## Photophysics of Phenalenone: Quantum-mechanical Investigation of Singlet-Triplet Intersystem Crossing

(Electronic Supplementary Information)

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### I ADIABATIC ELECTRONIC ENERGIES OF PHENALENONE



Figure S1: State energies (DFT/MRCI/TZVP, [eV]) computed at the optimized geometries of the  $S_0$ - $S_3$  and  $T_1$ - $T_3$  states of phenalenone. All energies are given relative to the ground state energy at  $S_0$  geometry. Zero-point vibrational energy corrected values are given in square brackets.

In figure S1 the complete set of calculated adiabatic electronic energies of phenalenone is shown. In addition to the data discussed in the paper this figure contains energies calculated at the optimized geometries of the higher excited states  $S_3$  and  $T_3$  which can briefly be characterized as follows.

The nuclear configuration obtained for  $S_3$  shows an elongation of the C1a-C3b, and C2-C3, C7-C8, C3a-C3, and C3b-C6a bonds by 5, 4, 4, and 3 pm, respectively, and a shortening of the C1-C2, C3-C3a, and C6a-C7 bonds by 4, 3, and 3 pm, respectively. Its adiabatic excitation energy is 3.59 eV, and thus 0.03 eV lower than its vertical excitation energy at the ground state geometry. At the TD-B3LYP level the relaxation energy of this state amounts to 0.26 eV.

The minimum molecular structure obtained for  $T_3$  exhibits an elongation of the C2-C3, C9-C1a, C1a-C3b, and C7-C8 bonds by 7, 5, 3, and 3 pm, respectively, and a shortening of the C3-C3b and C8-C9 bonds by 3 pm in each case. Its adiabatic excitation energy is 3.03 eV, and thus 0.2 eV lower than its vertical excitation energy at the ground state structure.

# II IMPACT OF USER DEFINED PARAMETERS ON INTERSYSTEM CROSSING RATES

As we have shown in the main paper, we obtain intersystem crossing rates  $k_{ISC}$  from an approximation to Fermi's golden rule expression:

$$k_{ISC}(i \to f) = \frac{\pi}{\hbar \eta} \sum_{\mathbf{v}'; |E_{f,\mathbf{v}'}-E_{i,\mathbf{q}}| \le \eta} \left| \left\langle \mathbf{0} \right| \left\langle i \right| \hat{H}_{SO} |f\rangle_{q_0=0} + \left( \nabla_{q} \left\langle i \right| \hat{H}_{SO} |f\rangle_{q_0=0} \right) \cdot \boldsymbol{q} |\mathbf{v}'\rangle \right|^2$$
(1)

Here, i and f are the initial and final electronic states, **0** and **v**' are the vibrational wave functions of the initial and the final vibronic states  $|i, 0\rangle$  and  $|f, v'\rangle$ .

The golden rule approach assumes that at sufficiently high adiabatic energy gaps between the initial and the final vibronic state, the final vibrational levels form a quasi-continuum. In this case, the (isoenergetic) transfer to the final state is irreversible on time scales accessible to experiment. Instead of treating a strictly isoenergetic transition, an interval of final states is considered in equation 1, taking into account all final states within  $\pm \eta$  of the vibronic energy of the initial level. Naturally, the results depend on the choice of  $\eta$ . As was shown by Tatchen *et al* [1] there is no unique choice for this parameter. On the one hand,  $\eta$  should be chosen as small as possible, because the transition  $i \rightarrow f$  should be isoenergetic. On the other hand,  $\eta$  should be chosen large enough to cover a sufficient number of acceptor states. We therefore tested a number of different  $\eta$  values to find a value that is as small as possible, while still yielding numerically stable and therefore meaningful results (see section II.A).

