdot 10^6$
F2	$8.81 \cdot 10^5$	$4.78 \cdot 10^4$	$2.23 \cdot 10^4$	$1.75 \cdot 10^6$	$6.32 \cdot 10^5$	$-2.70 \cdot 10^6$
F3	$1.47 \cdot 10^6$	$5.94 \cdot 10^4$	$1.93 \cdot 10^4$	$4.79 \cdot 10^6$	$7.84 \cdot 10^5$	$-1.43 \cdot 10^6$
F4	$-1.35 \cdot 10^6$	$-5.69 \cdot 10^4$	$-1.34 \cdot 10^4$	$-4.40 \cdot 10^6$	$-6.40 \cdot 10^5$	$2.21 \cdot 10^6$
F5	$-1.28 \cdot 10^6$	$-4.24 \cdot 10^4$	$-4.32 \cdot 10^3$	$-5.14 \cdot 10^6$	$-4.57 \cdot 10^5$	$4.76 \cdot 10^5$
F6	$-5.42 \cdot 10^5$	$-1.18 \cdot 10^4$	$7.45 \cdot 10^3$	$-2.87 \cdot 10^6$	$-4.76 \cdot 10^4$	$-4.33 \cdot 10^5$
F7	$4.35 \cdot 10^4$	$3.09 \cdot 10^4$	$2.14 \cdot 10^4$	$-2.39 \cdot 10^6$	$3.40 \cdot 10^5$	$-4.77 \cdot 10^6$
F8	$-1.45 \cdot 10^5$	$1.22 \cdot 10^3$	$4.09 \cdot 10^3$	$-1.10 \cdot 10^6$	$2.75 \cdot 10^4$	$-8.06 \cdot 10^5$
F9	$1.69 \cdot 10^4$	$8.73 \cdot 10^3$	$3.45 \cdot 10^3$	$-5.77 \cdot 10^5$	$4.57 \cdot 10^4$	$-1.62 \cdot 10^6$
F10	$1.96 \cdot 10^5$	$-9.91 \cdot 10^3$	$-2.25 \cdot 10^4$	$2.60 \cdot 10^6$	$-2.84 \cdot 10^5$	$1.82 \cdot 10^6$
F11	$7.61 \cdot 10^5$	$1.65 \cdot 10^4$	$-3.11 \cdot 10^3$	$3.85 \cdot 10^6$	$2.20 \cdot 10^5$	$1.54 \cdot 10^6$
F12	$-5.10 \cdot 10^4$	$-1.30 \cdot 10^4$	$-1.16 \cdot 10^4$	$9.14 \cdot 10^5$	$-1.76 \cdot 10^5$	$1.80 \cdot 10^6$
F13	$-1.02 \cdot 10^6$	$-5.85 \cdot 10^4$	$-3.78 \cdot 10^4$	$-1.46 \cdot 10^6$	$-9.45 \cdot 10^5$	$2.68 \cdot 10^6$
F14	$-1.11 \cdot 10^6$	$-5.84 \cdot 10^4$	$-2.70 \cdot 10^4$	$-2.38 \cdot 10^6$	$-8.02 \cdot 10^5$	$2.87 \cdot 10^6$
F15	$-1.01 \cdot 10^6$	$-4.75 \cdot 10^4$	$-1.89 \cdot 10^4$	$-2.69 \cdot 10^6$	$-6.21 \cdot 10^5$	$2.03 \cdot 10^6$
F16	$7.17 \cdot 10^5$	$4.75 \cdot 10^4$	$3.20 \cdot 10^4$	$4.28 \cdot 10^5$	$7.40 \cdot 10^5$	$-2.95 \cdot 10^6$
F17	$4.66 \cdot 10^5$	$5.34 \cdot 10^4$	$3.59 \cdot 10^4$	$-1.65 \cdot 10^6$	$7.07 \cdot 10^5$	$-5.67 \cdot 10^6$
F18	$-1.38 \cdot 10^5$	$1.05 \cdot 10^4$	$1.71 \cdot 10^4$	$-2.08 \cdot 10^6$	$2.31 \cdot 10^5$	$-1.81 \cdot 10^6$

TABLE SI-LXXVII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$
H1	$-7.33 \cdot 10^5$	$1.99 \cdot 10^4$	$-2.27 \cdot 10^6$
H2	$5.54 \cdot 10^5$	$2.53 \cdot 10^4$	$2.19 \cdot 10^6$
H3	$-3.18 \cdot 10^4$	$2.57 \cdot 10^4$	$-1.30 \cdot 10^5$
H4	$1.00 \cdot 10^6$	$4.38 \cdot 10^4$	$2.62 \cdot 10^6$
H5	$-3.69 \cdot 10^5$	$2.82 \cdot 10^3$	$-1.49 \cdot 10^6$
H6	$1.29 \cdot 10^6$	$3.27 \cdot 10^4$	$2.64 \cdot 10^6$
H7	$1.06 \cdot 10^6$	$2.89 \cdot 10^4$	$2.55 \cdot 10^6$
H8	$1.89 \cdot 10^6$	$3.42 \cdot 10^4$	$4.49 \cdot 10^6$
H9	$4.89 \cdot 10^5$	$4.04 \cdot 10^4$	$1.23 \cdot 10^6$
H10	$-6.61 \cdot 10^4$	$2.62 \cdot 10^3$	$-5.66 \cdot 10^5$
H11	$-1.34 \cdot 10^6$	$1.90 \cdot 10^4$	$-3.71 \cdot 10^6$
H12	$-5.06 \cdot 10^5$	$5.67 \cdot 10^3$	$-1.63 \cdot 10^6$
H13	$1.81 \cdot 10^5$	$5.29 \cdot 10^3$	$1.02 \cdot 10^4$
H14	$7.94 \cdot 10^5$	$1.70 \cdot 10^4$	$1.04 \cdot 10^6$
H15	$1.43 \cdot 10^4$	$-9.02 \cdot 10^4$	$7.83 \cdot 10^6$
H16	$5.97 \cdot 10^5$	$-8.69 \cdot 10^4$	$5.46 \cdot 10^6$
H17	$-8.58 \cdot 10^5$	$-7.45 \cdot 10^4$	$1.67 \cdot 10^6$
H18	$-2.79 \cdot 10^5$	$6.18 \cdot 10^3$	$-2.37 \cdot 10^6$
H19	$-2.63 \cdot 10^5$	$2.52 \cdot 10^3$	$-1.27 \cdot 10^6$
H20	$-3.34 \cdot 10^5$	$2.44 \cdot 10^3$	$-1.21 \cdot 10^6$
H21	$-1.18 \cdot 10^6$	$6.51 \cdot 10^3$	$-3.92 \cdot 10^6$
H22	$-2.69 \cdot 10^6$	$1.74 \cdot 10^4$	$-1.19 \cdot 10^7$
H23	$2.85 \cdot 10^5$	$3.59 \cdot 10^4$	$-3.36 \cdot 10^6$
H24	$-3.34 \cdot 10^6$	$-1.97 \cdot 10^5$	$-1.66 \cdot 10^6$

TABLE SI-LXXVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
C1	$-6.50 \cdot 10^5$	$8.98 \cdot 10^4$	$-8.00 \cdot 10^5$
C2	$4.74 \cdot 10^5$	$3.96 \cdot 10^4$	$1.57 \cdot 10^6$
C3	$-4.80 \cdot 10^6$	$2.85 \cdot 10^4$	$-1.55 \cdot 10^7$
C4	$-2.30 \cdot 10^6$	$8.44 \cdot 10^4$	$-7.68 \cdot 10^6$
C5	$-3.43 \cdot 10^5$	$4.09 \cdot 10^3$	$-1.63 \cdot 10^6$
C6	$1.81 \cdot 10^6$	$4.28 \cdot 10^4$	$4.18 \cdot 10^6$
C7	$4.15 \cdot 10^6$	$1.20 \cdot 10^5$	$1.01 \cdot 10^7$
C8	$-7.37 \cdot 10^5$	$8.29 \cdot 10^3$	$-3.42 \cdot 10^6$
C9	$9.34 \cdot 10^5$	$7.90 \cdot 10^4$	$2.24 \cdot 10^6$
C10	$-8.14 \cdot 10^4$	$3.87 \cdot 10^3$	$-7.78 \cdot 10^5$
C11	$-2.63 \cdot 10^6$	$3.71 \cdot 10^4$	$-7.29 \cdot 10^6$
C12	$-1.38 \cdot 10^6$	$1.32 \cdot 10^4$	$-4.81 \cdot 10^6$
C13	$-6.80 \cdot 10^5$	$6.19 \cdot 10^3$	$-2.32 \cdot 10^6$
C14	$1.40 \cdot 10^5$	$6.32 \cdot 10^3$	$-2.87 \cdot 10^5$
C15	$4.18 \cdot 10^5$	$1.31 \cdot 10^4$	$-6.81 \cdot 10^4$
C16	$-4.02 \cdot 10^5$	$-1.31 \cdot 10^5$	$6.12 \cdot 10^6$
C17	$-6.61 \cdot 10^5$	$5.98 \cdot 10^3$	$-3.27 \cdot 10^6$
C18	$-4.37 \cdot 10^5$	$3.47 \cdot 10^3$	$-1.91 \cdot 10^6$
C19	$-4.75 \cdot 10^5$	$3.50 \cdot 10^3$	$-1.76 \cdot 10^6$

TABLE SI-LXXIX: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
O1	$-1.18 \cdot 10^7$	$1.68 \cdot 10^5$	$-4.25 \cdot 10^7$
O2	$-1.10 \cdot 10^7$	$7.43 \cdot 10^4$	$-4.25 \cdot 10^7$
O3	$6.30 \cdot 10^6$	$3.32 \cdot 10^5$	$2.05 \cdot 10^7$
O4	$-3.77 \cdot 10^6$	$-4.15 \cdot 10^5$	$6.86 \cdot 10^6$
O5	$2.27 \cdot 10^5$	$6.22 \cdot 10^4$	$-3.93 \cdot 10^6$
O6	$1.43 \cdot 10^7$	$3.26 \cdot 10^5$	$3.14 \cdot 10^7$
O7	$8.25 \cdot 10^6$	$6.59 \cdot 10^4$	$1.04 \cdot 10^7$
O8	$-2.05 \cdot 10^6$	$-3.08 \cdot 10^5$	$-2.24 \cdot 10^6$
O9	$-4.91 \cdot 10^5$	$-2.25 \cdot 10^5$	$1.89 \cdot 10^7$
O10	$-2.25 \cdot 10^5$	$-8.29 \cdot 10^4$	$3.04 \cdot 10^6$
O11	$1.64 \cdot 10^6$	$3.86 \cdot 10^4$	$1.84 \cdot 10^6$
N1	$-1.43 \cdot 10^6$	$2.69 \cdot 10^4$	$-4.64 \cdot 10^6$
N2	$-1.71 \cdot 10^6$	$9.46 \cdot 10^3$	$-6.00 \cdot 10^6$
N3	$-2.16 \cdot 10^4$	$1.78 \cdot 10^4$	$-2.27 \cdot 10^6$
N4	$-2.00 \cdot 10^5$	$-2.34 \cdot 10^5$	$9.84 \cdot 10^6$
N5	$4.22 \cdot 10^6$	$1.05 \cdot 10^5$	$3.75 \cdot 10^6$
N6	$-1.68 \cdot 10^6$	$1.21 \cdot 10^4$	$-6.91 \cdot 10^6$

TABLE SI-LXXX: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
H1	$3.87 \cdot 10^5$	$1.82 \cdot 10^4$	$-2.90 \cdot 10^5$
H2	$-1.83 \cdot 10^5$	$-2.72 \cdot 10^3$	$-3.55 \cdot 10^5$
H3	$6.36 \cdot 10^5$	$3.39 \cdot 10^4$	$-7.58 \cdot 10^5$
H4	$-3.51 \cdot 10^5$	$-1.33 \cdot 10^4$	$-1.02 \cdot 10^5$
H5	$2.19 \cdot 10^4$	$1.56 \cdot 10^3$	$-5.28 \cdot 10^4$
H6	$-2.14 \cdot 10^4$	$7.98 \cdot 10^2$	$-1.24 \cdot 10^5$
H7	$9.03 \cdot 10^4$	$3.68 \cdot 10^3$	$-1.51 \cdot 10^4$
H8	$-4.73 \cdot 10^5$	$-1.12 \cdot 10^4$	$-1.67 \cdot 10^5$
H9	$-1.87 \cdot 10^4$	$3.89 \cdot 10^2$	$-5.54 \cdot 10^4$
H10	$-4.19 \cdot 10^5$	$-1.50 \cdot 10^4$	$9.08 \cdot 10^4$
H11	$-1.12 \cdot 10^5$	$-2.96 \cdot 10^3$	$-1.72 \cdot 10^5$
H12	$-8.52 \cdot 10^5$	$-7.07 \cdot 10^4$	$2.93 \cdot 10^6$
H13	$8.20 \cdot 10^3$	$5.89 \cdot 10^3$	$-3.34 \cdot 10^5$
H14	$6.52 \cdot 10^4$	$1.12 \cdot 10^3$	$1.22 \cdot 10^5$
H15	$-1.17 \cdot 10^6$	$-6.56 \cdot 10^4$	$1.07 \cdot 10^6$
H16	$6.97 \cdot 10^3$	$1.00 \cdot 10^3$	$-3.56 \cdot 10^4$
H17	$-1.18 \cdot 10^5$	$-6.47 \cdot 10^3$	$1.86 \cdot 10^5$
H18	$-3.06 \cdot 10^5$	$-2.78 \cdot 10^4$	$1.31 \cdot 10^6$
H19	$-6.96 \cdot 10^4$	$-7.24 \cdot 10^3$	$3.64 \cdot 10^5$
H20	$-4.55 \cdot 10^4$	$-9.56 \cdot 10^3$	$6.08 \cdot 10^5$
H21	$-4.71 \cdot 10^4$	$4.12 \cdot 10^2$	$-1.35 \cdot 10^5$
H22	$-1.29 \cdot 10^6$	$-4.38 \cdot 10^4$	$-1.45 \cdot 10^5$
H23	$-3.65 \cdot 10^3$	$7.93 \cdot 10^2$	$-7.08 \cdot 10^4$
H24	$7.65 \cdot 10^3$	$9.84 \cdot 10^2$	$-5.15 \cdot 10^4$
H25	$-1.90 \cdot 10^5$	$-8.00 \cdot 10^3$	$1.26 \cdot 10^5$
H26	$-8.85 \cdot 10^4$	$-7.32 \cdot 10^2$	$-1.43 \cdot 10^5$
H27	$-1.70 \cdot 10^5$	$-4.61 \cdot 10^3$	$-8.56 \cdot 10^4$
H28	$-3.64 \cdot 10^5$	$-1.25 \cdot 10^4$	$-2.61 \cdot 10^4$

TABLE SI-LXXXI: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
C1	$2.91 \cdot 10^5$	$2.70 \cdot 10^4$	$-1.08 \cdot 10^6$
C2	$1.50 \cdot 10^5$	$9.58 \cdot 10^3$	$-2.50 \cdot 10^5$
C3	$-4.05 \cdot 10^5$	$1.63 \cdot 10^4$	$-2.42 \cdot 10^6$
C4	$-2.22 \cdot 10^5$	$3.78 \cdot 10^3$	$-9.50 \cdot 10^5$
C5	$-5.31 \cdot 10^5$	$1.61 \cdot 10^4$	$-2.17 \cdot 10^6$
C6	$-8.90 \cdot 10^4$	$-2.55 \cdot 10^4$	$1.02 \cdot 10^6$
C7	$-3.98 \cdot 10^4$	$5.01 \cdot 10^3$	$-4.93 \cdot 10^5$
C8	$1.26 \cdot 10^5$	$9.03 \cdot 10^3$	$-2.79 \cdot 10^5$
C9	$-2.93 \cdot 10^5$	$-4.37 \cdot 10^3$	$-5.69 \cdot 10^5$
C10	$-8.69 \cdot 10^5$	$-3.84 \cdot 10^4$	$7.12 \cdot 10^5$
C11	$4.99 \cdot 10^4$	$6.45 \cdot 10^3$	$-3.31 \cdot 10^5$
C12	$-4.59 \cdot 10^4$	$5.97 \cdot 10^3$	$-4.99 \cdot 10^5$
C13	$1.22 \cdot 10^6$	$6.40 \cdot 10^4$	$-1.35 \cdot 10^6$
C14	$-5.01 \cdot 10^5$	$-1.56 \cdot 10^4$	$-3.91 \cdot 10^5$
C15	$-5.86 \cdot 10^5$	$-9.26 \cdot 10^3$	$-7.09 \cdot 10^5$
C16	$1.68 \cdot 10^4$	$1.71 \cdot 10^3$	$-7.86 \cdot 10^4$
C17	$-3.40 \cdot 10^5$	$9.61 \cdot 10^3$	$-1.59 \cdot 10^6$
C18	$-1.21 \cdot 10^4$	$1.20 \cdot 10^3$	$-1.27 \cdot 10^5$
C19	$6.33 \cdot 10^4$	$3.72 \cdot 10^3$	$-7.69 \cdot 10^4$
C20	$1.73 \cdot 10^4$	$2.56 \cdot 10^3$	$-1.41 \cdot 10^5$
C21	$-2.42 \cdot 10^6$	$-9.19 \cdot 10^4$	$9.76 \cdot 10^5$
C22	$-9.69 \cdot 10^5$	$-2.29 \cdot 10^4$	$-3.83 \cdot 10^5$
C23	$-2.01 \cdot 10^4$	$9.07 \cdot 10^2$	$-8.98 \cdot 10^4$
C24	$-4.62 \cdot 10^5$	$-1.86 \cdot 10^4$	$2.48 \cdot 10^5$
C25	$-2.69 \cdot 10^5$	$-6.57 \cdot 10^3$	$-4.28 \cdot 10^5$
C26	$3.23 \cdot 10^6$	$1.14 \cdot 10^5$	$5.77 \cdot 10^3$
C27	$-8.37 \cdot 10^3$	$2.14 \cdot 10^3$	$-1.86 \cdot 10^5$
C28	$1.24 \cdot 10^6$	$3.74 \cdot 10^4$	$4.08 \cdot 10^5$
C29	$-1.91 \cdot 10^5$	$-3.64 \cdot 10^4$	$2.32 \cdot 10^6$
C30	$-1.64 \cdot 10^5$	$2.81 \cdot 10^2$	$-3.67 \cdot 10^5$
C31	$1.02 \cdot 10^5$	$1.68 \cdot 10^3$	$1.99 \cdot 10^5$
C32	$-1.28 \cdot 10^6$	$-4.78 \cdot 10^4$	$-4.66 \cdot 10^5$
C33	$5.02 \cdot 10^5$	$4.63 \cdot 10^4$	$-1.59 \cdot 10^6$
C34	$6.86 \cdot 10^3$	$1.50 \cdot 10^3$	$-6.48 \cdot 10^4$
C35	$-1.81 \cdot 10^5$	$-9.52 \cdot 10^3$	$2.56 \cdot 10^5$
C36	$-4.51 \cdot 10^5$	$-2.68 \cdot 10^4$	$8.72 \cdot 10^5$
C37	$6.21 \cdot 10^5$	$3.06 \cdot 10^4$	$-4.99 \cdot 10^5$
C38	$-1.83 \cdot 10^5$	$-1.19 \cdot 10^4$	$4.31 \cdot 10^5$
C39	$1.83 \cdot 10^4$	$-8.55 \cdot 10^3$	$7.37 \cdot 10^5$
C40	$1.44 \cdot 10^5$	$-8.54 \cdot 10^3$	$7.51 \cdot 10^5$
C41	$-4.81 \cdot 10^4$	$1.31 \cdot 10^3$	$-1.87 \cdot 10^5$
C42	$-8.29 \cdot 10^5$	$-2.43 \cdot 10^4$	$-3.23 \cdot 10^5$
C43	$-2.00 \cdot 10^3$	$1.06 \cdot 10^3$	$-8.57 \cdot 10^4$
C44	$7.37 \cdot 10^3$	$1.22 \cdot 10^3$	$-6.98 \cdot 10^4$
C45	$-2.52 \cdot 10^5$	$-1.11 \cdot 10^4$	$2.04 \cdot 10^5$
C46	$-1.59 \cdot 10^5$	$-2.42 \cdot 10^3$	$-1.92 \cdot 10^5$
C47	$-2.29 \cdot 10^5$	$-5.94 \cdot 10^3$	$-1.33 \cdot 10^5$
C48	$-4.10 \cdot 10^5$	$-1.26 \cdot 10^4$	$-1.22 \cdot 10^5$

