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Synergic photoprotection of phenolic compounds present in tomato fruit cuticle: a spectroscopic investigation in solution

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mixtures of **pca** and **nch** in ethanol at different concentrations: 0.5 (black line), 5 (red line) and 10 mM (blue line).

Fig S4. Left: theoretical UV-Vis spectra of **pca** computed at TD-B3LYP(PCM, ethanol)/def2TZVP// B3LYP (PCM,ethanol)/def2TZVP level and the assignment of its more relevant transitions (in nm). Right: Frontier orbitals of **pca** implied in the main transitions computed at B3LYP(PCM, ethanol)/def2TZVP. Red and blue display occupied orbitals and green and yellow unoccupied orbitals.

Fig S5. Left: theoretical UV-Vis spectra of **nch** computed at TD-B3LYP(PCM, ethanol)/def2TZVP//B3LYP(PCM,ethanol)/def2TZVP level and the assignment of its more relevant transitions (in nm). Right: Frontier orbitals of **nch** implied in the main transitions computed at B3LYP(PCM, ethanol)/def2TZVP. Red and blue display occupied orbitals and green and yellow unoccupied orbitals.

Fig S6. (a,b) Bond distances (in Å) and (c,d) dihedral angles from optimized DFT//B3LYP(PCM, ethanol)/def2TZVP ground state (S_0) molecular structures of **pca** and **nch**, respectively.

Fig S7. Photostability of a 1:2 mixture of **pca** and **nch** (250 μM: 500 μM) in ethanol. UV-Vis spectra were recorded at different time intervals of solar irradiation of solution. The downwards arrows represent the absorbance difference before and after two hours of irradiation. The vertical dashed line indicates the critical wavelength. Molar extinction coefficient (ε) and maximum wavelengths are pointed in the graph.

Fig S8. ^{1}H-NMR spectra of **nch** in ethanol before and after 5 h of continuous irradiation at 365 nm. Coupling constants are shown.

Fig S9. Photostability of a 1:1 mixture of **pca** and **nch** in ethanol after subtracting **nch** UV-Vis spectrum. The downwards arrow represents the absorbance difference before and after two hours of irradiation.

Fig S10. Absorbance spectra of **pca** (black line) and **nch** (blue line) and fluorescence spectrum of **pca** (red line) in ethanol.

Fig S11. Stern-Volmer plot of the **pca** quenching by increasing concentrations of **nch**, where F_0 and F are fluorescence emission intensities in absence and presence of the quencher (**nch**). At low concentrations a linear fit was reached,

corresponding the slope of the line to K_{SV} (Stern-Volmer constant). At higher concentrations, data deviates from a linear to an exponential fit.

Fig S12. Schematic representation of all the **pca**-**nch** H-bonded and π-π stacked heterodimers analysed.

Fig S13. Geometries of the most stable **pca**-**nch** π-π stacked heterodimers. Under each dimer, their respective binding energy ($E_{binding}$(X,Y)) and binding free energies ($^{\Delta G^0_f}$(X,Y)) are shown. Energy values computed at the ωB97XD(PCM, ethanol)/ def2tzvp level are in kcal/mol. The nomenclature of the dimers is shown in FigS12.

Fig S14. Geometries of the most stable **pca**-**nch** H-bonded heterodimers. Under each dimer, their respective binding energy ($E_{binding}$(X,Y)) and binding free energies ($^{\Delta G^0_f}$(X,Y)) are shown. Energy values computed at the ωB97XD(PCM, ethanol)/ def2-TZVP level are in kcal/mol. The nomenclature of the dimers is shown in FigS12.

Fig S15. Power dependence studies of absorption bands of **pca** solution in ethanol excited at 312 nm at: (a) 335 (at time delay 1.8 ns), (b) 370 (at time delay 500 fs) (c) 390 (at time delay 1.8 ns) and (d) 625 nm (at time delay 1.8 ns). (e) Power dependence study of **nch** solution in ethanol (excited at 312 nm) at 420 nm (at time delay 500 fs).

Fig S16. TAS (left) and evolutionary associated difference spectra (EADS) computed by sequential fit (right) of (a) 500 μM **nch** and (c) a 1:1 mixture (500 μM: 500 μM) of **nch** and **pca** in ethanol (excitation at 365 nm).

Fig S17. (a) Predicted TAS map for an equimolar mixture of **pca** and **nch** in ethanol calculated as manual sum of the TAS maps of their individual compounds. (b) Experimental TAS map of an equimolar **pca**-**nch** mixture in methanol.