Another question concerns the number of vibrational acceptor modes taken into account in the summation in equation 1. In the case of undistorted phenalenone, only totally symmetric modes (which are necessarily in-plane-modes) contribute to the ISC rate. When vibronic spin-orbit coupling is taken into account, the symmetry of the molecule is lost and out-of-plane modes have to be treated as active, too. Unfortunately, these modes typically show rather low vibrational frequencies causing a drastic increase in the number of modes that have to be treated. In principle this problem could be solved by lowering the search interval  $\eta$ . However, if the search interval is chosen very small, the results become less numerically stable, i. e. they depend more sensitively on the energy gap between the initial and the final state. We therefore used a relatively large search interval in these calculations and made the calculations feasible by allowing only a limited number of vibrational excitations for the out-of-plane modes. This strategy has been successfully applied before [1,2,3] and introduces only minor errors as is confirmed by our test calculations shown in section II.B.

Finally, the intersystem crossing rates depend on the acceptor vibrational states within the search interval, which depend on the energy gap between the initial and the final vibronic state (energy gap rule). We therefore also examined the effect of varying the energy difference between the initial and the final state. This is especially important with regard to the uncertainties of our calculated energy gap between the initial and the final state. From the experimental data of Okutsu et al [4] and of Flors and Nonell [5] one obtains an S<sub>1</sub>-T<sub>1</sub> gap of 0.73 eV, while we calculated a gap of 0.45 eV (0.46 eV for the distance between the lowest vibronic levels). We therefore examined the sensitivity of our results with respect to variations of the S<sub>1</sub>-T<sub>1</sub> energy gap (see section II.C).

#### II.A Effect of the Interval Width $\eta$

In order to explore the effect of the interval width  $\eta$  on the calculated intersystem crossing rates we performed an extensive scan for the channel  $S_1 \rightarrow T_{1x}$ , using  $\eta$  values between 0.01 and 100 cm<sup>-1</sup>. Only inplane vibrational modes were taken into account as acceptor modes for this channel. As shown in table S1, basically identical results are obtained using  $\eta$  values between  $\approx 0.5$  and 10 cm<sup>-1</sup>. The number of acceptor levels is still relatively small, however, with  $\eta$  values of 0.5 and 1 cm<sup>-1</sup>. This results in low numerical stability with respect to variations of the S<sub>1</sub>-T<sub>1</sub> energy gap (see section II.C). With an  $\eta$  value of 5 cm<sup>-1</sup>, which yields more stable results, the number of acceptor levels is in the order of 10<sup>3</sup>.

In a less extensive scan we tested the effect of  $\eta$  on the ISC rates of the channel  $S_1 \rightarrow T_{1z}$  (lower part of table S1). Here, the ISC rates were calculated using the Herzberg-Teller approximation and in addition to in-plane vibrational modes, out-of-plane modes were taken into account as acceptor modes (with a max-

imum number of one vibrational excitation per mode). This increases the number of acceptor modes by several orders of magnitude. As for the  $S_1 \rightarrow T_{1x}$  channel, with  $\eta$  values between 0.5 and 10 cm<sup>-1</sup> the calculated intersystem crossing rates are basically identical.