TABLE SI-LXXXII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
O1	$1.15 \cdot 10^5$	$8.80 \cdot 10^4$	$-6.03 \cdot 10^6$
O2	$-7.16 \cdot 10^6$	$-3.22 \cdot 10^5$	$5.73 \cdot 10^6$
O3	$-5.43 \cdot 10^6$	$-1.23 \cdot 10^5$	$-3.86 \cdot 10^6$
O4	$1.49 \cdot 10^5$	$-1.10 \cdot 10^5$	$6.30 \cdot 10^6$
O5	$9.03 \cdot 10^6$	$2.39 \cdot 10^5$	$5.21 \cdot 10^6$
O6	$5.18 \cdot 10^6$	$2.69 \cdot 10^5$	$-5.54 \cdot 10^6$
N1	$-2.38 \cdot 10^6$	$-3.79 \cdot 10^4$	$-4.51 \cdot 10^6$
N2	$5.80 \cdot 10^5$	$9.23 \cdot 10^2$	$2.06 \cdot 10^6$
N3	$-4.22 \cdot 10^4$	$2.30 \cdot 10^3$	$-2.99 \cdot 10^5$
N4	$4.30 \cdot 10^4$	$3.73 \cdot 10^3$	$-1.50 \cdot 10^5$
F1	$6.57 \cdot 10^5$	$2.32 \cdot 10^4$	$-1.36 \cdot 10^4$
F2	$8.21 \cdot 10^5$	$1.98 \cdot 10^4$	$5.98 \cdot 10^5$
F3	$9.36 \cdot 10^5$	$2.53 \cdot 10^4$	$4.84 \cdot 10^5$
F4	$2.26 \cdot 10^5$	$1.19 \cdot 10^4$	$-1.82 \cdot 10^5$
F5	$-1.87 \cdot 10^4$	$-5.69 \cdot 10^3$	$2.38 \cdot 10^5$
F6	$-9.10 \cdot 10^4$	$-1.64 \cdot 10^4$	$7.40 \cdot 10^5$
F7	$5.06 \cdot 10^5$	$5.67 \cdot 10^3$	$7.54 \cdot 10^5$
F8	$9.30 \cdot 10^5$	$3.37 \cdot 10^4$	$2.76 \cdot 10^3$
F9	$3.91 \cdot 10^5$	$2.36 \cdot 10^4$	$-6.67 \cdot 10^5$

TABLE SI-LXXXIII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
H1	$-3.39 \cdot 10^4$	$-1.32 \cdot 10^4$	$1.71 \cdot 10^6$
H2	$-9.52 \cdot 10^3$	$7.81 \cdot 10^3$	$4.35 \cdot 10^6$
H3	$2.63 \cdot 10^4$	$5.10 \cdot 10^4$	$1.35 \cdot 10^7$
H4	$2.86 \cdot 10^5$	$2.99 \cdot 10^5$	$3.75 \cdot 10^7$
H5	$1.85 \cdot 10^5$	$1.81 \cdot 10^5$	$-7.74 \cdot 10^6$
H6	$1.40 \cdot 10^5$	$1.26 \cdot 10^5$	$-6.20 \cdot 10^6$
H7	$1.77 \cdot 10^5$	$1.36 \cdot 10^5$	$-1.14 \cdot 10^7$
H8	$-7.02 \cdot 10^4$	$-1.52 \cdot 10^5$	$-2.20 \cdot 10^7$
H9	$6.73 \cdot 10^5$	$7.87 \cdot 10^5$	$-5.45 \cdot 10^7$
H10	$7.28 \cdot 10^4$	$8.86 \cdot 10^4$	$-7.36 \cdot 10^6$
H11	$1.38 \cdot 10^4$	$8.92 \cdot 10^3$	$3.24 \cdot 10^6$
H12	$3.17 \cdot 10^4$	$1.15 \cdot 10^4$	$1.86 \cdot 10^7$
H13	$8.38 \cdot 10^4$	$7.02 \cdot 10^4$	$2.70 \cdot 10^7$
H14	$9.69 \cdot 10^4$	$1.02 \cdot 10^5$	$1.71 \cdot 10^7$
H15	$1.40 \cdot 10^5$	$1.76 \cdot 10^5$	$1.67 \cdot 10^7$
H16	$2.80 \cdot 10^5$	$4.96 \cdot 10^5$	$4.30 \cdot 10^7$
H17	$-5.64 \cdot 10^4$	$-7.24 \cdot 10^4$	$-1.03 \cdot 10^6$
H18	$1.56 \cdot 10^3$	$-1.73 \cdot 10^4$	$-2.62 \cdot 10^6$
H19	$1.15 \cdot 10^5$	$7.93 \cdot 10^4$	$-8.79 \cdot 10^6$
H20	$4.90 \cdot 10^5$	$4.24 \cdot 10^5$	$-3.48 \cdot 10^7$

TABLE SI-LXXXIV: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
C1	$-3.94 \cdot 10^4$	$-1.00 \cdot 10^4$	$3.48 \cdot 10^6$
C2	$-1.64 \cdot 10^4$	$9.16 \cdot 10^3$	$5.83 \cdot 10^6$
C3	$5.69 \cdot 10^3$	$4.11 \cdot 10^4$	$1.28 \cdot 10^7$
C4	$-2.22 \cdot 10^4$	$6.11 \cdot 10^4$	$2.11 \cdot 10^7$
C5	$1.07 \cdot 10^5$	$2.98 \cdot 10^5$	$7.74 \cdot 10^7$
C6	$4.60 \cdot 10^5$	$4.96 \cdot 10^5$	$7.76 \cdot 10^7$
C7	$6.54 \cdot 10^5$	$5.72 \cdot 10^5$	$1.21 \cdot 10^8$
C8	$2.43 \cdot 10^5$	$1.87 \cdot 10^5$	$3.76 \cdot 10^7$
C9	$2.55 \cdot 10^5$	$2.44 \cdot 10^5$	$-1.12 \cdot 10^7$
C10	$2.09 \cdot 10^5$	$1.89 \cdot 10^5$	$-9.56 \cdot 10^6$
C11	$2.76 \cdot 10^5$	$2.35 \cdot 10^5$	$-1.53 \cdot 10^7$
C12	$6.21 \cdot 10^5$	$5.51 \cdot 10^5$	$-3.70 \cdot 10^7$
C13	$9.62 \cdot 10^5$	$7.44 \cdot 10^5$	$-9.82 \cdot 10^7$
C14	$-1.90 \cdot 10^5$	$-3.45 \cdot 10^5$	$-4.59 \cdot 10^7$
C15	$-1.34 \cdot 10^6$	$-1.43 \cdot 10^6$	$-2.95 \cdot 10^7$
C16	$-5.29 \cdot 10^5$	$-5.37 \cdot 10^5$	$-4.47 \cdot 10^6$
C17	$3.31 \cdot 10^5$	$3.85 \cdot 10^5$	$-3.00 \cdot 10^7$
C18	$7.95 \cdot 10^4$	$9.14 \cdot 10^4$	$-6.15 \cdot 10^6$
C19	$2.36 \cdot 10^4$	$1.61 \cdot 10^4$	$5.22 \cdot 10^6$
C20	$2.94 \cdot 10^4$	$4.17 \cdot 10^3$	$2.16 \cdot 10^7$
C21	$6.02 \cdot 10^4$	$-3.22 \cdot 10^3$	$7.08 \cdot 10^7$
C22	$2.22 \cdot 10^5$	$1.88 \cdot 10^5$	$1.13 \cdot 10^8$
C23	$1.41 \cdot 10^5$	$1.32 \cdot 10^5$	$4.24 \cdot 10^7$
C24	$1.44 \cdot 10^5$	$1.54 \cdot 10^5$	$2.86 \cdot 10^7$
C25	$1.99 \cdot 10^5$	$2.42 \cdot 10^5$	$3.17 \cdot 10^7$
C26	$3.77 \cdot 10^5$	$5.28 \cdot 10^5$	$7.93 \cdot 10^7$
C27	$-6.02 \cdot 10^4$	$-8.58 \cdot 10^4$	$-2.20 \cdot 10^6$
C28	$-4.31 \cdot 10^3$	$-3.14 \cdot 10^4$	$-3.65 \cdot 10^6$
C29	$7.23 \cdot 10^4$	$2.88 \cdot 10^4$	$-8.49 \cdot 10^6$
C30	$1.78 \cdot 10^4$	$-7.46 \cdot 10^4$	$-1.58 \cdot 10^7$
C31	$4.06 \cdot 10^5$	$1.63 \cdot 10^5$	$-6.49 \cdot 10^7$
C32	$8.98 \cdot 10^5$	$7.70 \cdot 10^5$	$-7.03 \cdot 10^7$
C33	$1.60 \cdot 10^6$	$1.53 \cdot 10^6$	$-1.18 \cdot 10^8$
C34	$5.90 \cdot 10^5$	$5.94 \cdot 10^5$	$-4.12 \cdot 10^7$

TABLE SI-LXXXV: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$
O1	$-1.37 \cdot 10^6$	$-6.70 \cdot 10^5$	$1.54 \cdot 10^8$
O2	$8.03 \cdot 10^5$	$5.07 \cdot 10^5$	$3.03 \cdot 10^8$
O3	$3.94 \cdot 10^6$	$3.55 \cdot 10^6$	$-3.55 \cdot 10^8$
O4	$-4.73 \cdot 10^6$	$-4.58 \cdot 10^6$	$-5.95 \cdot 10^6$
O5	$-1.06 \cdot 10^6$	$-1.70 \cdot 10^6$	$-1.32 \cdot 10^8$
O6	$4.02 \cdot 10^6$	$4.09 \cdot 10^6$	$-3.19 \cdot 10^8$
N1	$4.84 \cdot 10^5$	$6.40 \cdot 10^5$	$2.79 \cdot 10^8$
N2	$2.34 \cdot 10^5$	$2.01 \cdot 10^5$	$3.85 \cdot 10^7$
F1	$1.78 \cdot 10^5$	$1.52 \cdot 10^5$	$2.05 \cdot 10^7$
F2	$5.25 \cdot 10^4$	$2.76 \cdot 10^4$	$2.62 \cdot 10^7$
F3	$2.04 \cdot 10^5$	$1.27 \cdot 10^5$	$1.94 \cdot 10^7$
F4	$-3.23 \cdot 10^5$	$-3.32 \cdot 10^5$	$-4.88 \cdot 10^6$
F5	$-2.45 \cdot 10^5$	$-2.63 \cdot 10^5$	$-1.41 \cdot 10^6$
F6	$-4.80 \cdot 10^5$	$-4.45 \cdot 10^5$	$2.17 \cdot 10^6$
F7	$4.81 \cdot 10^5$	$5.11 \cdot 10^5$	$-2.44 \cdot 10^7$
F8	$3.02 \cdot 10^5$	$3.09 \cdot 10^5$	$-3.03 \cdot 10^7$
F9	$3.37 \cdot 10^5$	$3.29 \cdot 10^5$	$-2.24 \cdot 10^7$
S1	$-1.04 \cdot 10^5$	$-4.07 \cdot 10^4$	$4.52 \cdot 10^6$
S2	$5.73 \cdot 10^5$	$5.61 \cdot 10^5$	$-2.78 \cdot 10^7$
S3	$-1.84 \cdot 10^5$	$-2.33 \cdot 10^5$	$-3.66 \cdot 10^6$

TABLE SI-LXXXVI: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
H1	$-2.30 \cdot 10^5$	$-1.63 \cdot 10^4$	$-5.27 \cdot 10^5$
H2	$-9.35 \cdot 10^4$	$-1.20 \cdot 10^4$	$2.34 \cdot 10^5$
H3	$8.77 \cdot 10^4$	$-1.48 \cdot 10^4$	$1.83 \cdot 10^6$
H4	$8.67 \cdot 10^5$	$-9.69 \cdot 10^3$	$7.35 \cdot 10^6$
H5	$-2.44 \cdot 10^5$	$-2.11 \cdot 10^3$	$-1.94 \cdot 10^6$
H6	$-9.42 \cdot 10^4$	$3.29 \cdot 10^3$	$-1.26 \cdot 10^6$
H7	$3.21 \cdot 10^4$	$1.22 \cdot 10^4$	$-1.36 \cdot 10^6$
H8	$5.92 \cdot 10^5$	$3.00 \cdot 10^4$	$6.08 \cdot 10^5$
H9	$5.05 \cdot 10^5$	$5.76 \cdot 10^3$	$2.82 \cdot 10^6$
H10	$3.11 \cdot 10^5$	$2.83 \cdot 10^2$	$2.12 \cdot 10^6$
H11	$1.78 \cdot 10^5$	$-9.31 \cdot 10^3$	$2.21 \cdot 10^6$
H12	$-7.29 \cdot 10^5$	$-4.26 \cdot 10^4$	$-7.42 \cdot 10^5$
H13	$1.39 \cdot 10^6$	$3.26 \cdot 10^4$	$4.02 \cdot 10^6$
H14	$2.51 \cdot 10^5$	$8.42 \cdot 10^3$	$9.82 \cdot 10^5$
H15	$4.34 \cdot 10^4$	$7.78 \cdot 10^3$	$2.10 \cdot 10^5$
H16	$-6.08 \cdot 10^4$	$8.99 \cdot 10^3$	$-4.85 \cdot 10^5$
H17	$-8.58 \cdot 10^4$	$1.06 \cdot 10^4$	$-9.52 \cdot 10^5$
H18	$-1.53 \cdot 10^4$	$1.35 \cdot 10^4$	$-1.20 \cdot 10^6$
H19	$2.12 \cdot 10^5$	$1.83 \cdot 10^4$	$-9.57 \cdot 10^5$
H20	$1.68 \cdot 10^6$	$6.84 \cdot 10^4$	$4.84 \cdot 10^5$

TABLE SI-LXXXVII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
C1	$-2.82 \cdot 10^5$	$-2.23 \cdot 10^4$	$-4.42 \cdot 10^5$
C2	$-1.49 \cdot 10^5$	$-1.78 \cdot 10^4$	$2.66 \cdot 10^5$
C3	$-4.83 \cdot 10^4$	$-2.23 \cdot 10^4$	$1.41 \cdot 10^6$
C4	$-3.81 \cdot 10^5$	$-5.68 \cdot 10^4$	$1.64 \cdot 10^6$
C5	$1.07 \cdot 10^5$	$-1.18 \cdot 10^5$	$1.04 \cdot 10^7$
C6	$1.74 \cdot 10^6$	$-1.96 \cdot 10^4$	$1.46 \cdot 10^7$
C7	$4.16 \cdot 10^6$	$5.04 \cdot 10^4$	$2.58 \cdot 10^7$
C8	$1.58 \cdot 10^6$	$2.81 \cdot 10^4$	$8.77 \cdot 10^6$
C9	$-2.99 \cdot 10^5$	$-6.69 \cdot 10^2$	$-2.60 \cdot 10^6$
C10	$-1.60 \cdot 10^5$	$4.01 \cdot 10^3$	$-1.93 \cdot 10^6$
C11	$-1.12 \cdot 10^5$	$1.10 \cdot 10^4$	$-2.42 \cdot 10^6$
C12	$-4.49 \cdot 10^5$	$1.68 \cdot 10^4$	$-6.08 \cdot 10^6$
C13	$-3.51 \cdot 10^5$	$7.03 \cdot 10^4$	$-1.18 \cdot 10^7$
C14	$8.69 \cdot 10^5$	$6.00 \cdot 10^4$	$-5.13 \cdot 10^5$
C15	$1.24 \cdot 10^6$	$5.74 \cdot 10^4$	$3.54 \cdot 10^6$
C16	$3.90 \cdot 10^5$	$9.89 \cdot 10^3$	$1.87 \cdot 10^6$
C17	$6.65 \cdot 10^5$	$6.12 \cdot 10^3$	$3.92 \cdot 10^6$
C18	$4.65 \cdot 10^5$	$9.18 \cdot 10^2$	$3.14 \cdot 10^6$
C19	$4.25 \cdot 10^5$	$-6.04 \cdot 10^3$	$3.62 \cdot 10^6$
C20	$1.27 \cdot 10^6$	$-3.05 \cdot 10^3$	$9.35 \cdot 10^6$
C21	$1.73 \cdot 10^6$	$-4.91 \cdot 10^4$	$1.78 \cdot 10^7$
C22	$-1.39 \cdot 10^6$	$-8.37 \cdot 10^4$	$-1.19 \cdot 10^6$
C23	$-4.62 \cdot 10^6$	$-1.50 \cdot 10^5$	$-1.93 \cdot 10^7$
C24	$-1.88 \cdot 10^6$	$-4.99 \cdot 10^4$	$-9.33 \cdot 10^6$
C25	$9.10 \cdot 10^5$	$3.28 \cdot 10^4$	$3.61 \cdot 10^6$
C26	$2.82 \cdot 10^5$	$1.37 \cdot 10^4$	$1.23 \cdot 10^6$
C27	$6.92 \cdot 10^4$	$1.26 \cdot 10^4$	$3.35 \cdot 10^5$
C28	$-8.85 \cdot 10^4$	$2.19 \cdot 10^4$	$-6.72 \cdot 10^5$
C29	$-3.33 \cdot 10^5$	$6.07 \cdot 10^4$	$-2.63 \cdot 10^6$
C30	$-1.04 \cdot 10^5$	$1.41 \cdot 10^4$	$-8.63 \cdot 10^5$
C31	$-1.26 \cdot 10^5$	$1.58 \cdot 10^4$	$-1.33 \cdot 10^6$
C32	$-1.59 \cdot 10^5$	$2.97 \cdot 10^4$	$-2.60 \cdot 10^6$
C33	$-4.03 \cdot 10^5$	$7.68 \cdot 10^4$	$-6.01 \cdot 10^6$
C34	$-1.29 \cdot 10^4$	$2.21 \cdot 10^4$	$-1.90 \cdot 10^6$
C35	$2.13 \cdot 10^5$	$2.88 \cdot 10^4$	$-1.85 \cdot 10^6$
C36	$9.47 \cdot 10^5$	$7.49 \cdot 10^4$	$-3.12 \cdot 10^6$