Fig S18. Frontier orbitals selected as active space in the CASSCF calculations of the conical intersections. Red/blue and green/yellow colors are used to represent occupied and virtual orbitals, respectively.

Cartesian coordinates (optimized at the B3LYP (PCM,ethanol)/def2-TZVP level) of all the stationary points collected in the main text associated with the absorption spectra calculation.

Cartesian coordinates (optimized at the ωB97XD(PCM,ethanol)/6-31+G(d,p) level) of all the stationary points collected in the main text associated with the S_0 and S_1 surface exploration for **nch**.

Cartesian coordinates of conical intersection computed at the CASSCF(12,11)(PCM,ethanol)/6-31+G(d,p) level of theory for **nch**.

Cartesian coordinates (optimized at the ωB97XD(PCM, ethanol)/def2-TZVP level) of all the stationary points associated to **pca**-**nch** heterodimers.

Table S1. Total electronic energies (E, in a.u.), zero point correction of the energy (ZPCE), thermal corrections to Gibbs free energies (TCGFE, in a.u.), and number of imaginary frequencies (NIMAG) of **pca-nch** heterodimers computed at ωB97XD(PCM, ethanol)/def2-TZVP level.

Structure	E	ZPCE	TCGFE	NIMAG
pca	-573.494641	0.154710	0.117440	0
nch	-955.001889	0.244371	0.197790	0
H ⋯ T´ conformer 1	-1528.508651	0.400328	0.334470	0
H ⋯ T´ conformer 2	-1528.511054	0.400346	0.335270	0
$(H \cdots H' + T \cdots T')_h$	-1528.513237	0.400880	0.338055	0
$(H \cdots H' + T \cdots T')_t$	-1528.511948	0.400919	0.338412	0
T ⋯ H´	-1528.508908	0.400917	0.337365	0
$(H \cdots T' + T \cdots H')_t$	-1528.516336	0.400901	0.339185	0
$O^A \cdots H^a$	-1528.513443	0.400566	0.337440	0
$O^A \cdots H^b + T \cdots T'$	-1528.516809	0.401341	0.338339	0
$O^C \cdots H^a + T \cdots T'$	-1528.512471	0.401057	0.338735	0
$H^1 \cdots O^\alpha + O^A \cdots H^a$	-1528.510070	0.400413	0.335016	0
$H^2 \cdots O^\alpha$	-1528.516242	0.401141	0.339165	0
$H^3 \cdots O^\alpha + H^4 \cdots O^\gamma$	-1528.515111	0.401112	0.338339	0
$H^4 \cdots O^\alpha + O^B \cdots H^a$	-1528.507940	0.400997	0.334149	0
$H^3 \cdots O^\gamma + H^4 \cdots O^\alpha$	-1528.517703	0.402500	0.342243	0

Values computed at 298.15K.

Table S2. Summary of the excited state lifetimes of solutions of **nch** and a 1:1 mixture of **pca** and **nch** after excitation at 365 nm in ethanol from a sequential fit. The first row indicates the pump wavelength. Errors are given as twice the standard error extracted from the Global fitting. We note the shorter τ_3 lifetime following photoexcitation at 365 nm (cf 1.15 ns (312 nm) versus 122 ps (365 nm)). We are unable to reconcile this difference.

	λ_{pump} = **365 nm**		
	τ_1 **(fs)**	τ_2 **(ps)**	τ_3 **(ps)**
nch	710 ± 90	3.73 ± 0.09	121.61 ± 4.68
mix	490 ± 90	2.42 ± 0.09	24.53 ± 0.76

Table S3. Total electronic energies[a] (E, in a.u.), zero point correction of the energy[b] (ZPCE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of all stationary points discussed in the main text.

Structure	E	ZPCE	TCGFE	NIMAG(ν)
s-trans-S_0	-954.698990	0.244824	0.197765	0
TS-S_0	-954.621345	0.240581	0.193807	1 (-894.2612)
s-cis-S_0	-954.691730	0.245070	0.200184	0
s-trans-S_1	-954.579602	0.241671	0.195240	0
TS-S_1	-954.574585	0.240481	0.194950	1 (-211.3240)
s-cis-S_1	-954.602026	0.284390	0.237911	0

[a]Computed at ωB97XD(PCM,ethanol)/6-31+G(d,p) level of theory. [b]Computed at 298.15 K. [c] If NIMAG=1, the imaginary frequency (ν), in parenthesis, is given in cm^{-1}.