channel		parameters &	results			
i→f	ΔE <sup>ad</sup> [eV]		vibr. SO # derivs.	interval η [cm <sup>-1</sup> ]	acceptors #v'	rate k <sub>ISC</sub> [s <sup>-1</sup> ]
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.01	2	8.56x10 <sup>6</sup>
$S_1 {\rightarrow} T_{1x}$	0.45	42.7	0	0.02	4	3.40x10 <sup>11</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.03	5	2.27x10 <sup>11</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.04	7	$1.70 x 10^{11}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.05	13	1.36x10 <sup>11</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.06	15	$1.18 \times 10^{11}$
$S_1 {\rightarrow} T_{1x}$	0.45	42.7	0	0.07	17	$1.01 \times 10^{11}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.08	18	8.86x10 <sup>10</sup>
$S_1 {\rightarrow} T_{1x}$	0.45	42.7	0	0.09	22	7.88x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.1	25	$7.09 x 10^{10}$
$S_1 {\rightarrow} T_{1x}$	0.45	42.7	0	0.2	52	3.62x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.3	76	$2.44 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.4	98	$1.84 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.5	122	$1.56 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.6	144	$1.34 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.7	163	$1.17 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.8	191	$1.04 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	0.9	213	9.34x10 <sup>9</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	1	235	8.56x10 <sup>9</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	2	497	$1.73 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	3	727	$2.24 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	4	991	2.05x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	5	$1.26 \times 10^{3}$	2.26x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	6	$1.49 \times 10^{3}$	$1.98 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	7	$1.77 \times 10^{3}$	$1.75 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	8	$2.02 \times 10^3$	$1.58 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	9	$2.25 \times 10^3$	$1.54 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	10	$2.51 \times 10^{3}$	3.32x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	15	$3.80 \times 10^3$	$4.44 x 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	20	$5.02 \times 10^3$	3.79x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	30	$7.53 \times 10^{3}$	5.68x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	40	$1.00 \times 10^4$	6.22x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	50	$1.25 \times 10^4$	5.96x10 <sup>10</sup>
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	60	$1.51 \times 10^{4}$	$5.24 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	70	$1.76 \times 10^4$	5.36x10 <sup>10</sup>
$S_1 {\rightarrow} T_{1x}$	0.45	42.7	0	80	2.01x10 <sup>4</sup>	$4.97 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	90	$2.27 \times 10^4$	$4.61 \times 10^{10}$
$S_1 \rightarrow T_{1x}$	0.45	42.7	0	100	$2.52 \times 10^4$	$4.55 \times 10^{10}$

channel		parameters &	results			
i→f	ΔE <sup>ad</sup> [eV]		vibr. SO # derivs.	interval η [cm <sup>-1</sup> ]	acceptors #v'	rate k <sub>ISC</sub> [s <sup>-1</sup> ]
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	0.5	$1.34 x 10^4$	7.93x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	$2.69 \times 10^4$	1.11x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	5	1.34x10 <sup>5</sup>	1.81x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	10	2.69x10 <sup>5</sup>	1.48x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	20	5.37x10 <sup>5</sup>	1.36x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	30	8.06x10 <sup>5</sup>	$1.44 x 10^8$
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	40	$1.08 \times 10^{6}$	1.43x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	50	$1.35 \times 10^{6}$	1.36x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	100	$2.72 \times 10^{6}$	1.60x10 <sup>8</sup>

Table S1: Calculated rate constants  $k_{ISC}$  for the channels  $S_1 \rightarrow T_{Ix}$  and  $S_1 \rightarrow T_{Iz}$ . Remaining columns: adiabatic electronic energy difference  $\Delta E^{ad}$ , direct SOME  $|\langle i|\hat{H}_{SO}|f\rangle|$ , number of derivatives with respect to out-of-plane modes (only included with a maximum excitation of one), width of the search interval 2  $\eta$  and number of accepting modes within the search interval.

#### II.B Maximum Excitation Degree for Out-of-Plane Modes

The restriction of out-of-plane vibrational functions to an excitation level of one seems to be very restrictive. Tatchen et al, however have shown that it is possible to obtain converged results with this approximation [1]. We performed similar test calculations, varying the number of maximally allowed outof-plane excitations within a computationally feasible range. For in-plane modes arbitrary excitations were allowed for. All 41 in-plane and 19 out-of-plane modes were taken into account in these calculations. To reduce the computational demands we used a relatively small search interval  $\eta$  of 1 cm<sup>-1</sup>. Derivatives of SOMEs along all out-of-plane modes were included in these calculations.

channel		param	results				
i→f	ΔE <sup>ad</sup> [eV]	$\begin{array}{c} \text{direct SO} \\ \left  \left\langle  i \right  \hat{H}_{SO} \right  f \left. \right\rangle \right   \left[ \text{cm}^{-1} \right. \\ \left. \right] \end{array}$	vibr. SO # derivs.	interval η [cm <sup>-1</sup> ]	max. oop excitation	acceptors #v'	rate k <sub>ISC</sub> [s <sup>-1</sup> ]
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	1	2.69x10 <sup>4</sup>	1.1164x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	2	9.14x10 <sup>4</sup>	1.1281x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	3	1.52x10 <sup>5</sup>	1.1314x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	4	1.97x10 <sup>5</sup>	1.1315x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	5	2.27x10 <sup>5</sup>	1.1315x10 <sup>8</sup>