TABLE SI-LXXXVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(1)}_{01}$	$\bar{\Phi}^{p(1)}_{02}$	$\bar{\Phi}^{p(1)}_{12}$
O1	$-3.86 \cdot 10^6$	$-4.73 \cdot 10^5$	$7.83 \cdot 10^6$
O2	$1.23 \cdot 10^7$	$2.39 \cdot 10^5$	$6.58 \cdot 10^7$
O3	$-5.59 \cdot 10^6$	$8.14 \cdot 10^4$	$-5.74 \cdot 10^7$
O4	$1.48 \cdot 10^6$	$8.74 \cdot 10^4$	$6.58 \cdot 10^6$
O5	$1.17 \cdot 10^7$	$1.20 \cdot 10^4$	$8.09 \cdot 10^7$
O6	$-1.44 \cdot 10^7$	$-3.86 \cdot 10^5$	$-7.39 \cdot 10^7$
N1	$7.30 \cdot 10^5$	$1.95 \cdot 10^5$	$-1.20 \cdot 10^7$
N2	$5.11 \cdot 10^5$	$9.87 \cdot 10^4$	$2.60 \cdot 10^6$
F1	$8.67 \cdot 10^5$	$2.57 \cdot 10^4$	$4.69 \cdot 10^6$
F2	$8.38 \cdot 10^5$	$1.17 \cdot 10^4$	$5.04 \cdot 10^6$
F3	$1.39 \cdot 10^6$	$2.42 \cdot 10^4$	$6.59 \cdot 10^6$
F4	$3.30 \cdot 10^5$	$7.93 \cdot 10^3$	$1.40 \cdot 10^6$
F5	$-1.29 \cdot 10^4$	$1.51 \cdot 10^4$	$-4.42 \cdot 10^5$
F6	$3.07 \cdot 10^5$	$-1.37 \cdot 10^4$	$2.67 \cdot 10^6$
F7	$-9.87 \cdot 10^5$	$-2.75 \cdot 10^4$	$-4.48 \cdot 10^6$
F8	$-1.15 \cdot 10^6$	$-4.09 \cdot 10^4$	$-5.53 \cdot 10^6$
F9	$-1.60 \cdot 10^6$	$-2.28 \cdot 10^4$	$-9.67 \cdot 10^6$
S1	$-7.13 \cdot 10^5$	$-5.08 \cdot 10^4$	$-1.59 \cdot 10^6$
S2	$-8.01 \cdot 10^5$	$-7.77 \cdot 10^3$	$-6.24 \cdot 10^6$
S3	$1.57 \cdot 10^6$	$1.81 \cdot 10^4$	$8.84 \cdot 10^6$

TABLE SI-LXXXIX: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{03}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$	$\bar{\Phi}_{13}^{p(1)}$	$\bar{\Phi}_{23}^{p(1)}$
H1	$-4.25 \cdot 10^4$	$-5.06 \cdot 10^4$	$-2.08 \cdot 10^4$	$-1.74 \cdot 10^6$	$-5.44 \cdot 10^5$	$-1.46 \cdot 10^6$
H2	$-9.32 \cdot 10^3$	$-5.80 \cdot 10^3$	$-8.57 \cdot 10^3$	$-9.01 \cdot 10^5$	$-3.72 \cdot 10^5$	$9.61 \cdot 10^4$
H3	$6.05 \cdot 10^3$	$4.20 \cdot 10^4$	$-6.95 \cdot 10^2$	$-9.18 \cdot 10^5$	$-4.80 \cdot 10^5$	$1.05 \cdot 10^6$
H4	$-1.63 \cdot 10^5$	$-5.18 \cdot 10^5$	$-1.15 \cdot 10^5$	$-2.68 \cdot 10^6$	$-2.64 \cdot 10^5$	$-6.50 \cdot 10^6$
H5	$-2.22 \cdot 10^4$	$-1.91 \cdot 10^5$	$-2.68 \cdot 10^4$	$1.26 \cdot 10^6$	$7.21 \cdot 10^5$	$-8.70 \cdot 10^5$
H6	$-1.12 \cdot 10^4$	$-2.13 \cdot 10^4$	$4.41 \cdot 10^3$	$6.88 \cdot 10^5$	$4.23 \cdot 10^5$	$-6.99 \cdot 10^5$
H7	$-4.04 \cdot 10^2$	$8.93 \cdot 10^4$	$2.69 \cdot 10^4$	$5.91 \cdot 10^5$	$3.39 \cdot 10^5$	$-3.28 \cdot 10^5$
H8	$-2.57 \cdot 10^4$	$-8.57 \cdot 10^5$	$-1.60 \cdot 10^5$	$3.27 \cdot 10^6$	$1.46 \cdot 10^6$	$9.45 \cdot 10^5$
H9	$3.71 \cdot 10^4$	$-6.42 \cdot 10^4$	$-5.65 \cdot 10^3$	$1.66 \cdot 10^6$	$4.92 \cdot 10^5$	$1.26 \cdot 10^6$
H10	$1.20 \cdot 10^4$	$-1.44 \cdot 10^5$	$-2.91 \cdot 10^4$	$6.66 \cdot 10^5$	$1.71 \cdot 10^5$	$9.18 \cdot 10^5$
H11	$4.58 \cdot 10^3$	$-2.59 \cdot 10^5$	$-5.76 \cdot 10^4$	$3.32 \cdot 10^5$	$1.59 \cdot 10^4$	$1.31 \cdot 10^6$
H12	$9.01 \cdot 10^4$	$4.73 \cdot 10^5$	$1.29 \cdot 10^5$	$3.71 \cdot 10^6$	$1.32 \cdot 10^6$	$1.02 \cdot 10^6$
H13	$1.81 \cdot 10^5$	$-1.05 \cdot 10^6$	$-3.10 \cdot 10^5$	$-3.01 \cdot 10^6$	$-3.36 \cdot 10^6$	$1.94 \cdot 10^7$
H14	$3.64 \cdot 10^4$	$-9.22 \cdot 10^4$	$-3.25 \cdot 10^4$	$-3.83 \cdot 10^5$	$-5.15 \cdot 10^5$	$3.15 \cdot 10^6$
H15	$-5.21 \cdot 10^2$	$-1.38 \cdot 10^4$	$-3.48 \cdot 10^3$	$-3.23 \cdot 10^4$	$-1.95 \cdot 10^4$	$-1.05 \cdot 10^5$
H16	$-5.20 \cdot 10^4$	$-3.64 \cdot 10^4$	$-1.42 \cdot 10^3$	$-3.16 \cdot 10^5$	$2.33 \cdot 10^5$	$-3.53 \cdot 10^6$
H17	$-9.05 \cdot 10^4$	$-1.08 \cdot 10^5$	$-1.90 \cdot 10^4$	$-1.18 \cdot 10^6$	$8.06 \cdot 10^4$	$-5.16 \cdot 10^6$
H18	$-1.07 \cdot 10^5$	$-6.54 \cdot 10^5$	$-2.47 \cdot 10^5$	$-1.16 \cdot 10^7$	$-5.15 \cdot 10^6$	$5.51 \cdot 10^6$
H19	$-3.42 \cdot 10^4$	$-1.24 \cdot 10^4$	$-5.17 \cdot 10^3$	$-8.93 \cdot 10^5$	$-1.79 \cdot 10^5$	$-1.81 \cdot 10^6$
H20	$-4.40 \cdot 10^4$	$-1.21 \cdot 10^5$	$-2.66 \cdot 10^4$	$-7.24 \cdot 10^5$	$-6.32 \cdot 10^4$	$-1.89 \cdot 10^6$
H21	$-2.13 \cdot 10^4$	$-5.74 \cdot 10^4$	$-1.55 \cdot 10^4$	$-6.39 \cdot 10^5$	$-1.72 \cdot 10^5$	$-7.13 \cdot 10^5$
H22	$-2.13 \cdot 10^4$	$-1.47 \cdot 10^5$	$-5.01 \cdot 10^4$	$-2.03 \cdot 10^6$	$-8.94 \cdot 10^5$	$9.44 \cdot 10^5$
H23	$-1.25 \cdot 10^4$	$7.47 \cdot 10^3$	$-5.09 \cdot 10^3$	$-9.22 \cdot 10^5$	$-3.53 \cdot 10^5$	$-2.15 \cdot 10^5$
H24	$-1.92 \cdot 10^4$	$8.96 \cdot 10^4$	$1.14 \cdot 10^4$	$-1.30 \cdot 10^6$	$-4.50 \cdot 10^5$	$-9.40 \cdot 10^5$
H25	$-3.33 \cdot 10^4$	$-3.68 \cdot 10^5$	$-8.22 \cdot 10^4$	$-3.63 \cdot 10^5$	$-7.23 \cdot 10^4$	$3.69 \cdot 10^4$
H26	$-6.53 \cdot 10^4$	$-4.26 \cdot 10^5$	$-9.19 \cdot 10^4$	$-6.34 \cdot 10^5$	$2.13 \cdot 10^4$	$-1.56 \cdot 10^6$
H27	$-3.12 \cdot 10^4$	$-2.24 \cdot 10^5$	$-4.87 \cdot 10^4$	$-3.14 \cdot 10^5$	$-3.86 \cdot 10^3$	$-6.28 \cdot 10^5$
H28	$-1.37 \cdot 10^4$	$-1.06 \cdot 10^5$	$-2.63 \cdot 10^4$	$-4.38 \cdot 10^5$	$-1.53 \cdot 10^5$	$-2.69 \cdot 10^4$
H29	$-1.11 \cdot 10^4$	$-8.82 \cdot 10^4$	$-2.49 \cdot 10^4$	$-6.62 \cdot 10^5$	$-2.76 \cdot 10^5$	$2.26 \cdot 10^5$
H30	$-1.30 \cdot 10^4$	$-1.70 \cdot 10^5$	$-4.20 \cdot 10^4$	$-5.23 \cdot 10^5$	$-2.28 \cdot 10^5$	$4.28 \cdot 10^5$

TABLE SI-XC: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for hydrogen atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{03}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$	$\bar{\Phi}_{13}^{p(1)}$	$\bar{\Phi}_{23}^{p(1)}$
C1	$-2.26 \cdot 10^5$	$-2.52 \cdot 10^5$	$-1.29 \cdot 10^5$	$-1.15 \cdot 10^7$	$-3.98 \cdot 10^6$	$-5.94 \cdot 10^6$
C2	$-4.59 \cdot 10^4$	$-8.82 \cdot 10^3$	$-3.61 \cdot 10^4$	$-4.29 \cdot 10^6$	$-1.75 \cdot 10^6$	$2.27 \cdot 10^5$
C3	$-3.45 \cdot 10^4$	$-2.97 \cdot 10^4$	$-2.11 \cdot 10^4$	$-2.09 \cdot 10^6$	$-7.71 \cdot 10^5$	$-6.74 \cdot 10^5$
C4	$-1.10 \cdot 10^4$	$1.66 \cdot 10^3$	$-1.05 \cdot 10^4$	$-1.29 \cdot 10^6$	$-5.50 \cdot 10^5$	$2.66 \cdot 10^5$
C5	$3.01 \cdot 10^3$	$4.33 \cdot 10^4$	$-4.07 \cdot 10^3$	$-1.34 \cdot 10^6$	$-6.65 \cdot 10^5$	$1.17 \cdot 10^6$
C6	$-3.03 \cdot 10^5$	$-7.87 \cdot 10^5$	$-1.79 \cdot 10^5$	$-5.64 \cdot 10^6$	$-7.32 \cdot 10^5$	$-1.29 \cdot 10^7$
C7	$-4.50 \cdot 10^5$	$-8.72 \cdot 10^5$	$-1.54 \cdot 10^5$	$-4.12 \cdot 10^6$	$1.13 \cdot 10^6$	$-2.39 \cdot 10^7$
C8	$-1.43 \cdot 10^5$	$-2.80 \cdot 10^5$	$-3.95 \cdot 10^4$	$-3.10 \cdot 10^5$	$8.50 \cdot 10^5$	$-7.83 \cdot 10^6$
C9	$-3.37 \cdot 10^4$	$-5.65 \cdot 10^5$	$-1.02 \cdot 10^4$	$1.11 \cdot 10^7$	$5.54 \cdot 10^6$	$-3.16 \cdot 10^6$
C10	$-2.81 \cdot 10^4$	$-6.77 \cdot 10^4$	$2.68 \cdot 10^4$	$3.58 \cdot 10^6$	$1.98 \cdot 10^6$	$-2.21 \cdot 10^6$
C11	$-2.34 \cdot 10^4$	$-1.36 \cdot 10^5$	$-1.07 \cdot 10^4$	$1.58 \cdot 10^6$	$9.12 \cdot 10^5$	$-1.22 \cdot 10^6$
C12	$-1.36 \cdot 10^4$	$-1.33 \cdot 10^4$	$1.02 \cdot 10^4$	$1.02 \cdot 10^6$	$6.13 \cdot 10^5$	$-9.31 \cdot 10^5$
C13	$-4.28 \cdot 10^3$	$9.51 \cdot 10^4$	$3.29 \cdot 10^4$	$9.59 \cdot 10^5$	$5.56 \cdot 10^5$	$-6.59 \cdot 10^5$
C14	$-2.30 \cdot 10^4$	$-1.51 \cdot 10^6$	$-2.76 \cdot 10^5$	$6.78 \cdot 10^6$	$2.89 \cdot 10^6$	$2.41 \cdot 10^6$
C15	$7.63 \cdot 10^4$	$-2.56 \cdot 10^6$	$-5.47 \cdot 10^5$	$6.02 \cdot 10^6$	$1.26 \cdot 10^6$	$1.28 \cdot 10^7$
C16	$4.00 \cdot 10^4$	$-9.62 \cdot 10^5$	$-2.19 \cdot 10^5$	$1.13 \cdot 10^6$	$-1.73 \cdot 10^5$	$6.16 \cdot 10^6$
C17	$1.44 \cdot 10^5$	$-9.89 \cdot 10^5$	$-1.54 \cdot 10^5$	$1.03 \cdot 10^7$	$3.50 \cdot 10^6$	$6.84 \cdot 10^6$
C18	$4.83 \cdot 10^4$	$-7.21 \cdot 10^5$	$-1.43 \cdot 10^5$	$3.36 \cdot 10^6$	$9.61 \cdot 10^5$	$4.03 \cdot 10^6$
C19	$3.39 \cdot 10^4$	$-2.35 \cdot 10^5$	$-4.31 \cdot 10^4$	$1.79 \cdot 10^6$	$5.11 \cdot 10^5$	$1.83 \cdot 10^6$
C20	$1.56 \cdot 10^4$	$-2.27 \cdot 10^5$	$-4.65 \cdot 10^4$	$9.14 \cdot 10^5$	$2.29 \cdot 10^5$	$1.36 \cdot 10^6$
C21	$8.75 \cdot 10^3$	$-3.38 \cdot 10^5$	$-7.34 \cdot 10^4$	$6.50 \cdot 10^5$	$1.06 \cdot 10^5$	$1.71 \cdot 10^6$
C22	$1.64 \cdot 10^5$	$8.22 \cdot 10^5$	$2.32 \cdot 10^5$	$7.40 \cdot 10^6$	$2.71 \cdot 10^6$	$1.93 \cdot 10^6$
C23	$2.48 \cdot 10^5$	$2.61 \cdot 10^6$	$6.17 \cdot 10^5$	$6.12 \cdot 10^6$	$2.21 \cdot 10^6$	$1.72 \cdot 10^6$
C24	$9.17 \cdot 10^4$	$1.11 \cdot 10^6$	$2.48 \cdot 10^5$	$8.48 \cdot 10^5$	$1.87 \cdot 10^5$	$1.17 \cdot 10^6$
C25	$1.48 \cdot 10^5$	$-5.20 \cdot 10^5$	$-1.63 \cdot 10^5$	$-1.22 \cdot 10^6$	$-2.00 \cdot 10^6$	$1.25 \cdot 10^7$
C26	$4.04 \cdot 10^4$	$-1.01 \cdot 10^5$	$-3.47 \cdot 10^4$	$-3.10 \cdot 10^5$	$-5.17 \cdot 10^5$	$3.21 \cdot 10^6$
C27	$-8.68 \cdot 10^2$	$-2.53 \cdot 10^4$	$-6.41 \cdot 10^3$	$-5.99 \cdot 10^4$	$-3.70 \cdot 10^4$	$-1.97 \cdot 10^5$
C28	$-5.27 \cdot 10^4$	$-3.26 \cdot 10^4$	-4.88	$-2.68 \cdot 10^5$	$2.61 \cdot 10^5$	$-3.84 \cdot 10^6$
C29	$-1.84 \cdot 10^5$	$-8.34 \cdot 10^4$	$2.81 \cdot 10^3$	$-1.36 \cdot 10^6$	$7.18 \cdot 10^5$	$-1.33 \cdot 10^7$
C30	$-3.34 \cdot 10^5$	$-2.65 \cdot 10^5$	$-4.58 \cdot 10^4$	$-4.96 \cdot 10^6$	$4.56 \cdot 10^4$	$-1.98 \cdot 10^7$
C31	$-1.39 \cdot 10^5$	$-1.66 \cdot 10^5$	$-3.39 \cdot 10^4$	$-2.28 \cdot 10^6$	$-1.07 \cdot 10^5$	$-7.59 \cdot 10^6$
C32	$-9.44 \cdot 10^4$	$-1.44 \cdot 10^5$	$-3.76 \cdot 10^4$	$-2.27 \cdot 10^6$	$-4.42 \cdot 10^5$	$-4.34 \cdot 10^6$
C33	$-1.05 \cdot 10^5$	$-2.57 \cdot 10^5$	$-7.63 \cdot 10^4$	$-3.72 \cdot 10^6$	$-1.12 \cdot 10^6$	$-3.20 \cdot 10^6$
C34	$-2.51 \cdot 10^5$	$-6.31 \cdot 10^5$	$-2.05 \cdot 10^5$	$-1.07 \cdot 10^7$	$-3.59 \cdot 10^6$	$-6.10 \cdot 10^6$
C35	$-4.56 \cdot 10^4$	$-8.34 \cdot 10^4$	$-2.10 \cdot 10^4$	$-1.06 \cdot 10^6$	$-2.00 \cdot 10^5$	$-2.03 \cdot 10^6$
C36	$-3.04 \cdot 10^4$	$-8.07 \cdot 10^4$	$-2.21 \cdot 10^4$	$-9.38 \cdot 10^5$	$-2.58 \cdot 10^5$	$-1.00 \cdot 10^6$
C37	$-3.90 \cdot 10^4$	$-1.52 \cdot 10^5$	$-4.77 \cdot 10^4$	$-2.02 \cdot 10^6$	$-7.51 \cdot 10^5$	$-3.45 \cdot 10^5$
C38	$-3.28 \cdot 10^4$	$-1.95 \cdot 10^5$	$-4.84 \cdot 10^4$	$-9.79 \cdot 10^5$	$-3.07 \cdot 10^5$	$-4.61 \cdot 10^5$
C39	$-2.18 \cdot 10^4$	$3.85 \cdot 10^3$	$-7.27 \cdot 10^3$	$-1.24 \cdot 10^6$	$-4.36 \cdot 10^5$	$-6.41 \cdot 10^5$
C40	$-4.15 \cdot 10^4$	$-3.18 \cdot 10^5$	$-7.08 \cdot 10^4$	$-5.53 \cdot 10^5$	$-8.00 \cdot 10^4$	$-6.48 \cdot 10^5$
C41	$-1.55 \cdot 10^4$	$-1.34 \cdot 10^5$	$-3.40 \cdot 10^4$	$-6.12 \cdot 10^5$	$-2.36 \cdot 10^5$	$1.26 \cdot 10^5$