Table S4. S_0 and S_1 electronic energies (E, in a.u.) of intersection (CI) discussed in the text computed at CASSCF(12,11)(PCM,ethanol)/ cc-pVTZ.

Structure	**E S_0**	**E S_1**
CI	-949.6632309	-949.66377154

The Full Width Half Maximum (FWHM) of our instrument response provides the minimum value for lifetimes acquired through the fitting procedure. It also is a required input as an initial guess in the fitting. Solvent only scans under the same experimental conditions as the data were collected and then fitted with Equation 1.[1]

$$F_{cc} = \exp\left[-\frac{-t_d + \left(t_0(\omega)\right)^2}{\tau^2}\right] \qquad 1.$$

Here, t_d is pump-probe time delay, $t_0(\omega)$ is the temporal overlap between the pump and probe (for a given ω) and τ is the pump pulse duration (τ = 100 fs for Figure S1a, 180 fs for Figure S1b). Applying this fitting procedure takes into account the winged gaussian observed in Figure S1b which form part of the instrument response.

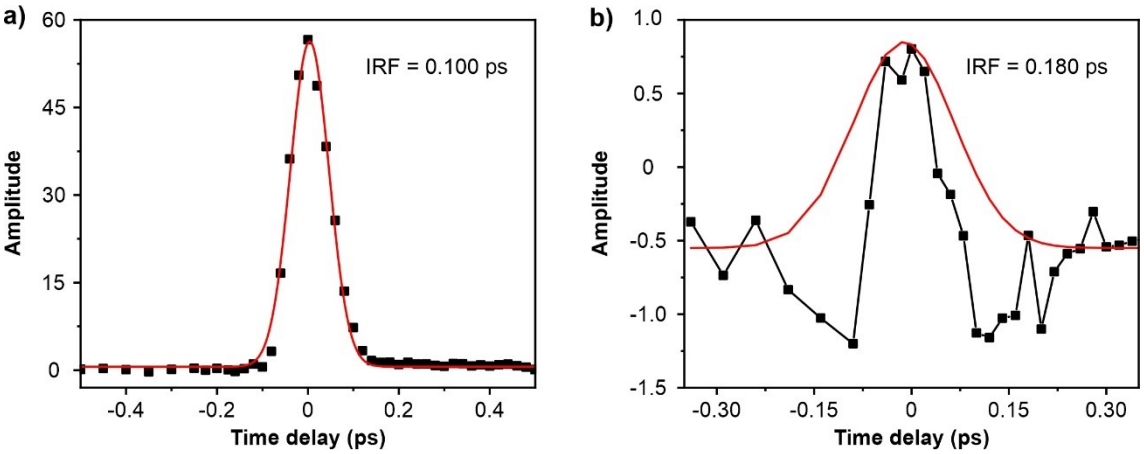


Fig S1. Solvent only transients following excitation at (a) 312 nm (integrated over 355-360 nm) (black squares) of ethanol and its curve fitting (overlaid red line). Solvent only transients following excitation at (b) 365 nm (integrated over 420-425 nm) (black squares) of ethanol and its pump-probe cross-correlation, FCC, with its curve fitting (overlaid red line). The instrument response function (IRF) corresponds to the FWHM parameter of the curve fitting.