Table S2: Calculated rate constants  $k_{ISC}$  for the channels  $S_1 \rightarrow T_{1z}$ . Remaining columns: adiabatic electronic energy difference  $\Delta E^{ad}$ , direct SOME  $|\langle i|\hat{H}_{SO}|f\rangle|$ , number of derivatives with respect to out-of-plane modes, width of the search interval 2  $\eta$ , maximum excitation level for out-of-plane vibrational modes and number of accepting modes within the search interval.

The results in table S2 show that already with a maximum excitation level of one, practically converged results can be obtained. Increasing the excitation level to at most 5 per out-of-plane mode increases the computation time by a factor of  $\approx 25$ , while changing the calculated ISC rates by only about 1 %.

#### II.C Uncertainty of the Adiabatic Energy Difference

Due to their dependence on the vibrational wave functions, our calculated ISC rates depend on the adiabatic energy difference between the involved states. The accuracy of the calculated values for this energy gap is limited by (a) inaccuracies of the (TD)DFT methods used for geometry optimization and (b) inaccuracies of the DFT/MRCI method used for calculating the electronic energies. Our calculated purely

electronic energy difference between the  $S_1$  and  $T_1$  states is 0.45 eV. Experimentally, using fluorescence data from ref. [4] and phosphorescence data from ref. [5], one obtains a significantly larger gap of 0.73 eV. It seemed therefore mandatory to examine the effect of the  $S_1$ - $T_1$  energy gap on our calculated ISC rates. Because the relevant channel is the  $S_1 \rightarrow T_{1x}$  channel, we performed a series of ISC rate calculations for this channel: we varied the adiabatic electronic energy difference over a very wide range, up to the experimentally observed energy gap of 0.73 eV. All in-plane vibrational modes were taken into account and different search intervals ( $\eta$ =0.1 to 10.0 cm<sup>-1</sup>) were applied. The results of these extensive scans are shown in figure S2.



Figure S2: Calculated intersystem crossing rates  $S_1 \rightarrow T_{1x}$  for different values of the energy gap  $S_1$ - $T_1$  and different widths of the search interval 2  $\eta$ . The energy gap is given in eV relative to our calculated value of 0.45 eV.

Generally all calculated ISC rates decrease with increasing energy gap, due to the increasing dominance of vibrational wave functions in the final state which overlap weakly with the vibrational wave function of the initial state.

The curves obtained with smaller widths of the search interval ( $\eta$ =0.5 – 1 cm<sup>-1</sup>) exhibit a high sensitivity of the calculated ISC rates with respect to the energy gap, which shows up as large jumps in the curves. Using  $\eta$  values of 5 to 10 cm<sup>-1</sup>, the curves are much smoother and exhibit an almost continuous decrease of the ISC rates with increasing energy gap. At the experimentally determined energy gap the ISC rates are about one order of magnitude smaller than at our calculated energy gap, but still of the order of 10<sup>9</sup> s<sup>-1</sup>, which is very fast.

#### **III DERIVATIVES OF SPIN-ORBIT MATRIX ELEMENTS**

Here we present details of the derivatives of the spin-orbit matrix elements used for calculation of the ISC rates via the channel  $S_1 \rightarrow T_{1z}$ . In table S3 derivatives of the spin-orbit matrix element  $\langle S_1 | \hat{H}_{SO} | T_{1z} \rangle$  along out-of-plane vibrational modes of the  $S_1$  state of phenalenone are collected. As can be seen, the largest derivative is obtained along the lowest-frequency vibrational mode, which involves a large out-of-plane movement of the carbonyl O atom. A scan along this mode, applying elongations of up to 2 in dimensionless harmonic oscillator coordinates, shows that a vibration along this mode induces significant  $n\pi^*-\pi\pi^*$  mixing.