TABLE SI-XCI: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for carbon atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(1)}$	$\bar{\Phi}_{02}^{p(1)}$	$\bar{\Phi}_{03}^{p(1)}$	$\bar{\Phi}_{12}^{p(1)}$	$\bar{\Phi}_{13}^{p(1)}$	$\bar{\Phi}_{23}^{p(1)}$
O1	$-1.08 \cdot 10^5$	$2.52 \cdot 10^6$	$2.71 \cdot 10^5$	$-3.31 \cdot 10^7$	$-1.43 \cdot 10^7$	$6.02 \cdot 10^6$
O2	$-8.34 \cdot 10^5$	$-8.95 \cdot 10^5$	$-8.81 \cdot 10^4$	$-4.55 \cdot 10^6$	$3.90 \cdot 10^6$	$-5.23 \cdot 10^7$
O3	$2.11 \cdot 10^5$	$2.74 \cdot 10^6$	$8.87 \cdot 10^5$	$2.87 \cdot 10^7$	$1.38 \cdot 10^7$	$-5.33 \cdot 10^6$
O4	$4.42 \cdot 10^5$	$-6.39 \cdot 10^6$	$-1.49 \cdot 10^6$	$7.82 \cdot 10^6$	$-2.43 \cdot 10^6$	$4.98 \cdot 10^7$
O5	$1.71 \cdot 10^5$	$-6.67 \cdot 10^6$	$-1.36 \cdot 10^6$	$2.17 \cdot 10^7$	$6.46 \cdot 10^6$	$2.85 \cdot 10^7$
O6	$6.64 \cdot 10^5$	$8.05 \cdot 10^6$	$1.78 \cdot 10^6$	$4.83 \cdot 10^6$	$7.27 \cdot 10^5$	$1.20 \cdot 10^7$
N1	$1.75 \cdot 10^4$	$-3.56 \cdot 10^5$	$-9.65 \cdot 10^4$	$-8.33 \cdot 10^5$	$-7.65 \cdot 10^5$	$-2.10 \cdot 10^6$
N2	$-8.27 \cdot 10^5$	$-9.40 \cdot 10^5$	$-2.58 \cdot 10^5$	$-2.02 \cdot 10^7$	$-3.88 \cdot 10^6$	$-4.01 \cdot 10^7$
F1	$-9.21 \cdot 10^4$	$-2.49 \cdot 10^5$	$-4.22 \cdot 10^4$	$-2.90 \cdot 10^5$	$4.77 \cdot 10^5$	$-4.57 \cdot 10^6$
F2	$-7.38 \cdot 10^4$	$-5.95 \cdot 10^4$	$-4.30 \cdot 10^3$	$-4.99 \cdot 10^5$	$3.03 \cdot 10^5$	$-4.83 \cdot 10^6$
F3	$-9.20 \cdot 10^4$	$-1.52 \cdot 10^5$	$-5.47 \cdot 10^3$	$1.08 \cdot 10^6$	$1.21 \cdot 10^6$	$-5.12 \cdot 10^6$
F4	$5.76 \cdot 10^4$	$6.87 \cdot 10^5$	$1.56 \cdot 10^5$	$8.27 \cdot 10^5$	$2.64 \cdot 10^5$	$1.27 \cdot 10^6$
F5	$5.20 \cdot 10^4$	$5.92 \cdot 10^5$	$1.35 \cdot 10^5$	$8.49 \cdot 10^5$	$2.67 \cdot 10^5$	$3.49 \cdot 10^5$
F6	$6.52 \cdot 10^4$	$9.44 \cdot 10^5$	$1.93 \cdot 10^5$	$-1.25 \cdot 10^6$	$-7.16 \cdot 10^5$	$1.30 \cdot 10^6$
F7	$5.79 \cdot 10^4$	$-5.80 \cdot 10^5$	$-1.37 \cdot 10^5$	$8.63 \cdot 10^5$	$-2.89 \cdot 10^5$	$5.26 \cdot 10^6$
F8	$1.36 \cdot 10^4$	$-5.37 \cdot 10^5$	$-1.17 \cdot 10^5$	$9.81 \cdot 10^5$	$1.45 \cdot 10^5$	$2.73 \cdot 10^6$
F9	$1.77 \cdot 10^4$	$-7.79 \cdot 10^5$	$-1.90 \cdot 10^5$	$-6.31 \cdot 10^5$	$-7.84 \cdot 10^5$	$5.46 \cdot 10^6$
S1	$2.05 \cdot 10^4$	$1.34 \cdot 10^5$	$-8.01 \cdot 10^2$	$-2.75 \cdot 10^6$	$-1.46 \cdot 10^6$	$3.29 \cdot 10^6$
S2	$7.04 \cdot 10^3$	$3.29 \cdot 10^5$	$9.55 \cdot 10^4$	$1.99 \cdot 10^6$	$1.09 \cdot 10^6$	$-7.76 \cdot 10^5$
S3	$1.60 \cdot 10^3$	$-8.24 \cdot 10^5$	$-1.82 \cdot 10^5$	$8.99 \cdot 10^5$	$7.78 \cdot 10^4$	$3.54 \cdot 10^6$

TABLE SI-XCII: Values of the KD–dependent components of $\bar{\Phi}^{p(1)}$ (expressed in ppm au) for the other atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

$\bar{\Phi}^{p(0)}$

Atom	$\bar{\Phi}^{p(0)}_{01}$
H1	$4.37 \cdot 10^1$
H2	-4.66
H3	$1.22 \cdot 10^2$
H4	$-1.58 \cdot 10^2$
H5	$-1.15 \cdot 10^2$
H6	$-1.47 \cdot 10^2$
H7	$-1.78 \cdot 10^2$
H8	-3.26
H9	$-9.76 \cdot 10^1$
H10	$-1.38 \cdot 10^2$
H11	$-1.53 \cdot 10^2$
H12	$-5.75 \cdot 10^1$
H13	$-7.10 \cdot 10^1$
H14	-2.37
H15	$-2.52 \cdot 10^2$
H16	$-1.24 \cdot 10^2$
H17	$-1.13 \cdot 10^2$
H18	$-3.06 \cdot 10^1$
H19	$1.43 \cdot 10^2$
H20	$5.99 \cdot 10^1$
H21	$9.11 \cdot 10^1$
H22	3.17
H23	$-1.28 \cdot 10^2$
H24	$-6.04 \cdot 10^1$
H25	$1.39 \cdot 10^2$

TABLE SI-XCIII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$
C1	$5.21 \cdot 10^1$
C2	$-5.82 \cdot 10^1$
C3	$-2.89 \cdot 10^2$
C4	$-5.40 \cdot 10^2$
C5	$-1.96 \cdot 10^2$
C6	$-1.01 \cdot 10^2$
C7	$-2.46 \cdot 10^2$
C8	$-2.46 \cdot 10^2$
C9	$-2.05 \cdot 10^2$
C10	$-6.18 \cdot 10^1$
C11	$-1.98 \cdot 10^2$
C12	$-3.55 \cdot 10^2$
C13	$-2.39 \cdot 10^1$
C14	$3.01 \cdot 10^2$
C15	$1.26 \cdot 10^2$

TABLE SI-XCIV: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$
O1	$6.07 \cdot 10^2$
O2	$-1.36 \cdot 10^3$
O3	$1.07 \cdot 10^2$
O4	$-9.57 \cdot 10^1$
O5	$-1.17 \cdot 10^3$
O6	$1.30 \cdot 10^3$
O7	$6.83 \cdot 10^1$
O8	4.24

TABLE SI-XCV: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **1**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$
H1	-5.42
H2	-4.01
H3	$-2.49 \cdot 10^2$
H4	$-1.43 \cdot 10^2$
H5	$-1.25 \cdot 10^2$
H6	-7.51
H7	$-3.63 \cdot 10^1$
H8	-2.01
H9	$-5.39 \cdot 10^1$
H10	$-7.31 \cdot 10^1$
H11	$-3.43 \cdot 10^2$
H12	-3.60
H13	$1.60 \cdot 10^1$
H14	-2.74
H15	$-3.39 \cdot 10^1$
H16	$-6.20 \cdot 10^1$
H17	$5.33 \cdot 10^1$
H18	$-3.21 \cdot 10^1$
H19	$-3.91 \cdot 10^1$
H20	$9.28 \cdot 10^1$
H21	$-7.93 \cdot 10^1$
H22	$-6.95 \cdot 10^1$
H23	$-1.43 \cdot 10^2$
H24	$-2.81 \cdot 10^1$
H25	$1.14 \cdot 10^2$
H26	$1.01 \cdot 10^2$
H27	4.40
H28	$-6.44 \cdot 10^1$
H29	$9.52 \cdot 10^1$
H30	$4.82 \cdot 10^1$
H31	$-4.84 \cdot 10^1$

TABLE SI-XCVI: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$
C1	-7.43
C2	-5.82
C3	-8.68
C4	$-1.09 \cdot 10^{1}$
C5	-4.94
C6	$-2.11 \cdot 10^{2}$
C7	$-8.33 \cdot 10^{1}$
C8	$-3.49 \cdot 10^{2}$
C9	$2.28 \cdot 10^{2}$
C10	-7.24
C11	$-2.57 \cdot 10^{1}$
C12	$-5.72 \cdot 10^{1}$
C13	$-5.84 \cdot 10^{1}$
C14	$-8.81 \cdot 10^{-1}$
C15	$2.39 \cdot 10^{2}$
C16	$-1.65 \cdot 10^{1}$
C17	$-1.10 \cdot 10^{2}$
C18	$-1.26 \cdot 10^{2}$
C19	$-1.06 \cdot 10^{1}$
C20	$-1.00 \cdot 10^{2}$
C21	$-4.01 \cdot 10^{2}$
C22	$4.49 \cdot 10^{1}$
C23	$-2.80 \cdot 10^{2}$
C24	-4.50
C25	$9.36 \cdot 10^{1}$
C26	2.21
C27	$-1.03 \cdot 10^{1}$
C28	2.73
C29	$-1.28 \cdot 10^{2}$
C30	$1.95 \cdot 10^{1}$
C31	$9.53 \cdot 10^{1}$
C32	$-8.00 \cdot 10^{1}$
C33	$5.11 \cdot 10^{1}$

TABLE SI-XCVII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$
O1	$-8.57 \cdot 10^1$
O2	$-1.28 \cdot 10^3$
O3	$-1.99 \cdot 10^2$
O4	$-1.36 \cdot 10^3$
O5	$9.72 \cdot 10^2$
O6	$1.28 \cdot 10^3$
N1	$1.49 \cdot 10^2$
N2	$-4.38 \cdot 10^2$
N3	$-1.03 \cdot 10^1$
N4	$-1.74 \cdot 10^1$

TABLE SI-XCVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **2**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$	$\bar{\Phi}_{02}^{p(0)}$	$\bar{\Phi}_{12}^{p(0)}$
H1	$1.24 \cdot 10^{3}$	6.11	$2.53 \cdot 10^{3}$
H2	$4.38 \cdot 10^{2}$	1.62	$-1.15 \cdot 10^{2}$
H3	$2.88 \cdot 10^{2}$	$9.30 \cdot 10^{-1}$	$-6.43 \cdot 10^{2}$
H4	$3.40 \cdot 10^{1}$	$1.58 \cdot 10^{-1}$	$-2.50 \cdot 10^{2}$
H5	$-1.52 \cdot 10^{1}$	$5.24 \cdot 10^{-2}$	$-1.86 \cdot 10^{2}$
H6	$-2.49 \cdot 10^{2}$	$-2.18 \cdot 10^{-1}$	$9.65 \cdot 10^{1}$
H7	$-4.50 \cdot 10^{2}$	$-2.82 \cdot 10^{-1}$	$1.11 \cdot 10^{3}$
H8	$-1.47 \cdot 10^{3}$	$1.56 \cdot 10^{-1}$	$6.00 \cdot 10^{3}$
H9	$3.43 \cdot 10^{2}$	$-2.40 \cdot 10^{-2}$	$-4.08 \cdot 10^{2}$
H10	$1.63 \cdot 10^{2}$	$-6.38 \cdot 10^{-1}$	$-4.28 \cdot 10^{2}$
H11	$4.36 \cdot 10^{2}$	$-4.19 \cdot 10^{-1}$	$-1.41 \cdot 10^{3}$
H12	$-1.11 \cdot 10^{2}$	-1.91	$2.32 \cdot 10^{1}$
H13	$-5.25 \cdot 10^{2}$	-1.26	$1.82 \cdot 10^{3}$
H14	$-2.82 \cdot 10^{2}$	$-9.63 \cdot 10^{-1}$	$1.17 \cdot 10^{3}$
H15	$-3.35 \cdot 10^{2}$	$-1.95 \cdot 10^{-1}$	$2.45 \cdot 10^{3}$
H16	$1.43 \cdot 10^{2}$	$9.87 \cdot 10^{-1}$	$1.02 \cdot 10^{3}$
H17	$1.23 \cdot 10^{2}$	$3.22 \cdot 10^{-1}$	$3.65 \cdot 10^{2}$
H18	$-2.15 \cdot 10^{2}$	$3.68 \cdot 10^{-1}$	$1.46 \cdot 10^{3}$
H19	$5.34 \cdot 10^{2}$	$-3.45 \cdot 10^{-1}$	$-1.43 \cdot 10^{3}$
H20	$3.64 \cdot 10^{2}$	2.01	$1.12 \cdot 10^{2}$
H21	$-7.49 \cdot 10^{1}$	-2.12	$-1.05 \cdot 10^{3}$
H22	$2.28 \cdot 10^{2}$	-1.11	$-1.54 \cdot 10^{3}$
H23	$1.77 \cdot 10^{2}$	-1.73	$-2.55 \cdot 10^{3}$
H24	$-5.02 \cdot 10^{1}$	1.33	$2.44 \cdot 10^{3}$
H25	$1.48 \cdot 10^{2}$	1.29	$1.16 \cdot 10^{3}$
H26	$-1.79 \cdot 10^{2}$	$5.09 \cdot 10^{-1}$	$2.22 \cdot 10^{3}$
H27	$2.26 \cdot 10^{1}$	$7.01 \cdot 10^{-1}$	$-6.38 \cdot 10^{2}$
H28	$2.07 \cdot 10^{2}$	$7.25 \cdot 10^{-1}$	$-1.64 \cdot 10^{3}$
H29	$-1.79 \cdot 10^{2}$	$1.72 \cdot 10^{-1}$	$-1.39 \cdot 10^{3}$

TABLE SI-XCIX: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$	$\bar{\Phi}_{02}^{p(0)}$	$\bar{\Phi}_{12}^{p(0)}$
C1	$1.71 \cdot 10^3$	6.36	$-6.58 \cdot 10^2$
C2	$6.82 \cdot 10^2$	2.38	$-6.44 \cdot 10^2$
C3	$4.61 \cdot 10^2$	1.50	$-1.02 \cdot 10^3$
C4	$4.26 \cdot 10^2$	1.47	$-1.75 \cdot 10^3$
C5	$1.19 \cdot 10^2$	$5.39 \cdot 10^{-1}$	$-9.25 \cdot 10^2$
C6	$3.59 \cdot 10^1$	$1.89 \cdot 10^{-1}$	$-3.34 \cdot 10^2$
C7	-9.24	$9.21 \cdot 10^{-2}$	$-2.76 \cdot 10^2$
C8	$-4.50 \cdot 10^1$	$1.81 \cdot 10^{-1}$	$-7.01 \cdot 10^2$
C9	$-3.07 \cdot 10^2$	$-1.05 \cdot 10^{-1}$	$-7.68 \cdot 10^2$
C10	$-4.01 \cdot 10^2$	$-3.51 \cdot 10^{-1}$	$1.51 \cdot 10^2$
C11	$-6.64 \cdot 10^2$	$-5.19 \cdot 10^{-1}$	$1.19 \cdot 10^3$
C12	$-1.73 \cdot 10^3$	-1.12	$3.89 \cdot 10^3$
C13	$-5.39 \cdot 10^2$	$2.26 \cdot 10^{-1}$	$-2.75 \cdot 10^3$
C14	$8.73 \cdot 10^2$	3.25	$-4.73 \cdot 10^3$
C15	$3.89 \cdot 10^2$	$-6.29 \cdot 10^{-1}$	$-1.02 \cdot 10^3$
C16	$7.23 \cdot 10^2$	-3.24	$-2.70 \cdot 10^3$
C17	$-2.02 \cdot 10^2$	-3.76	$-9.58 \cdot 10^1$
C18	$-1.16 \cdot 10^3$	-5.04	$3.70 \cdot 10^3$
C19	$-4.95 \cdot 10^2$	-1.25	$2.19 \cdot 10^3$
C20	$8.36 \cdot 10^1$	$7.08 \cdot 10^{-1}$	$1.05 \cdot 10^3$
C21	$7.89 \cdot 10^2$	1.42	$6.56 \cdot 10^2$
C22	$1.02 \cdot 10^3$	$-7.07 \cdot 10^{-1}$	$-2.74 \cdot 10^3$
C23	$1.02 \cdot 10^3$	-4.32	$-6.05 \cdot 10^3$
C24	$8.60 \cdot 10^2$	4.08	$-4.07 \cdot 10^3$
C25	$7.96 \cdot 10^2$	4.09	$-5.31 \cdot 10^1$
C26	$6.36 \cdot 10^2$	5.25	$4.34 \cdot 10^3$
C27	$1.94 \cdot 10^2$	-2.06	$-2.26 \cdot 10^3$
C28	$2.33 \cdot 10^1$	1.49	$2.35 \cdot 10^3$
C29	$9.47 \cdot 10^1$	$8.76 \cdot 10^{-1}$	$-1.62 \cdot 10^3$