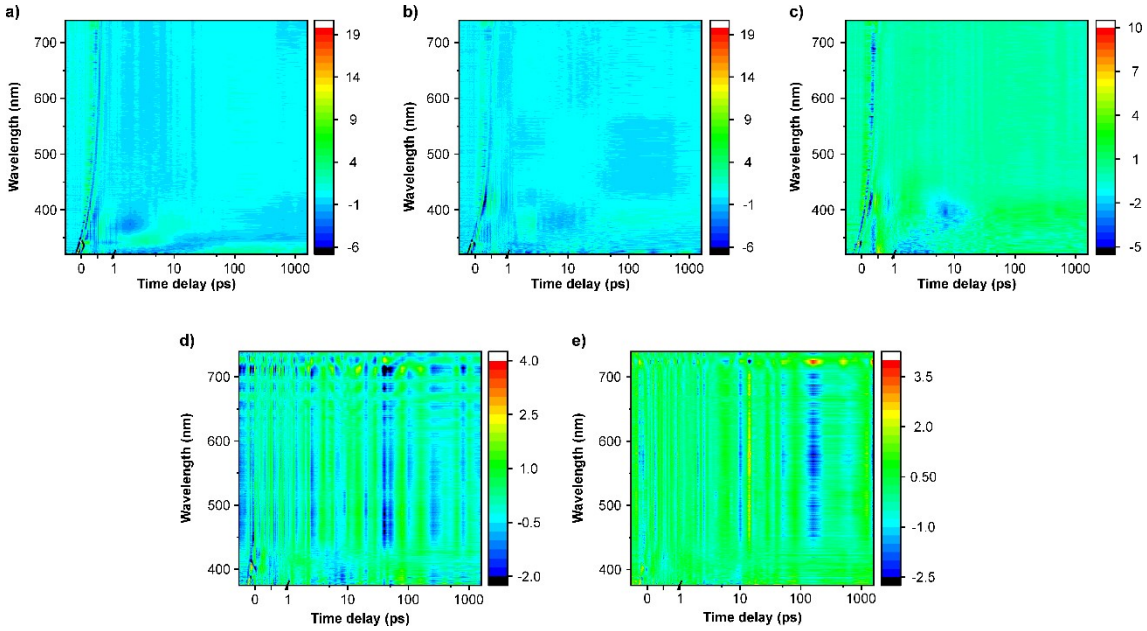


Fig S2. Residuals for (a) 500 μM **pca**, (b) 500 μM **nch** and (c) a 1:1 mixture (500 μM : 500 μM) of **nch** and **pca** in ethanol after excitation at 312 nm. Residuals for (d) 500 μM **nch** and (e) a 1:1 mixture (500 μM: 500 μM) of **nch** and **pca** in ethanol after excitation at 365 nm. Residuals have not been chirp-corrected.

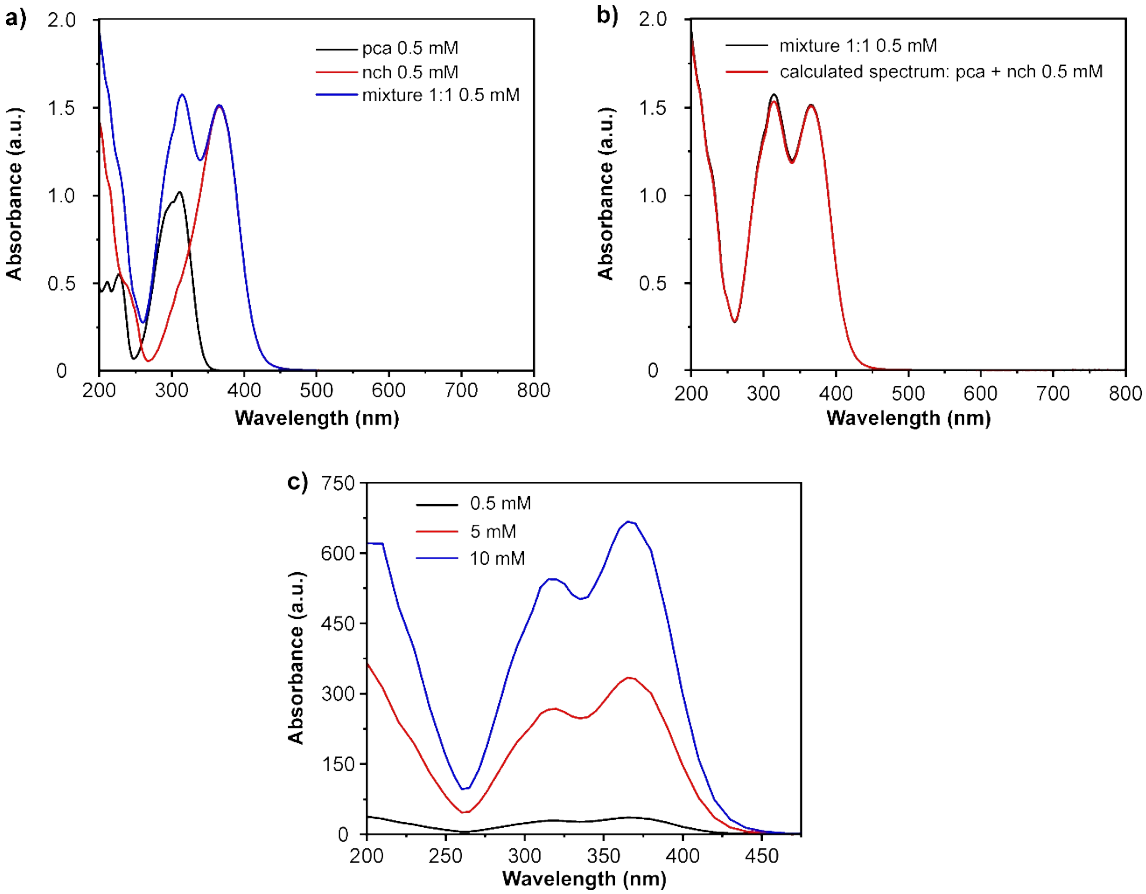


Fig S3. (a) UV-Vis spectra of **pca**, **nch** and a 1:1 mixture of both in ethanol. (b) Difference between the experimental mixture spectrum and the calculated spectrum as sum of **pca** and **nch** UV-Vis spectra. (c) UV-Vis spectra of 1:1 mixtures of **pca** and **nch** in ethanol at different concentrations: 0.5 (black line), 5 (red line) and 10 mM (blue line).