Mode	v <sub>i</sub> /cm <sup>-1</sup>	$\partial rac{\left\langle S_{1} \middle  \hat{H}_{SO} \middle  T_{1z} \right\rangle}{\partial q_{i}}$	Mode	<b>v</b> <sub>i</sub> /cm <sup>-1</sup>	$\partial rac{\left\langle S_{1} \middle  \hat{H}_{SO} \middle  T_{1z}  ight angle}{\partial q_{i}}$	
1	105	2.11	25	867	0.22	¥¥.
6	352	-1.45	17	621	-0.18	
15	560	-1.29	18	680	-0.17	
4	226	1.20	9	460	-0.12	
21	781	0.66	20	751	0.12	
2	163	-0.49	27	892	0.12	
12	509	-0.40	26	878	0.10	
22	803	0.38	29	976	0.07	
3	202	-0.28	28	966	-0.05	
10	470	0.25				

*Table S3: Derivatives of SOMEs*  $\langle S_1 | \hat{H}_{SO} | T_{1z} \rangle$  along out-of-plane vibrational modes of the  $S_1$  state. Derivatives are sorted in decreasing order.

To test the effect of the different derivatives in table S3 on the total ISC rate, we have performed ISC rate calculations including an increasing number of derivatives in the Herzberg-Teller expansion, starting with the largest derivatives. The results are shown in table S4 and reveal that the largest derivative accounts for the major part of the Herzberg-Teller driven ISC via the channel  $S_1 \rightarrow T_{1z}$ . Including the remaining derivatives increases the ISC rate further by a factor of  $\approx 10$  from  $2x10^7$  to  $1x10^8$  s<sup>-1</sup>.

channel	parameters & settings					results	
i->f	ΔE <sup>ad</sup> [eV]	$\begin{array}{c} \textbf{direct SO} \\ \left  \left\langle  \textbf{i} \right  \hat{\textbf{H}}_{\textbf{SO}} \right  \textbf{f}  \left. \right\rangle \right   [\textbf{cm}^{-1} \\ \textbf{j} \end{array}$	vibr. SO # derivs.	interval η [cm <sup>-1</sup> ]	max. oop excitation	acceptors #v'	rate k <sub>ISC</sub> [s <sup>-1</sup> ]
$S_1 \rightarrow T_{1z}$	0.45	0.0	0	1	1	26871	0.0
$S_1 \rightarrow T_{1z}$	0.45	0.0	1	1	1	26871	2.20x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	2	1	1	26871	3.61x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	3	1	1	26871	4.29x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	4	1	1	26871	5.71x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	5	1	1	26871	9.41x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	6	1	1	26871	9.52x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	7	1	1	26871	9.53x10 <sup>7</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	8	1	1	26871	1.21x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	9	1	1	26871	1.21x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	10	1	1	26871	1.25x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	11	1	1	26871	$1.77 \times 10^{8}$
$S_1 \rightarrow T_{1z}$	0.45	0.0	12	1	1	26871	1.79x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	13	1	1	26871	1.79x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	14	1	1	26871	1.80x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	15	1	1	26871	1.83x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	16	1	1	26871	1.56x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	17	1	1	26871	$1.42 \times 10^{8}$
$S_1 \rightarrow T_{1z}$	0.45	0.0	18	1	1	26871	1.43x10 <sup>8</sup>
$S_1 \rightarrow T_{1z}$	0.45	0.0	19	1	1	26871	$1.40 \times 10^{8}$

Table S4: Calculated rate constants  $k_{ISC}$  for the channel  $S_1 \rightarrow T_{1z}$ . Remaining columns: adiabatic electronic energy difference  $\Delta E^{ad}$ , direct SOME  $|\langle i|\hat{H}_{SO}|f\rangle|$ , number of derivatives with respect to out-of-plane modes, width of the search interval 2  $\eta$ , maximum excitation level for out-of-plane vibrational modes and number of accepting modes within the search interval. Derivatives of SOMEs were included in the order shown in table S3.

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