TABLE SI-C: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
O1	$3.02 \cdot 10^{2}$	$-1.88 \cdot 10^{1}$	$-1.49 \cdot 10^{4}$
O2	$-2.80 \cdot 10^{2}$	5.34	$1.08 \cdot 10^{4}$
O3	$9.37 \cdot 10^{2}$	4.87	$-1.76 \cdot 10^{4}$
O4	$-6.16 \cdot 10^{1}$	$1.18 \cdot 10^{1}$	$1.97 \cdot 10^{4}$
O5	$3.73 \cdot 10^{3}$	-2.48	$-9.06 \cdot 10^{3}$
O6	$-4.78 \cdot 10^{3}$	$-1.19 \cdot 10^{1}$	$1.75 \cdot 10^{4}$
N1	$3.95 \cdot 10^{3}$	$1.31 \cdot 10^{1}$	$-8.73 \cdot 10^{3}$
N2	$-3.56 \cdot 10^{3}$	-2.92	$1.49 \cdot 10^{3}$
N3	$9.53 \cdot 10^{1}$	$3.74 \cdot 10^{-1}$	$-5.20 \cdot 10^{2}$
N4	$-5.69 \cdot 10^{1}$	$4.47 \cdot 10^{-2}$	$-3.21 \cdot 10^{2}$

TABLE SI-CI: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **3**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$
H1	$2.13 \cdot 10^2$
H2	$-1.14 \cdot 10^1$
H3	$-2.62 \cdot 10^1$
H4	-3.71
H5	$2.28 \cdot 10^1$
H6	$5.54 \cdot 10^1$
H7	$7.36 \cdot 10^1$
H8	$1.78 \cdot 10^2$
H9	$2.89 \cdot 10^2$
H10	$3.25 \cdot 10^2$
H11	$5.89 \cdot 10^2$
H12	$-5.98 \cdot 10^1$
H13	$-4.39 \cdot 10^2$
H14	$-2.93 \cdot 10^2$
H15	$-4.84 \cdot 10^2$
H16	$1.22 \cdot 10^2$
H17	$-5.12 \cdot 10^1$
H18	$-2.24 \cdot 10^2$
H19	$1.92 \cdot 10^2$
H20	$2.95 \cdot 10^1$
H21	$1.46 \cdot 10^2$
H22	$1.72 \cdot 10^2$
H23	$1.12 \cdot 10^1$
H24	$2.29 \cdot 10^2$
H25	$1.73 \cdot 10^2$
H26	$5.16 \cdot 10^2$
H27	$3.38 \cdot 10^2$
H28	$2.90 \cdot 10^2$
H29	$2.43 \cdot 10^2$

TABLE SI-CII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$
C1	$-2.28 \cdot 10^1$
C2	$-3.69 \cdot 10^1$
C3	$-4.16 \cdot 10^1$
C4	$-3.78 \cdot 10^1$
C5	-1.29
C6	$2.59 \cdot 10^1$
C7	$7.94 \cdot 10^1$
C8	$8.41 \cdot 10^1$
C9	$1.13 \cdot 10^2$
C10	$2.49 \cdot 10^2$
C11	$1.30 \cdot 10^2$
C12	$-8.35 \cdot 10^1$
C13	$4.86 \cdot 10^2$
C14	$8.83 \cdot 10^2$
C15	$-1.32 \cdot 10^2$
C16	$-1.12 \cdot 10^3$
C17	$-5.13 \cdot 10^2$
C18	$-5.74 \cdot 10^1$
C19	$-7.61 \cdot 10^1$
C20	$2.97 \cdot 10^2$
C21	$4.36 \cdot 10^2$
C22	$1.56 \cdot 10^2$
C23	$2.08 \cdot 10^2$
C24	$8.24 \cdot 10^2$
C25	$9.70 \cdot 10^2$
C26	$1.29 \cdot 10^3$
C27	$4.03 \cdot 10^2$

TABLE SI-CIII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}_{01}^{p(0)}$
O1	$3.95 \cdot 10^3$
O2	$-4.26 \cdot 10^3$
O3	$-2.16 \cdot 10^3$
O4	$4.75 \cdot 10^2$
O5	$3.29 \cdot 10^2$
O6	$2.80 \cdot 10^3$
N1	$-3.37 \cdot 10^2$
N2	$4.80 \cdot 10^2$

TABLE SI-CIV: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **4**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{03}$	$\bar{\Phi}^{p(0)}_{12}$	$\bar{\Phi}^{p(0)}_{13}$	$\bar{\Phi}^{p(0)}_{23}$
H1	$6.72 \cdot 10^2$	7.43	-2.12	$-2.78 \cdot 10^3$	$-9.16 \cdot 10^2$	$9.66 \cdot 10^3$
H2	$9.71 \cdot 10^1$	$-3.07 \cdot 10^1$	-5.25	$-2.59 \cdot 10^3$	$-9.33 \cdot 10^2$	$-7.07 \cdot 10^3$
H3	$3.52 \cdot 10^2$	-7.44	-2.93	$-1.40 \cdot 10^3$	$-1.00 \cdot 10^3$	$1.49 \cdot 10^4$
H4	$-2.44 \cdot 10^2$	$2.39 \cdot 10^1$	-3.60	$1.68 \cdot 10^4$	$-1.55 \cdot 10^3$	$1.34 \cdot 10^4$
H5	$2.10 \cdot 10^2$	5.05	-3.59	$2.73 \cdot 10^3$	$-1.09 \cdot 10^3$	$2.51 \cdot 10^4$
H6	$-4.17 \cdot 10^2$	2.24	-4.14	$4.77 \cdot 10^3$	$-1.31 \cdot 10^2$	$9.55 \cdot 10^3$
H7	$2.93 \cdot 10^2$	2.36	-3.72	$-6.24 \cdot 10^3$	$-1.96 \cdot 10^2$	$3.93 \cdot 10^4$
H8	$3.56 \cdot 10^2$	8.20	$-4.03 \cdot 10^{-1}$	$-1.44 \cdot 10^4$	$1.42 \cdot 10^3$	$1.35 \cdot 10^4$
H9	$-4.07 \cdot 10^2$	-8.54	-3.95	$-9.46 \cdot 10^3$	$1.85 \cdot 10^3$	$-2.31 \cdot 10^4$
H10	$-4.62 \cdot 10^2$	-4.21	-3.14	$-1.28 \cdot 10^3$	$8.32 \cdot 10^2$	$-7.04 \cdot 10^3$
H11	$-9.09 \cdot 10^1$	7.70	3.87	$4.75 \cdot 10^3$	$5.43 \cdot 10^1$	$-1.12 \cdot 10^4$
H12	$-4.70 \cdot 10^2$	-3.36	-2.77	$1.71 \cdot 10^3$	$4.59 \cdot 10^2$	$-5.50 \cdot 10^3$
H13	$-5.48 \cdot 10^2$	$-1.28 \cdot 10^1$	1.07	$6.68 \cdot 10^3$	$1.24 \cdot 10^1$	$-2.07 \cdot 10^4$

TABLE SI-CV: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{03}$	$\bar{\Phi}^{p(0)}_{12}$	$\bar{\Phi}^{p(0)}_{13}$	$\bar{\Phi}^{p(0)}_{23}$
C1	$6.47 \cdot 10^2$	$-1.12 \cdot 10^1$	-5.11	$-2.92 \cdot 10^3$	$-1.62 \cdot 10^3$	$1.83 \cdot 10^4$
C2	$1.53 \cdot 10^2$	$1.46 \cdot 10^1$	-7.34	$9.47 \cdot 10^3$	$-2.05 \cdot 10^3$	$4.45 \cdot 10^4$
C3	$-2.78 \cdot 10^2$	5.26	-7.48	$2.68 \cdot 10^3$	$-4.63 \cdot 10^2$	$3.70 \cdot 10^4$
C4	$-3.83 \cdot 10^2$	-2.20	-4.21	$-9.44 \cdot 10^3$	$1.80 \cdot 10^3$	$-5.01 \cdot 10^3$
C5	$9.84 \cdot 10^2$	$4.66 \cdot 10^1$	$1.27 \cdot 10^1$	$-2.68 \cdot 10^3$	$5.75 \cdot 10^2$	$-5.29 \cdot 10^3$
C6	$-1.39 \cdot 10^2$	$1.45 \cdot 10^1$	7.74	$8.47 \cdot 10^3$	$1.35 \cdot 10^2$	$-2.10 \cdot 10^4$
C7	$-1.32 \cdot 10^3$	$-1.67 \cdot 10^1$	6.35	$2.04 \cdot 10^4$	$8.12 \cdot 10^1$	$-5.47 \cdot 10^4$
C8	$5.02 \cdot 10^2$	$1.88 \cdot 10^1$	4.10	$-3.47 \cdot 10^3$	$2.77 \cdot 10^2$	$9.39 \cdot 10^2$
C9	$-6.71 \cdot 10^2$	$-1.25 \cdot 10^1$	$9.23 \cdot 10^{-1}$	$8.39 \cdot 10^3$	$4.40 \cdot 10^1$	$-2.44 \cdot 10^4$
C10	$-1.07 \cdot 10^3$	3.44	-8.37	$1.26 \cdot 10^4$	$-1.77 \cdot 10^2$	$1.01 \cdot 10^4$
C11	$-8.19 \cdot 10^2$	-5.22	-5.30	$2.03 \cdot 10^3$	$9.00 \cdot 10^2$	$-6.94 \cdot 10^3$
C12	$-4.27 \cdot 10^2$	-4.36	-4.50	$-1.16 \cdot 10^4$	$2.18 \cdot 10^3$	$-1.37 \cdot 10^4$
C13	$-3.53 \cdot 10^2$	4.05	-2.81	$6.64 \cdot 10^3$	$-3.42 \cdot 10^2$	$4.52 \cdot 10^3$
C14	$-2.32 \cdot 10^1$	$-6.19 \cdot 10^{-1}$	-1.07	$-5.49 \cdot 10^3$	$7.91 \cdot 10^2$	$-6.50 \cdot 10^3$
C15	$-1.26 \cdot 10^3$	$-5.52 \cdot 10^1$	-2.18	$1.03 \cdot 10^4$	$-2.66 \cdot 10^2$	$-4.79 \cdot 10^4$
C16	$-1.04 \cdot 10^3$	$-2.50 \cdot 10^1$	2.24	$1.27 \cdot 10^4$	$1.38 \cdot 10^1$	$-3.95 \cdot 10^4$
C17	$-9.87 \cdot 10^2$	$-9.35 \cdot 10^{-1}$	8.44	$1.94 \cdot 10^4$	$9.19 \cdot 10^1$	$-4.78 \cdot 10^4$
C18	$-3.51 \cdot 10^2$	$-1.99 \cdot 10^1$	-1.64	$2.07 \cdot 10^3$	$-1.33 \cdot 10^2$	$-1.47 \cdot 10^4$
C19	$-2.14 \cdot 10^2$	7.03	3.56	$6.70 \cdot 10^3$	7.80	$-1.42 \cdot 10^4$

TABLE SI-CVI: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{03}$	$\bar{\Phi}^{p(0)}_{12}$	$\bar{\Phi}^{p(0)}_{13}$	$\bar{\Phi}^{p(0)}_{23}$
O1	$2.07 \cdot 10^{3}$	-8.59	$-1.73 \cdot 10^{1}$	$-1.78 \cdot 10^{3}$	$-6.16 \cdot 10^{3}$	$1.27 \cdot 10^{5}$
O2	$-2.26 \cdot 10^{3}$	-7.16	$-1.87 \cdot 10^{1}$	$2.18 \cdot 10^{3}$	$2.66 \cdot 10^{3}$	$1.07 \cdot 10^{4}$
O3	$4.35 \cdot 10^{3}$	$1.45 \cdot 10^{2}$	$3.16 \cdot 10^{1}$	$-4.02 \cdot 10^{4}$	$3.00 \cdot 10^{3}$	$1.71 \cdot 10^{4}$
O4	$-4.65 \cdot 10^{3}$	$-1.20 \cdot 10^{2}$	5.85	$5.34 \cdot 10^{4}$	$6.23 \cdot 10^{1}$	$-1.73 \cdot 10^{5}$
O5	$-1.24 \cdot 10^{3}$	$3.48 \cdot 10^{1}$	$-2.26 \cdot 10^{1}$	$3.55 \cdot 10^{4}$	$-3.76 \cdot 10^{3}$	$9.13 \cdot 10^{4}$
O6	$1.43 \cdot 10^{3}$	$3.11 \cdot 10^{1}$	$-6.32 \cdot 10^{-1}$	$-5.85 \cdot 10^{4}$	$6.39 \cdot 10^{3}$	$-1.45 \cdot 10^{4}$
O7	$-1.71 \cdot 10^{3}$	$-1.51 \cdot 10^{2}$	$-1.36 \cdot 10^{1}$	$7.60 \cdot 10^{3}$	$-2.10 \cdot 10^{3}$	$-7.75 \cdot 10^{4}$
O8	$-5.92 \cdot 10^{2}$	$7.75 \cdot 10^{1}$	$3.18 \cdot 10^{1}$	$4.06 \cdot 10^{4}$	$2.92 \cdot 10^{2}$	$-8.91 \cdot 10^{4}$
F1	$3.98 \cdot 10^{2}$	$1.45 \cdot 10^{1}$	2.01	$-2.00 \cdot 10^{3}$	$2.38 \cdot 10^{1}$	$1.21 \cdot 10^{3}$
F2	$2.13 \cdot 10^{2}$	9.74	2.43	$-7.18 \cdot 10^{2}$	$1.11 \cdot 10^{2}$	$-7.10 \cdot 10^{2}$
F3	$4.64 \cdot 10^{2}$	$1.30 \cdot 10^{1}$	2.93	$-5.97 \cdot 10^{3}$	$4.47 \cdot 10^{2}$	$3.43 \cdot 10^{3}$
F4	$-4.02 \cdot 10^{2}$	$-1.41 \cdot 10^{1}$	$1.99 \cdot 10^{-1}$	$4.07 \cdot 10^{3}$	$-4.09 \cdot 10^{1}$	$-1.51 \cdot 10^{4}$
F5	$-7.24 \cdot 10^{2}$	$-1.12 \cdot 10^{1}$	$-7.12 \cdot 10^{-1}$	$7.95 \cdot 10^{3}$	$1.35 \cdot 10^{2}$	$-2.29 \cdot 10^{4}$
F6	$-2.98 \cdot 10^{2}$	-4.05	1.03	$4.36 \cdot 10^{3}$	$1.65 \cdot 10^{1}$	$-1.17 \cdot 10^{4}$
F7	$-3.40 \cdot 10^{2}$	6.50	-1.26	$8.25 \cdot 10^{3}$	$-3.71 \cdot 10^{2}$	$-2.48 \cdot 10^{3}$
F8	$-2.47 \cdot 10^{2}$	$8.02 \cdot 10^{-1}$	-1.61	$3.26 \cdot 10^{3}$	$-5.83 \cdot 10^{1}$	$5.68 \cdot 10^{2}$
F9	$-3.29 \cdot 10^{1}$	3.24	-2.18	$2.56 \cdot 10^{3}$	$-4.38 \cdot 10^{2}$	$1.16 \cdot 10^{4}$
F10	$3.16 \cdot 10^{1}$	-2.03	-1.00	$-4.31 \cdot 10^{3}$	$5.00 \cdot 10^{2}$	$-8.21 \cdot 10^{3}$
F11	$1.94 \cdot 10^{2}$	4.37	$3.24 \cdot 10^{-1}$	$-5.96 \cdot 10^{3}$	$5.94 \cdot 10^{2}$	$1.01 \cdot 10^{3}$
F12	$-1.42 \cdot 10^{2}$	-2.52	-1.07	$-1.64 \cdot 10^{3}$	$4.21 \cdot 10^{2}$	$-5.71 \cdot 10^{3}$
F13	$-1.38 \cdot 10^{2}$	$-1.33 \cdot 10^{1}$	-1.91	$-3.05 \cdot 10^{2}$	$-9.02 \cdot 10^{1}$	$-9.71 \cdot 10^{3}$
F14	$-5.70 \cdot 10^{1}$	$-1.31 \cdot 10^{1}$	$-9.09 \cdot 10^{-1}$	$6.96 \cdot 10^{1}$	$-3.02 \cdot 10^{2}$	$-2.04 \cdot 10^{3}$
F15	$-2.95 \cdot 10^{2}$	$-1.13 \cdot 10^{1}$	$-7.95 \cdot 10^{-1}$	$2.19 \cdot 10^{3}$	1.22	$-1.13 \cdot 10^{4}$
F16	$1.20 \cdot 10^{2}$	8.91	3.69	$1.07 \cdot 10^{3}$	$1.28 \cdot 10^{2}$	$-4.69 \cdot 10^{3}$
F17	$-1.80 \cdot 10^{2}$	9.91	2.04	$7.00 \cdot 10^{3}$	$-1.51 \cdot 10^{2}$	$-9.62 \cdot 10^{3}$
F18	$-2.10 \cdot 10^{2}$	$8.25 \cdot 10^{-1}$	1.60	$4.31 \cdot 10^{3}$	6.61	$-9.75 \cdot 10^{3}$

TABLE SI-CVII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **5**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
H1	$-2.20 \cdot 10^2$	4.92	$-6.06 \cdot 10^2$
H2	$2.97 \cdot 10^2$	1.84	$8.72 \cdot 10^2$
H3	$2.18 \cdot 10^2$	3.21	$-2.88 \cdot 10^2$
H4	$1.08 \cdot 10^3$	3.44	$3.99 \cdot 10^2$
H5	$-1.37 \cdot 10^2$	2.93	$4.21 \cdot 10^2$
H6	$1.19 \cdot 10^3$	1.66	$1.62 \cdot 10^3$
H7	$1.04 \cdot 10^3$	2.11	$8.00 \cdot 10^2$
H8	$1.90 \cdot 10^3$	5.22	$1.70 \cdot 10^3$
H9	$7.15 \cdot 10^2$	3.75	$-1.25 \cdot 10^2$
H10	$7.97 \cdot 10^1$	1.99	$3.51 \cdot 10^2$
H11	$-9.52 \cdot 10^2$	5.82	$2.41 \cdot 10^2$
H12	$-2.21 \cdot 10^2$	2.77	$-1.60 \cdot 10^2$
H13	$3.18 \cdot 10^2$	2.33	$5.36 \cdot 10^2$
H14	$1.04 \cdot 10^3$	5.34	$1.46 \cdot 10^3$
H15	$-4.36 \cdot 10^3$	$-3.21 \cdot 10^1$	$3.48 \cdot 10^3$
H16	$-1.07 \cdot 10^3$	$-2.00 \cdot 10^1$	$-2.27 \cdot 10^3$
H17	$-3.42 \cdot 10^3$	$-2.61 \cdot 10^1$	$7.26 \cdot 10^2$
H18	$7.23 \cdot 10^2$	9.66	$-1.52 \cdot 10^2$
H19	$9.49 \cdot 10^1$	3.46	$-1.79 \cdot 10^1$
H20	$-9.45 \cdot 10^1$	2.28	$-5.55 \cdot 10^1$
H21	$-7.15 \cdot 10^2$	5.86	$6.79 \cdot 10^2$
H22	$9.88 \cdot 10^2$	$2.94 \cdot 10^1$	$-3.57 \cdot 10^3$
H23	$1.51 \cdot 10^3$	$1.96 \cdot 10^1$	$4.67 \cdot 10^3$
H24	$-9.52 \cdot 10^3$	$-8.76 \cdot 10^1$	$-2.98 \cdot 10^3$

TABLE SI-CVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
C1	$-2.77 \cdot 10^2$	$1.16 \cdot 10^1$	$5.51 \cdot 10^2$
C2	$5.28 \cdot 10^2$	3.83	$3.52 \cdot 10^2$
C3	$-3.00 \cdot 10^3$	$2.26 \cdot 10^1$	$2.21 \cdot 10^3$
C4	$-7.07 \cdot 10^1$	$1.85 \cdot 10^1$	$-3.56 \cdot 10^3$
C5	$-4.82 \cdot 10^1$	3.85	$6.23 \cdot 10^2$
C6	$1.76 \cdot 10^3$	3.77	$1.66 \cdot 10^3$
C7	$4.10 \cdot 10^3$	8.41	$2.86 \cdot 10^3$
C8	$-1.51 \cdot 10^2$	7.78	$1.33 \cdot 10^3$
C9	$1.43 \cdot 10^3$	7.25	$-4.19 \cdot 10^2$
C10	$1.23 \cdot 10^2$	2.84	$5.22 \cdot 10^2$
C11	$-1.85 \cdot 10^3$	$1.15 \cdot 10^1$	$4.35 \cdot 10^2$
C12	$-3.57 \cdot 10^2$	8.83	$-8.38 \cdot 10^2$
C13	$-2.34 \cdot 10^2$	4.12	$-2.53 \cdot 10^2$
C14	$3.45 \cdot 10^2$	3.24	$7.08 \cdot 10^2$
C15	$7.50 \cdot 10^2$	5.73	$1.38 \cdot 10^3$
C16	$-4.43 \cdot 10^3$	$-4.03 \cdot 10^1$	$-2.28 \cdot 10^1$
C17	$3.33 \cdot 10^2$	9.14	$-3.26 \cdot 10^2$
C18	$5.58 \cdot 10^1$	4.62	$-1.06 \cdot 10^2$
C19	$-1.08 \cdot 10^2$	3.42	$-1.22 \cdot 10^2$

TABLE SI-CIX: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
O1	$-3.92 \cdot 10^2$	$8.09 \cdot 10^1$	$-1.80 \cdot 10^4$
O2	$-4.74 \cdot 10^3$	$7.84 \cdot 10^1$	$1.05 \cdot 10^4$
O3	$5.67 \cdot 10^3$	$2.90 \cdot 10^1$	$5.69 \cdot 10^3$
O4	$-1.39 \cdot 10^4$	$-1.34 \cdot 10^2$	$-8.34 \cdot 10^3$
O5	$-3.81 \cdot 10^3$	$-2.20 \cdot 10^1$	$1.94 \cdot 10^4$
O6	$1.40 \cdot 10^4$	$3.11 \cdot 10^1$	$1.52 \cdot 10^4$
O7	$1.53 \cdot 10^4$	$8.16 \cdot 10^1$	$7.25 \cdot 10^2$
O8	$6.64 \cdot 10^1$	$-4.85 \cdot 10^1$	$-2.91 \cdot 10^4$
O9	$-1.20 \cdot 10^4$	$-8.26 \cdot 10^1$	$1.01 \cdot 10^4$
O10	$-2.11 \cdot 10^3$	$-2.33 \cdot 10^1$	$-1.69 \cdot 10^3$
O11	$2.18 \cdot 10^3$	$1.19 \cdot 10^1$	$3.57 \cdot 10^3$
N1	$-4.10 \cdot 10^2$	8.93	$-1.23 \cdot 10^3$
N2	$-9.65 \cdot 10^2$	9.54	$1.31 \cdot 10^3$
N3	$6.81 \cdot 10^2$	$1.07 \cdot 10^1$	$2.38 \cdot 10^3$
N4	$-5.39 \cdot 10^3$	$-6.34 \cdot 10^1$	$-4.98 \cdot 10^3$
N5	$5.90 \cdot 10^3$	$3.51 \cdot 10^1$	$1.01 \cdot 10^4$
N6	$1.35 \cdot 10^2$	$1.55 \cdot 10^1$	$-1.26 \cdot 10^3$

TABLE SI-CX: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **6**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
H1	$-2.85 \cdot 10^{2}$	-4.09	$2.16 \cdot 10^{3}$
H2	$6.21 \cdot 10^{1}$	$-3.16 \cdot 10^{-1}$	$7.20 \cdot 10^{2}$
H3	$4.05 \cdot 10^{1}$	$2.50 \cdot 10^{1}$	$-5.35 \cdot 10^{3}$
H4	$8.25 \cdot 10^{1}$	-2.57	$1.92 \cdot 10^{3}$
H5	$-1.87 \cdot 10^{1}$	$-4.65 \cdot 10^{-1}$	$1.72 \cdot 10^{2}$
H6	4.86	$3.63 \cdot 10^{-2}$	$1.24 \cdot 10^{2}$
H7	$-8.72 \cdot 10^{1}$	-2.42	$7.50 \cdot 10^{2}$
H8	$-1.63 \cdot 10^{2}$	-9.32	$-2.00 \cdot 10^{3}$
H9	$3.58 \cdot 10^{1}$	-1.68	$2.26 \cdot 10^{1}$
H10	$-1.92 \cdot 10^{2}$	$-1.20 \cdot 10^{1}$	$1.02 \cdot 10^{3}$
H11	$4.89 \cdot 10^{2}$	3.76	$-7.21 \cdot 10^{2}$
H12	$-1.12 \cdot 10^{3}$	$-6.09 \cdot 10^{1}$	$1.44 \cdot 10^{4}$
H13	$-3.40 \cdot 10^{1}$	4.52	$-1.98 \cdot 10^{3}$
H14	$-1.22 \cdot 10^{2}$	-5.16	$1.17 \cdot 10^{3}$
H15	$2.26 \cdot 10^{2}$	$-1.43 \cdot 10^{1}$	$9.44 \cdot 10^{3}$
H16	$-2.03 \cdot 10^{1}$	-2.00	$3.00 \cdot 10^{2}$
H17	$-9.26 \cdot 10^{1}$	-5.96	$9.98 \cdot 10^{2}$
H18	$-5.54 \cdot 10^{2}$	$-3.05 \cdot 10^{1}$	$6.38 \cdot 10^{3}$
H19	$-1.52 \cdot 10^{2}$	-8.08	$1.76 \cdot 10^{3}$
H20	$-2.58 \cdot 10^{2}$	$-1.27 \cdot 10^{1}$	$2.92 \cdot 10^{3}$
H21	$1.70 \cdot 10^{2}$	-1.12	$-3.53 \cdot 10^{2}$
H22	$-5.80 \cdot 10^{2}$	$-2.92 \cdot 10^{1}$	$4.96 \cdot 10^{3}$
H23	$-9.21 \cdot 10^{-1}$	$-9.34 \cdot 10^{-4}$	$6.91 \cdot 10^{1}$
H24	-6.77	$-1.32 \cdot 10^{-1}$	$8.07 \cdot 10^{1}$
H25	$-1.00 \cdot 10^{2}$	-6.68	$8.45 \cdot 10^{2}$
H26	$-4.98 \cdot 10^{1}$	$-5.45 \cdot 10^{-1}$	$-4.20 \cdot 10^{2}$
H27	$-8.01 \cdot 10^{1}$	-3.26	$3.03 \cdot 10^{2}$
H28	$-1.65 \cdot 10^{2}$	-8.41	$1.41 \cdot 10^{3}$

TABLE SI-CXI: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
C1	$-3.06 \cdot 10^{2}$	$-1.50 \cdot 10^{1}$	$3.66 \cdot 10^{3}$
C2	$-1.64 \cdot 10^{2}$	-6.58	$1.63 \cdot 10^{3}$
C3	$2.23 \cdot 10^{2}$	-1.51	$2.29 \cdot 10^{3}$
C4	$9.43 \cdot 10^{1}$	$-4.35 \cdot 10^{-2}$	$1.00 \cdot 10^{3}$
C5	$-4.71 \cdot 10^{2}$	$1.20 \cdot 10^{1}$	$-8.08 \cdot 10^{3}$
C6	$1.38 \cdot 10^{3}$	$2.01 \cdot 10^{1}$	$3.38 \cdot 10^{2}$
C7	$1.01 \cdot 10^{1}$	$-3.08 \cdot 10^{-1}$	$4.85 \cdot 10^{2}$
C8	$-1.36 \cdot 10^{2}$	-5.71	$1.41 \cdot 10^{3}$
C9	$1.06 \cdot 10^{2}$	$-4.64 \cdot 10^{-1}$	$1.14 \cdot 10^{3}$
C10	$-4.84 \cdot 10^{2}$	$-3.30 \cdot 10^{1}$	$4.32 \cdot 10^{3}$
C11	$-4.57 \cdot 10^{1}$	-1.67	$6.15 \cdot 10^{2}$
C12	$6.95 \cdot 10^{1}$	-6.21	$7.24 \cdot 10^{2}$
C13	$1.27 \cdot 10^{2}$	$4.81 \cdot 10^{1}$	$-1.07 \cdot 10^{4}$
C14	$1.52 \cdot 10^{2}$	-2.40	$2.37 \cdot 10^{3}$
C15	$-3.12 \cdot 10^{2}$	-6.71	$-8.91 \cdot 10^{2}$
C16	$-1.43 \cdot 10^{1}$	$-3.31 \cdot 10^{-1}$	$1.53 \cdot 10^{2}$
C17	$5.74 \cdot 10^{2}$	-7.29	$6.56 \cdot 10^{2}$
C18	1.37	$8.11 \cdot 10^{-3}$	$1.21 \cdot 10^{2}$
C19	$-7.78 \cdot 10^{1}$	-3.44	$7.81 \cdot 10^{2}$
C20	$-1.59 \cdot 10^{1}$	$-4.05 \cdot 10^{-1}$	$2.16 \cdot 10^{2}$
C21	$-1.14 \cdot 10^{3}$	$-7.63 \cdot 10^{1}$	$7.07 \cdot 10^{3}$
C22	$-3.60 \cdot 10^{2}$	$-1.89 \cdot 10^{1}$	$-3.46 \cdot 10^{3}$
C23	$2.94 \cdot 10^{1}$	-2.49	$1.49 \cdot 10^{2}$
C24	$-2.31 \cdot 10^{2}$	$-1.54 \cdot 10^{1}$	$1.76 \cdot 10^{3}$
C25	$9.09 \cdot 10^{2}$	6.55	$-9.67 \cdot 10^{2}$
C26	$6.86 \cdot 10^{2}$	$9.20 \cdot 10^{1}$	$-1.52 \cdot 10^{4}$
C27	-1.69	$-7.81 \cdot 10^{-2}$	$1.87 \cdot 10^{2}$
C28	$2.19 \cdot 10^{2}$	$3.08 \cdot 10^{1}$	$-3.79 \cdot 10^{3}$
C29	$-1.02 \cdot 10^{3}$	$-5.14 \cdot 10^{1}$	$1.13 \cdot 10^{4}$
C30	$-1.04 \cdot 10^{2}$	$2.14 \cdot 10^{-1}$	$-1.26 \cdot 10^{3}$
C31	$-1.97 \cdot 10^{2}$	-8.48	$1.89 \cdot 10^{3}$
C32	$4.30 \cdot 10^{2}$	-7.05	$6.75 \cdot 10^{3}$
C33	$7.63 \cdot 10^{1}$	$3.69 \cdot 10^{1}$	$-1.44 \cdot 10^{4}$
C34	$-2.18 \cdot 10^{1}$	-2.69	$3.87 \cdot 10^{2}$
C35	$-1.32 \cdot 10^{2}$	-8.63	$1.40 \cdot 10^{3}$
C36	$-4.11 \cdot 10^{2}$	$-2.57 \cdot 10^{1}$	$4.53 \cdot 10^{3}$
C37	$1.58 \cdot 10^{2}$	$2.45 \cdot 10^{1}$	$-6.36 \cdot 10^{3}$
C38	$-1.95 \cdot 10^{2}$	$-1.18 \cdot 10^{1}$	$2.19 \cdot 10^{3}$
C39	$-3.59 \cdot 10^{2}$	$-1.71 \cdot 10^{1}$	$3.81 \cdot 10^{3}$
C40	$4.61 \cdot 10^{2}$	9.41	$3.19 \cdot 10^{2}$
C41	$1.07 \cdot 10^{2}$	-2.88	$3.44 \cdot 10^{-1}$
C42	$-3.84 \cdot 10^{2}$	$-1.68 \cdot 10^{1}$	$2.10 \cdot 10^{3}$
C43	-2.14	$-2.73 \cdot 10^{-2}$	$8.72 \cdot 10^{1}$
C44	-7.08	$-1.36 \cdot 10^{-1}$	$9.70 \cdot 10^{1}$
C45	$-1.40 \cdot 10^{2}$	-9.45	$1.27 \cdot 10^{3}$
C46	$-8.38 \cdot 10^{1}$	-1.78	$-3.43 \cdot 10^{2}$
C47	$-1.09 \cdot 10^{2}$	-4.23	$3.21 \cdot 10^{2}$
C48	$-1.89 \cdot 10^{2}$	-8.70	$1.18 \cdot 10^{3}$

TABLE SI-CXII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
O1	$-1.47 \cdot 10^2$	$-2.65 \cdot 10^1$	$8.41 \cdot 10^3$
O2	$-4.06 \cdot 10^3$	$-2.59 \cdot 10^2$	$4.01 \cdot 10^4$
O3	$-2.60 \cdot 10^3$	$-9.18 \cdot 10^1$	$-3.02 \cdot 10^3$
O4	$2.53 \cdot 10^3$	$3.83 \cdot 10^1$	$1.29 \cdot 10^4$
O5	$2.75 \cdot 10^3$	$2.31 \cdot 10^2$	$-3.03 \cdot 10^4$
O6	$5.60 \cdot 10^2$	$2.02 \cdot 10^2$	$-4.49 \cdot 10^4$
N1	$1.35 \cdot 10^3$	$-5.55 \cdot 10^{-1}$	$8.51 \cdot 10^3$
N2	$-1.79 \cdot 10^3$	$-8.94 \cdot 10^1$	$1.78 \cdot 10^4$
N3	$1.16 \cdot 10^1$	$9.03 \cdot 10^{-3}$	$2.89 \cdot 10^2$
N4	$-3.82 \cdot 10^1$	-1.17	$3.99 \cdot 10^2$
F1	$8.79 \cdot 10^1$	$1.76 \cdot 10^1$	$-2.50 \cdot 10^3$
F2	$2.90 \cdot 10^2$	$2.10 \cdot 10^1$	$-2.62 \cdot 10^3$
F3	$-2.93 \cdot 10^1$	$1.68 \cdot 10^1$	$-5.46 \cdot 10^2$
F4	$1.04 \cdot 10^2$	$1.01 \cdot 10^1$	$-3.50 \cdot 10^3$
F5	$2.55 \cdot 10^2$	3.75	$2.37 \cdot 10^2$
F6	$1.23 \cdot 10^2$	$-7.30 \cdot 10^{-1}$	$2.52 \cdot 10^3$
F7	$4.50 \cdot 10^2$	$1.59 \cdot 10^1$	$-1.76 \cdot 10^3$
F8	$3.33 \cdot 10^2$	$2.93 \cdot 10^1$	$-6.23 \cdot 10^3$
F9	$-2.14 \cdot 10^1$	$1.67 \cdot 10^1$	$-3.43 \cdot 10^3$

TABLE SI-CXIII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **7**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
H1	$-2.14 \cdot 10^{1}$	$-7.46 \cdot 10^{-1}$	$-1.07 \cdot 10^{4}$
H2	$-1.99 \cdot 10^{1}$	-4.73	$-1.90 \cdot 10^{4}$
H3	$-2.79 \cdot 10^{1}$	$-1.02 \cdot 10^{1}$	$-4.48 \cdot 10^{4}$
H4	$2.52 \cdot 10^{1}$	-4.05	$-8.60 \cdot 10^{4}$
H5	$5.16 \cdot 10^{1}$	$-1.51 \cdot 10^{1}$	$1.91 \cdot 10^{4}$
H6	$4.14 \cdot 10^{1}$	$8.42 \cdot 10^{-1}$	$9.17 \cdot 10^{3}$
H7	$6.00 \cdot 10^{1}$	$2.86 \cdot 10^{1}$	$6.20 \cdot 10^{3}$
H8	3.46	$1.08 \cdot 10^{2}$	$-2.47 \cdot 10^{4}$
H9	$3.16 \cdot 10^{2}$	$-1.64 \cdot 10^{2}$	$3.58 \cdot 10^{5}$
H10	$6.80 \cdot 10^{1}$	$-1.85 \cdot 10^{1}$	$8.76 \cdot 10^{4}$
H11	$4.15 \cdot 10^{1}$	2.35	$4.61 \cdot 10^{4}$
H12	$4.79 \cdot 10^{1}$	$1.53 \cdot 10^{1}$	$2.48 \cdot 10^{4}$
H13	$2.46 \cdot 10^{1}$	$1.18 \cdot 10^{1}$	$-2.76 \cdot 10^{4}$
H14	5.00	-1.19	$-3.77 \cdot 10^{4}$
H15	$-1.06 \cdot 10^{1}$	$-1.80 \cdot 10^{1}$	$-5.42 \cdot 10^{4}$
H16	$-1.22 \cdot 10^{2}$	$-8.37 \cdot 10^{1}$	$-1.79 \cdot 10^{5}$
H17	-1.72	$3.94 \cdot 10^{1}$	$-3.34 \cdot 10^{3}$
H18	9.34	$2.82 \cdot 10^{1}$	$-3.24 \cdot 10^{3}$
H19	$4.24 \cdot 10^{1}$	$3.08 \cdot 10^{1}$	$1.91 \cdot 10^{3}$
H20	$1.49 \cdot 10^{2}$	$-7.50 \cdot 10^{-1}$	$4.45 \cdot 10^{4}$

TABLE SI-CXIV: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
C1	$-3.13 \cdot 10^{1}$	-3.30	$-1.95 \cdot 10^{4}$
C2	$-2.89 \cdot 10^{1}$	-6.52	$-2.63 \cdot 10^{4}$
C3	$-4.01 \cdot 10^{1}$	$-1.24 \cdot 10^{1}$	$-4.88 \cdot 10^{4}$
C4	$-8.96 \cdot 10^{1}$	$-2.44 \cdot 10^{1}$	$-9.05 \cdot 10^{4}$
C5	$-2.07 \cdot 10^{2}$	$-7.17 \cdot 10^{1}$	$-2.82 \cdot 10^{5}$
C6	$1.37 \cdot 10^{1}$	$-1.35 \cdot 10^{1}$	$-1.82 \cdot 10^{5}$
C7	$1.81 \cdot 10^{2}$	$8.66 \cdot 10^{1}$	$-1.40 \cdot 10^{5}$
C8	$1.08 \cdot 10^{2}$	$6.53 \cdot 10^{1}$	$-1.22 \cdot 10^{4}$
C9	$7.19 \cdot 10^{1}$	$-1.69 \cdot 10^{1}$	$2.48 \cdot 10^{4}$
C10	$6.11 \cdot 10^{1}$	-2.11	$1.53 \cdot 10^{4}$
C11	$8.55 \cdot 10^{1}$	$1.39 \cdot 10^{1}$	$1.66 \cdot 10^{4}$
C12	$1.86 \cdot 10^{2}$	-5.02	$5.29 \cdot 10^{4}$
C13	$3.10 \cdot 10^{2}$	$7.29 \cdot 10^{1}$	$7.45 \cdot 10^{4}$
C14	$-1.56 \cdot 10^{1}$	$2.01 \cdot 10^{2}$	$-5.31 \cdot 10^{4}$
C15	$-3.55 \cdot 10^{2}$	$3.52 \cdot 10^{2}$	$-1.78 \cdot 10^{5}$
C16	$-1.42 \cdot 10^{2}$	$1.22 \cdot 10^{2}$	$-6.11 \cdot 10^{4}$
C17	$2.89 \cdot 10^{2}$	$-1.03 \cdot 10^{2}$	$3.67 \cdot 10^{5}$
C18	$1.03 \cdot 10^{2}$	$-2.08 \cdot 10^{1}$	$1.31 \cdot 10^{5}$
C19	$6.79 \cdot 10^{1}$	1.49	$7.63 \cdot 10^{4}$
C20	$7.89 \cdot 10^{1}$	$1.49 \cdot 10^{1}$	$6.32 \cdot 10^{4}$
C21	$1.67 \cdot 10^{2}$	$2.19 \cdot 10^{1}$	$1.12 \cdot 10^{5}$
C22	$4.52 \cdot 10^{1}$	$2.09 \cdot 10^{1}$	$-1.31 \cdot 10^{5}$
C23	$2.09 \cdot 10^{1}$	9.99	$-6.27 \cdot 10^{4}$
C24	2.90	-2.95	$-6.36 \cdot 10^{4}$
C25	$-1.74 \cdot 10^{1}$	$-2.07 \cdot 10^{1}$	$-9.26 \cdot 10^{4}$
C26	$-1.09 \cdot 10^{2}$	$-6.77 \cdot 10^{1}$	$-2.57 \cdot 10^{5}$
C27	1.41	$5.40 \cdot 10^{1}$	$-5.94 \cdot 10^{3}$
C28	$1.21 \cdot 10^{1}$	$4.20 \cdot 10^{1}$	$-5.00 \cdot 10^{3}$
C29	$3.57 \cdot 10^{1}$	$4.98 \cdot 10^{1}$	$-3.35 \cdot 10^{3}$
C30	$4.35 \cdot 10^{1}$	$1.30 \cdot 10^{2}$	$-1.68 \cdot 10^{4}$
C31	$1.83 \cdot 10^{2}$	$2.43 \cdot 10^{2}$	$-1.43 \cdot 10^{4}$
C32	$2.75 \cdot 10^{2}$	-4.39	$8.71 \cdot 10^{4}$
C33	$4.82 \cdot 10^{2}$	$-2.28 \cdot 10^{2}$	$2.88 \cdot 10^{5}$
C34	$1.84 \cdot 10^{2}$	$-1.06 \cdot 10^{2}$	$1.31 \cdot 10^{5}$

TABLE SI-CXV: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
O1	$-1.03 \cdot 10^3$	$-1.03 \cdot 10^2$	$-7.66 \cdot 10^5$
O2	$5.79 \cdot 10^2$	$2.64 \cdot 10^2$	$4.29 \cdot 10^4$
O3	$1.19 \cdot 10^3$	$-3.94 \cdot 10^2$	$6.07 \cdot 10^5$
O4	$-1.47 \cdot 10^3$	$7.74 \cdot 10^2$	$-6.39 \cdot 10^5$
O5	$-4.62 \cdot 10^1$	$1.04 \cdot 10^3$	$-2.29 \cdot 10^5$
O6	$1.34 \cdot 10^3$	$-8.98 \cdot 10^2$	$1.13 \cdot 10^6$
N1	$-2.52 \cdot 10^2$	$-7.93 \cdot 10^1$	$-6.55 \cdot 10^5$
N2	$5.72 \cdot 10^2$	$-1.49 \cdot 10^2$	$7.06 \cdot 10^5$
F1	$5.78 \cdot 10^1$	$2.95 \cdot 10^1$	$-1.95 \cdot 10^4$
F2	$5.09 \cdot 10^1$	$1.93 \cdot 10^1$	$1.21 \cdot 10^4$
F3	$1.22 \cdot 10^2$	$1.09 \cdot 10^2$	$1.14 \cdot 10^4$
F4	$-9.55 \cdot 10^1$	$6.35 \cdot 10^1$	$-4.53 \cdot 10^4$
F5	$-3.53 \cdot 10^1$	$9.61 \cdot 10^1$	$-7.30 \cdot 10^3$
F6	$-1.54 \cdot 10^2$	$7.07 \cdot 10^1$	$-6.36 \cdot 10^4$
F7	$1.42 \cdot 10^2$	$-7.78 \cdot 10^1$	$9.49 \cdot 10^4$
F8	$1.13 \cdot 10^2$	$-9.51 \cdot 10^1$	$1.16 \cdot 10^5$
F9	$1.01 \cdot 10^2$	$-4.70 \cdot 10^1$	$5.89 \cdot 10^4$
S1	$-6.32 \cdot 10^1$	-1.33	$-2.94 \cdot 10^4$
S2	$1.63 \cdot 10^2$	$-5.62 \cdot 10^1$	$7.09 \cdot 10^4$
S3	-9.68	$1.22 \cdot 10^2$	$-1.24 \cdot 10^4$

TABLE SI-CXVI: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **8**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
H1	-1.29	-2.74	$-9.54 \cdot 10^{2}$
H2	$1.20 \cdot 10^{1}$	-1.29	$-9.81 \cdot 10^{2}$
H3	$6.96 \cdot 10^{1}$	$2.83 \cdot 10^{-1}$	$-2.25 \cdot 10^{3}$
H4	$2.91 \cdot 10^{2}$	8.24	$-6.18 \cdot 10^{3}$
H5	$-9.11 \cdot 10^{1}$	-2.32	$1.16 \cdot 10^{3}$
H6	$-6.80 \cdot 10^{1}$	-1.37	$1.25 \cdot 10^{3}$
H7	$-8.17 \cdot 10^{1}$	-1.71	$2.27 \cdot 10^{3}$
H8	$3.80 \cdot 10^{1}$	-1.79	$2.61 \cdot 10^{3}$
H9	$1.65 \cdot 10^{2}$	3.48	$-2.43 \cdot 10^{3}$
H10	$1.05 \cdot 10^{2}$	2.33	$-1.81 \cdot 10^{3}$
H11	$7.25 \cdot 10^{1}$	1.84	$-2.09 \cdot 10^{3}$
H12	$-2.06 \cdot 10^{2}$	-2.78	$-4.70 \cdot 10^{2}$
H13	$7.71 \cdot 10^{2}$	$1.09 \cdot 10^{1}$	$-1.14 \cdot 10^{4}$
H14	$1.71 \cdot 10^{2}$	3.42	$-2.31 \cdot 10^{3}$
H15	$5.24 \cdot 10^{1}$	2.22	$-1.72 \cdot 10^{2}$
H16	$-3.22 \cdot 10^{1}$	$9.35 \cdot 10^{-1}$	$1.43 \cdot 10^{3}$
H17	$-7.99 \cdot 10^{1}$	$-1.50 \cdot 10^{-1}$	$2.38 \cdot 10^{3}$
H18	$-9.65 \cdot 10^{1}$	-1.24	$2.87 \cdot 10^{3}$
H19	$-5.00 \cdot 10^{1}$	-1.75	$2.32 \cdot 10^{3}$
H20	$2.19 \cdot 10^{2}$	-2.43	$1.30 \cdot 10^{3}$

TABLE SI-CXVII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
C1	1.71	-3.45	$-1.40 \cdot 10^{3}$
C2	$1.57 \cdot 10^{1}$	-2.02	$-1.41 \cdot 10^{3}$
C3	$5.40 \cdot 10^{1}$	-1.23	$-2.44 \cdot 10^{3}$
C4	$6.58 \cdot 10^{1}$	-5.35	$-4.88 \cdot 10^{3}$
C5	$3.70 \cdot 10^{2}$	-2.42	$-1.47 \cdot 10^{4}$
C6	$5.93 \cdot 10^{2}$	$1.59 \cdot 10^{1}$	$-1.24 \cdot 10^{4}$
C7	$1.29 \cdot 10^{3}$	$3.90 \cdot 10^{1}$	$-2.02 \cdot 10^{4}$
C8	$5.03 \cdot 10^{2}$	$1.47 \cdot 10^{1}$	$-7.24 \cdot 10^{3}$
C9	$-1.27 \cdot 10^{2}$	-2.99	$1.80 \cdot 10^{3}$
C10	$-1.03 \cdot 10^{2}$	-2.11	$1.82 \cdot 10^{3}$
C11	$-1.37 \cdot 10^{2}$	-2.68	$2.92 \cdot 10^{3}$
C12	$-3.34 \cdot 10^{2}$	-6.60	$6.22 \cdot 10^{3}$
C13	$-7.11 \cdot 10^{2}$	$-1.32 \cdot 10^{1}$	$1.65 \cdot 10^{4}$
C14	$-5.12 \cdot 10^{1}$	-4.25	$7.10 \cdot 10^{3}$
C15	$2.92 \cdot 10^{2}$	-4.83	$4.36 \cdot 10^{3}$
C16	$1.90 \cdot 10^{2}$	-2.01	$-3.26 \cdot 10^{2}$
C17	$2.18 \cdot 10^{2}$	4.75	$-3.34 \cdot 10^{3}$
C18	$1.56 \cdot 10^{2}$	3.51	$-2.66 \cdot 10^{3}$
C19	$1.50 \cdot 10^{2}$	3.64	$-3.18 \cdot 10^{3}$
C20	$4.27 \cdot 10^{2}$	$1.05 \cdot 10^{1}$	$-7.90 \cdot 10^{3}$
C21	$6.19 \cdot 10^{2}$	$1.79 \cdot 10^{1}$	$-1.56 \cdot 10^{4}$
C22	$-3.84 \cdot 10^{2}$	-5.36	$-1.23 \cdot 10^{3}$
C23	$-1.36 \cdot 10^{3}$	$-2.99 \cdot 10^{1}$	$9.41 \cdot 10^{3}$
C24	$-5.69 \cdot 10^{2}$	$-1.32 \cdot 10^{1}$	$4.96 \cdot 10^{3}$
C25	$6.69 \cdot 10^{2}$	$1.34 \cdot 10^{1}$	$-8.89 \cdot 10^{3}$
C26	$2.21 \cdot 10^{2}$	5.29	$-2.65 \cdot 10^{3}$
C27	$8.61 \cdot 10^{1}$	3.58	$-2.93 \cdot 10^{2}$
C28	$-1.30 \cdot 10^{1}$	3.50	$2.41 \cdot 10^{3}$
C29	$-1.15 \cdot 10^{2}$	6.95	$8.37 \cdot 10^{3}$
C30	$-6.19 \cdot 10^{1}$	1.14	$2.45 \cdot 10^{3}$
C31	$-1.10 \cdot 10^{2}$	$9.43 \cdot 10^{-3}$	$3.42 \cdot 10^{3}$
C32	$-2.17 \cdot 10^{2}$	-1.46	$6.60 \cdot 10^{3}$
C33	$-4.96 \cdot 10^{2}$	-2.32	$1.63 \cdot 10^{4}$
C34	$-1.52 \cdot 10^{2}$	-2.01	$4.62 \cdot 10^{3}$
C35	$-1.25 \cdot 10^{2}$	-2.89	$4.59 \cdot 10^{3}$
C36	$-1.68 \cdot 10^{2}$	-6.58	$9.16 \cdot 10^{3}$

TABLE SI-CXVIII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{12}$
O1	$4.33 \cdot 10^{2}$	$-5.26 \cdot 10^{1}$	$-3.78 \cdot 10^{4}$
O2	$3.99 \cdot 10^{3}$	$1.15 \cdot 10^{2}$	$-5.61 \cdot 10^{4}$
O3	$-3.17 \cdot 10^{3}$	$-6.19 \cdot 10^{1}$	$5.29 \cdot 10^{4}$
O4	$1.01 \cdot 10^{3}$	$-1.15 \cdot 10^{1}$	$4.56 \cdot 10^{3}$
O5	$3.89 \cdot 10^{3}$	$9.22 \cdot 10^{1}$	$-6.82 \cdot 10^{4}$
O6	$-4.17 \cdot 10^{3}$	$-1.07 \cdot 10^{2}$	$3.52 \cdot 10^{4}$
N1	$-9.75 \cdot 10^{2}$	$-1.64 \cdot 10^{1}$	$3.57 \cdot 10^{4}$
N2	$8.78 \cdot 10^{2}$	$2.82 \cdot 10^{1}$	$-4.57 \cdot 10^{3}$
F1	$2.79 \cdot 10^{2}$	$1.13 \cdot 10^{1}$	$-3.58 \cdot 10^{3}$
F2	$2.60 \cdot 10^{2}$	7.89	$-3.97 \cdot 10^{3}$
F3	$4.61 \cdot 10^{2}$	9.34	$-6.35 \cdot 10^{3}$
F4	$1.15 \cdot 10^{2}$	$-9.98 \cdot 10^{-1}$	$-2.04 \cdot 10^{2}$
F5	$-9.45 \cdot 10^{-1}$	$7.06 \cdot 10^{-4}$	$2.19 \cdot 10^{3}$
F6	$2.97 \cdot 10^{2}$	-3.44	$-3.85 \cdot 10^{3}$
F7	$-3.12 \cdot 10^{2}$	-6.20	$2.64 \cdot 10^{3}$
F8	$-2.26 \cdot 10^{2}$	$-1.00 \cdot 10^{1}$	$6.90 \cdot 10^{2}$
F9	$-6.00 \cdot 10^{2}$	$-1.10 \cdot 10^{1}$	$7.28 \cdot 10^{3}$
S1	-7.42	-8.46	$-2.95 \cdot 10^{3}$
S2	$-2.93 \cdot 10^{2}$	-7.52	$3.68 \cdot 10^{3}$
S3	$5.09 \cdot 10^{2}$	$1.12 \cdot 10^{1}$	$-7.57 \cdot 10^{3}$

TABLE SI-CXIX: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **9**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{03}$	$\bar{\Phi}^{p(0)}_{12}$	$\bar{\Phi}^{p(0)}_{13}$	$\bar{\Phi}^{p(0)}_{23}$
H1	-3.62	$-3.19 \cdot 10^{1}$	-5.27	$-6.42 \cdot 10^{2}$	$1.45 \cdot 10^{2}$	$1.37 \cdot 10^{3}$
H2	$5.33 \cdot 10^{-1}$	-8.48	-2.09	$-3.44 \cdot 10^{2}$	$7.77 \cdot 10^{1}$	$-2.36 \cdot 10^{2}$
H3	1.85	6.74	$-4.77 \cdot 10^{-1}$	$-3.77 \cdot 10^{2}$	$6.41 \cdot 10^{1}$	$-8.65 \cdot 10^{2}$
H4	$-4.49 \cdot 10^{1}$	$-2.43 \cdot 10^{2}$	$-2.35 \cdot 10^{1}$	$-9.13 \cdot 10^{2}$	$9.19 \cdot 10^{1}$	$9.21 \cdot 10^{3}$
H5	$-1.08 \cdot 10^{1}$	$-1.11 \cdot 10^{2}$	-6.23	$5.72 \cdot 10^{2}$	$-9.18 \cdot 10^{1}$	$5.63 \cdot 10^{2}$
H6	-8.60	$-4.35 \cdot 10^{1}$	$-6.49 \cdot 10^{-1}$	$2.85 \cdot 10^{2}$	$-8.58 \cdot 10^{1}$	$1.44 \cdot 10^{3}$
H7	-8.92	$-1.20 \cdot 10^{1}$	3.03	$2.07 \cdot 10^{2}$	$-1.13 \cdot 10^{2}$	$1.94 \cdot 10^{3}$
H8	-9.20	$-3.24 \cdot 10^{2}$	$-2.69 \cdot 10^{1}$	$1.56 \cdot 10^{3}$	$-7.90 \cdot 10^{1}$	$-5.93 \cdot 10^{3}$
H9	$2.34 \cdot 10^{1}$	$2.22 \cdot 10^{1}$	$6.95 \cdot 10^{-1}$	$7.23 \cdot 10^{2}$	$5.15 \cdot 10^{1}$	$-5.56 \cdot 10^{3}$
H10	5.29	$-2.78 \cdot 10^{1}$	-3.60	$3.01 \cdot 10^{2}$	8.17	$-2.51 \cdot 10^{3}$
H11	-1.12	$-6.90 \cdot 10^{1}$	-8.01	$1.73 \cdot 10^{2}$	4.20	$-2.34 \cdot 10^{3}$
H12	$6.77 \cdot 10^{1}$	$1.79 \cdot 10^{2}$	$1.94 \cdot 10^{1}$	$1.60 \cdot 10^{3}$	$1.64 \cdot 10^{2}$	$-1.10 \cdot 10^{4}$
H13	$-5.69 \cdot 10^{1}$	$-1.49 \cdot 10^{2}$	$-2.93 \cdot 10^{1}$	$-1.66 \cdot 10^{3}$	$-4.28 \cdot 10^{2}$	$-6.76 \cdot 10^{3}$
H14	$-2.08 \cdot 10^{1}$	5.35	$-6.40 \cdot 10^{-1}$	$-3.17 \cdot 10^{2}$	$-2.05 \cdot 10^{2}$	$1.84 \cdot 10^{3}$
H15	$-1.99 \cdot 10^{1}$	9.37	1.64	$-1.21 \cdot 10^{2}$	$-1.81 \cdot 10^{2}$	$4.22 \cdot 10^{3}$
H16	$-3.32 \cdot 10^{1}$	$-1.25 \cdot 10^{1}$	$6.11 \cdot 10^{-1}$	$-2.17 \cdot 10^{2}$	$-2.11 \cdot 10^{2}$	$9.04 \cdot 10^{3}$
H17	$-2.87 \cdot 10^{1}$	$-5.67 \cdot 10^{1}$	-4.83	$-4.58 \cdot 10^{2}$	$-4.62 \cdot 10^{1}$	$8.56 \cdot 10^{3}$
H18	$-1.46 \cdot 10^{1}$	$-2.96 \cdot 10^{2}$	$-4.60 \cdot 10^{1}$	$-4.42 \cdot 10^{3}$	$9.01 \cdot 10^{2}$	$-5.90 \cdot 10^{3}$
H19	-4.74	$-1.04 \cdot 10^{1}$	-1.95	$-3.33 \cdot 10^{2}$	$5.98 \cdot 10^{1}$	$2.18 \cdot 10^{3}$
H20	$-1.19 \cdot 10^{1}$	$-5.82 \cdot 10^{1}$	-5.62	$-2.52 \cdot 10^{2}$	$2.23 \cdot 10^{1}$	$2.71 \cdot 10^{3}$
H21	-3.85	$-2.72 \cdot 10^{1}$	-3.29	$-2.30 \cdot 10^{2}$	$4.61 \cdot 10^{1}$	$8.18 \cdot 10^{2}$
H22	-3.80	$-6.26 \cdot 10^{1}$	-9.15	$-7.70 \cdot 10^{2}$	$1.56 \cdot 10^{2}$	$-9.99 \cdot 10^{2}$
H23	$8.93 \cdot 10^{-1}$	-4.11	-1.68	$-3.50 \cdot 10^{2}$	$8.36 \cdot 10^{1}$	$1.54 \cdot 10^{1}$
H24	4.75	$2.43 \cdot 10^{1}$	$4.23 \cdot 10^{-1}$	$-4.94 \cdot 10^{2}$	$1.34 \cdot 10^{2}$	$4.13 \cdot 10^{2}$
H25	$-1.30 \cdot 10^{1}$	$-1.38 \cdot 10^{2}$	$-1.38 \cdot 10^{1}$	$-6.51 \cdot 10^{1}$	$2.38 \cdot 10^{1}$	$-2.75 \cdot 10^{2}$
H26	$-2.25 \cdot 10^{1}$	$-1.80 \cdot 10^{2}$	$-1.67 \cdot 10^{1}$	$-1.49 \cdot 10^{2}$	$1.44 \cdot 10^{1}$	$2.08 \cdot 10^{3}$
H27	$-1.09 \cdot 10^{1}$	$-9.21 \cdot 10^{1}$	-8.72	$-7.17 \cdot 10^{1}$	$1.02 \cdot 10^{1}$	$7.95 \cdot 10^{2}$
H28	-4.11	$-4.14 \cdot 10^{1}$	-4.60	$-1.49 \cdot 10^{2}$	$3.04 \cdot 10^{1}$	$3.01 \cdot 10^{1}$
H29	-2.86	$-3.46 \cdot 10^{1}$	-4.37	$-2.43 \cdot 10^{2}$	$4.91 \cdot 10^{1}$	$-2.40 \cdot 10^{2}$
H30	-5.25	$-6.08 \cdot 10^{1}$	-6.89	$-1.77 \cdot 10^{2}$	$3.61 \cdot 10^{1}$	$-4.92 \cdot 10^{2}$

TABLE SI-CXX: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for hydrogen atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{03}$	$\bar{\Phi}^{p(0)}_{12}$	$\bar{\Phi}^{p(0)}_{13}$	$\bar{\Phi}^{p(0)}_{23}$
C1	$-1.13 \cdot 10^{1}$	$-1.77 \cdot 10^{2}$	$-3.23 \cdot 10^{1}$	$-4.27 \cdot 10^{3}$	$9.89 \cdot 10^{2}$	$4.45 \cdot 10^{3}$
C2	3.23	$-3.41 \cdot 10^{1}$	-9.32	$-1.64 \cdot 10^{3}$	$3.74 \cdot 10^{2}$	$-9.59 \cdot 10^{2}$
C3	$-5.29 \cdot 10^{-1}$	$-2.60 \cdot 10^{1}$	-5.37	$-7.85 \cdot 10^{2}$	$1.83 \cdot 10^{2}$	$3.34 \cdot 10^{2}$
C4	1.28	-8.72	-2.67	$-4.98 \cdot 10^{2}$	$1.12 \cdot 10^{2}$	$-4.63 \cdot 10^{2}$
C5	2.66	4.50	-1.34	$-5.40 \cdot 10^{2}$	$1.03 \cdot 10^{2}$	$-1.11 \cdot 10^{3}$
C6	$-7.62 \cdot 10^{1}$	$-3.79 \cdot 10^{2}$	$-3.83 \cdot 10^{1}$	$-1.98 \cdot 10^{3}$	$2.37 \cdot 10^{2}$	$1.79 \cdot 10^{4}$
C7	$-1.66 \cdot 10^{2}$	$-4.69 \cdot 10^{2}$	$-3.50 \cdot 10^{1}$	$-1.55 \cdot 10^{3}$	$-4.45 \cdot 10^{2}$	$4.21 \cdot 10^{4}$
C8	$-7.20 \cdot 10^{1}$	$-1.78 \cdot 10^{2}$	-9.31	$-1.62 \cdot 10^{2}$	$-3.65 \cdot 10^{2}$	$1.69 \cdot 10^{4}$
C9	$-1.45 \cdot 10^{1}$	$-4.98 \cdot 10^{2}$	$-1.52 \cdot 10^{1}$	$4.87 \cdot 10^{3}$	$-5.36 \cdot 10^{2}$	$-4.91 \cdot 10^{3}$
C10	$-2.18 \cdot 10^{1}$	$-1.72 \cdot 10^{2}$	-1.68	$1.52 \cdot 10^{3}$	$-3.04 \cdot 10^{2}$	$2.77 \cdot 10^{3}$
C11	$-1.36 \cdot 10^{1}$	$-1.11 \cdot 10^{2}$	-4.36	$6.90 \cdot 10^{2}$	$-1.36 \cdot 10^{2}$	$1.42 \cdot 10^{3}$
C12	$-1.14 \cdot 10^{1}$	$-5.73 \cdot 10^{1}$	$-3.38 \cdot 10^{-1}$	$4.22 \cdot 10^{2}$	$-1.23 \cdot 10^{2}$	$1.93 \cdot 10^{3}$
C13	$-1.20 \cdot 10^{1}$	$-2.82 \cdot 10^{1}$	3.26	$3.59 \cdot 10^{2}$	$-1.52 \cdot 10^{2}$	$2.53 \cdot 10^{3}$
C14	-4.33	$-5.58 \cdot 10^{2}$	$-4.60 \cdot 10^{1}$	$3.18 \cdot 10^{3}$	$-1.30 \cdot 10^{2}$	$-1.33 \cdot 10^{4}$
C15	$1.35 \cdot 10^{1}$	$-6.56 \cdot 10^{2}$	$-7.51 \cdot 10^{1}$	$2.88 \cdot 10^{3}$	$3.73 \cdot 10^{1}$	$-2.78 \cdot 10^{4}$
C16	$-6.75 \cdot 10^{-1}$	$-2.20 \cdot 10^{2}$	$-2.85 \cdot 10^{1}$	$5.61 \cdot 10^{2}$	8.10	$-9.77 \cdot 10^{3}$
C17	$9.07 \cdot 10^{1}$	$-2.04 \cdot 10^{2}$	$-1.98 \cdot 10^{1}$	$4.59 \cdot 10^{3}$	$1.14 \cdot 10^{2}$	$-2.94 \cdot 10^{4}$
C18	$2.25 \cdot 10^{1}$	$-1.63 \cdot 10^{2}$	$-1.88 \cdot 10^{1}$	$1.53 \cdot 10^{3}$	$2.97 \cdot 10^{1}$	$-1.17 \cdot 10^{4}$
C19	$1.84 \cdot 10^{1}$	$-3.11 \cdot 10^{1}$	-4.75	$7.95 \cdot 10^{2}$	$3.20 \cdot 10^{1}$	$-6.14 \cdot 10^{3}$
C20	6.31	$-4.78 \cdot 10^{1}$	-5.93	$4.16 \cdot 10^{2}$	9.40	$-3.53 \cdot 10^{3}$
C21	$5.32 \cdot 10^{-1}$	$-8.73 \cdot 10^{1}$	$-1.01 \cdot 10^{1}$	$3.18 \cdot 10^{2}$	4.82	$-3.44 \cdot 10^{3}$
C22	$1.21 \cdot 10^{2}$	$2.90 \cdot 10^{2}$	$3.41 \cdot 10^{1}$	$3.18 \cdot 10^{3}$	$2.58 \cdot 10^{2}$	$-2.04 \cdot 10^{4}$
C23	$1.73 \cdot 10^{2}$	$7.23 \cdot 10^{2}$	$8.58 \cdot 10^{1}$	$2.50 \cdot 10^{3}$	$4.46 \cdot 10^{2}$	$-2.03 \cdot 10^{4}$
C24	$5.86 \cdot 10^{1}$	$2.99 \cdot 10^{2}$	$3.44 \cdot 10^{1}$	$3.01 \cdot 10^{2}$	$1.89 \cdot 10^{2}$	$-5.92 \cdot 10^{3}$
C25	$-7.90 \cdot 10^{1}$	$2.70 \cdot 10^{1}$	-5.31	$-1.13 \cdot 10^{3}$	$-8.05 \cdot 10^{2}$	$6.34 \cdot 10^{3}$
C26	$-3.54 \cdot 10^{1}$	$2.13 \cdot 10^{1}$	1.17	$-3.79 \cdot 10^{2}$	$-3.53 \cdot 10^{2}$	$4.97 \cdot 10^{3}$
C27	$-3.19 \cdot 10^{1}$	$1.73 \cdot 10^{1}$	2.65	$-1.99 \cdot 10^{2}$	$-2.89 \cdot 10^{2}$	$6.80 \cdot 10^{3}$
C28	$-4.80 \cdot 10^{1}$	3.86	2.68	$-2.85 \cdot 10^{2}$	$-3.54 \cdot 10^{2}$	$1.25 \cdot 10^{4}$
C29	$-1.24 \cdot 10^{2}$	$1.71 \cdot 10^{1}$	6.01	$-9.46 \cdot 10^{2}$	$-8.17 \cdot 10^{2}$	$3.49 \cdot 10^{4}$
C30	$-9.63 \cdot 10^{1}$	$-1.38 \cdot 10^{2}$	$-1.35 \cdot 10^{1}$	$-1.95 \cdot 10^{3}$	$-8.40 \cdot 10^{1}$	$3.17 \cdot 10^{4}$
C31	$-3.63 \cdot 10^{1}$	$-8.76 \cdot 10^{1}$	-8.83	$-8.56 \cdot 10^{2}$	$2.90 \cdot 10^{1}$	$1.14 \cdot 10^{4}$
C32	$-1.75 \cdot 10^{1}$	$-7.57 \cdot 10^{1}$	-9.18	$-8.27 \cdot 10^{2}$	$1.39 \cdot 10^{2}$	$5.46 \cdot 10^{3}$
C33	$-1.55 \cdot 10^{1}$	$-1.26 \cdot 10^{2}$	$-1.65 \cdot 10^{1}$	$-1.36 \cdot 10^{3}$	$2.90 \cdot 10^{2}$	$3.35 \cdot 10^{3}$
C34	$-3.13 \cdot 10^{1}$	$-3.13 \cdot 10^{2}$	$-4.39 \cdot 10^{1}$	$-3.95 \cdot 10^{3}$	$8.70 \cdot 10^{2}$	$5.63 \cdot 10^{3}$
C35	-9.10	$-4.23 \cdot 10^{1}$	-4.88	$-3.82 \cdot 10^{2}$	$6.21 \cdot 10^{1}$	$2.59 \cdot 10^{3}$
C36	-5.33	$-3.84 \cdot 10^{1}$	-4.70	$-3.38 \cdot 10^{2}$	$6.87 \cdot 10^{1}$	$1.14 \cdot 10^{3}$
C37	-5.72	$-6.88 \cdot 10^{1}$	-9.40	$-7.44 \cdot 10^{2}$	$1.61 \cdot 10^{2}$	$2.22 \cdot 10^{2}$
C38	-8.67	$-7.96 \cdot 10^{1}$	-8.83	$-3.38 \cdot 10^{2}$	$6.76 \cdot 10^{1}$	$5.45 \cdot 10^{2}$
C39	$3.80 \cdot 10^{-1}$	-7.62	-2.42	$-4.65 \cdot 10^{2}$	$1.12 \cdot 10^{2}$	$3.99 \cdot 10^{2}$
C40	$-1.43 \cdot 10^{1}$	$-1.28 \cdot 10^{2}$	$-1.25 \cdot 10^{1}$	$-1.46 \cdot 10^{2}$	$2.71 \cdot 10^{1}$	$7.76 \cdot 10^{2}$
C41	-4.75	$-5.11 \cdot 10^{1}$	-5.88	$-2.14 \cdot 10^{2}$	$4.35 \cdot 10^{1}$	$-1.40 \cdot 10^{2}$

TABLE SI-CXXI: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for carbon atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

Atom	$\bar{\Phi}^{p(0)}_{01}$	$\bar{\Phi}^{p(0)}_{02}$	$\bar{\Phi}^{p(0)}_{03}$	$\bar{\Phi}^{p(0)}_{12}$	$\bar{\Phi}^{p(0)}_{13}$	$\bar{\Phi}^{p(0)}_{23}$
O1	$1.48 \cdot 10^{2}$	$5.98 \cdot 10^{2}$	$1.35 \cdot 10^{1}$	$-1.30 \cdot 10^{4}$	$3.21 \cdot 10^{3}$	$-1.67 \cdot 10^{4}$
O2	$-4.58 \cdot 10^{2}$	$-5.08 \cdot 10^{2}$	$-1.60 \cdot 10^{1}$	$-2.65 \cdot 10^{3}$	$-2.58 \cdot 10^{3}$	$1.21 \cdot 10^{5}$
O3	$6.43 \cdot 10^{1}$	$-1.20 \cdot 10^{2}$	$9.60 \cdot 10^{1}$	$1.19 \cdot 10^{4}$	$-1.51 \cdot 10^{3}$	$-8.94 \cdot 10^{3}$
O4	$1.94 \cdot 10^{1}$	$-1.17 \cdot 10^{3}$	$-1.76 \cdot 10^{2}$	$3.48 \cdot 10^{3}$	$-1.07 \cdot 10^{2}$	$-7.14 \cdot 10^{4}$
O5	$6.07 \cdot 10^{1}$	$-1.84 \cdot 10^{3}$	$-1.94 \cdot 10^{2}$	$1.02 \cdot 10^{4}$	$4.17 \cdot 10^{1}$	$-7.69 \cdot 10^{4}$
O6	$3.56 \cdot 10^{2}$	$2.01 \cdot 10^{3}$	$2.45 \cdot 10^{2}$	$1.43 \cdot 10^{3}$	$9.21 \cdot 10^{2}$	$-3.41 \cdot 10^{4}$
N1	$-2.30 \cdot 10^{2}$	$3.15 \cdot 10^{2}$	$2.36 \cdot 10^{1}$	$-1.79 \cdot 10^{3}$	$-2.19 \cdot 10^{3}$	$5.24 \cdot 10^{4}$
N2	$-1.44 \cdot 10^{2}$	$-5.25 \cdot 10^{2}$	$-6.85 \cdot 10^{1}$	$-7.41 \cdot 10^{3}$	$1.25 \cdot 10^{3}$	$5.01 \cdot 10^{4}$
F1	$-3.99 \cdot 10^{1}$	$-1.41 \cdot 10^{2}$	-9.33	$-8.84 \cdot 10^{1}$	$-1.56 \cdot 10^{2}$	$8.70 \cdot 10^{3}$
F2	$-4.08 \cdot 10^{1}$	$-2.70 \cdot 10^{1}$	$-3.07 \cdot 10^{-1}$	$-2.90 \cdot 10^{2}$	$-2.34 \cdot 10^{2}$	$1.13 \cdot 10^{4}$
F3	$-6.73 \cdot 10^{1}$	$-1.72 \cdot 10^{2}$	-4.25	$3.58 \cdot 10^{2}$	$-4.76 \cdot 10^{2}$	$1.41 \cdot 10^{4}$
F4	$1.90 \cdot 10^{1}$	$1.42 \cdot 10^{2}$	$2.11 \cdot 10^{1}$	$2.55 \cdot 10^{2}$	$-3.62 \cdot 10^{1}$	$-1.31 \cdot 10^{3}$
F5	$3.81 \cdot 10^{1}$	$1.72 \cdot 10^{2}$	$1.90 \cdot 10^{1}$	$3.42 \cdot 10^{2}$	$1.27 \cdot 10^{2}$	$-4.18 \cdot 10^{3}$
F6	$4.81 \cdot 10^{1}$	$2.68 \cdot 10^{2}$	$2.66 \cdot 10^{1}$	$-5.48 \cdot 10^{2}$	$2.79 \cdot 10^{2}$	$-4.49 \cdot 10^{3}$
F7	4.71	$-7.18 \cdot 10^{1}$	$-1.44 \cdot 10^{1}$	$3.42 \cdot 10^{2}$	$-3.09 \cdot 10^{1}$	$-7.09 \cdot 10^{3}$
F8	$4.60 \cdot 10^{-1}$	$-1.39 \cdot 10^{2}$	$-1.61 \cdot 10^{1}$	$4.83 \cdot 10^{2}$	7.71	$-5.39 \cdot 10^{3}$
F9	$-1.25 \cdot 10^{1}$	$-2.05 \cdot 10^{2}$	$-2.59 \cdot 10^{1}$	$-1.96 \cdot 10^{2}$	$2.85 \cdot 10^{1}$	$-6.12 \cdot 10^{3}$
S1	5.49	$2.24 \cdot 10^{1}$	-1.16	$-1.14 \cdot 10^{3}$	$1.88 \cdot 10^{2}$	$-2.64 \cdot 10^{3}$
S2	$-2.07 \cdot 10^{1}$	$-2.15 \cdot 10^{1}$	$1.09 \cdot 10^{1}$	$7.19 \cdot 10^{2}$	$-3.18 \cdot 10^{2}$	$4.78 \cdot 10^{3}$
S3	-7.23	$-2.37 \cdot 10^{2}$	$-2.63 \cdot 10^{1}$	$5.00 \cdot 10^{2}$	$1.42 \cdot 10^{1}$	$-6.53 \cdot 10^{3}$

TABLE SI-CXXII: Values of the KD–dependent components of $\bar{\Phi}^{p(0)}$ (expressed in ppm au) for the other atoms of complex **10**. Subscripts in the Table header represent the KD for which the contribution is computed, with 0 representing the ground KD and higher numbers the corresponding excited KD.

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