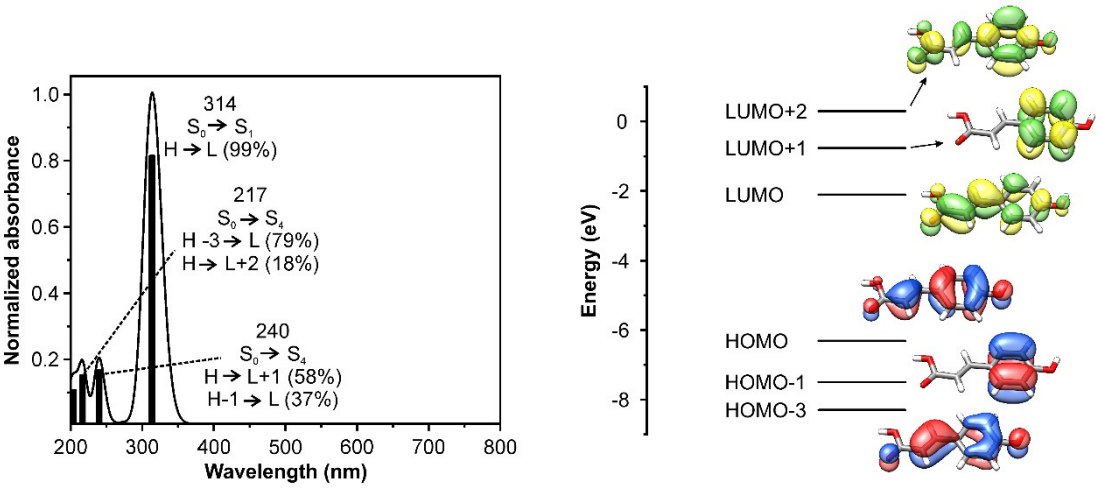


Fig S4. Left: theoretical UV-Vis spectra of **pca** computed at TD-B3LYP(PCM, ethanol)/def2TZVP// B3LYP (PCM,ethanol)/def2TZVP level and the assignment of its more relevant transitions (in nm). Right: Frontier orbitals of **pca** implied in the main transitions computed at B3LYP(PCM, ethanol)/def2TZVP. Red and blue display occupied orbitals and green and yellow unoccupied orbitals.

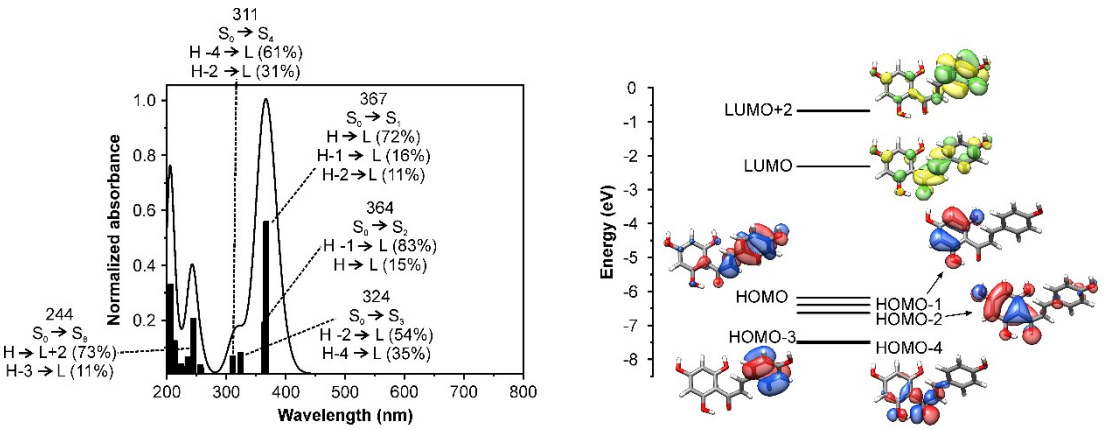
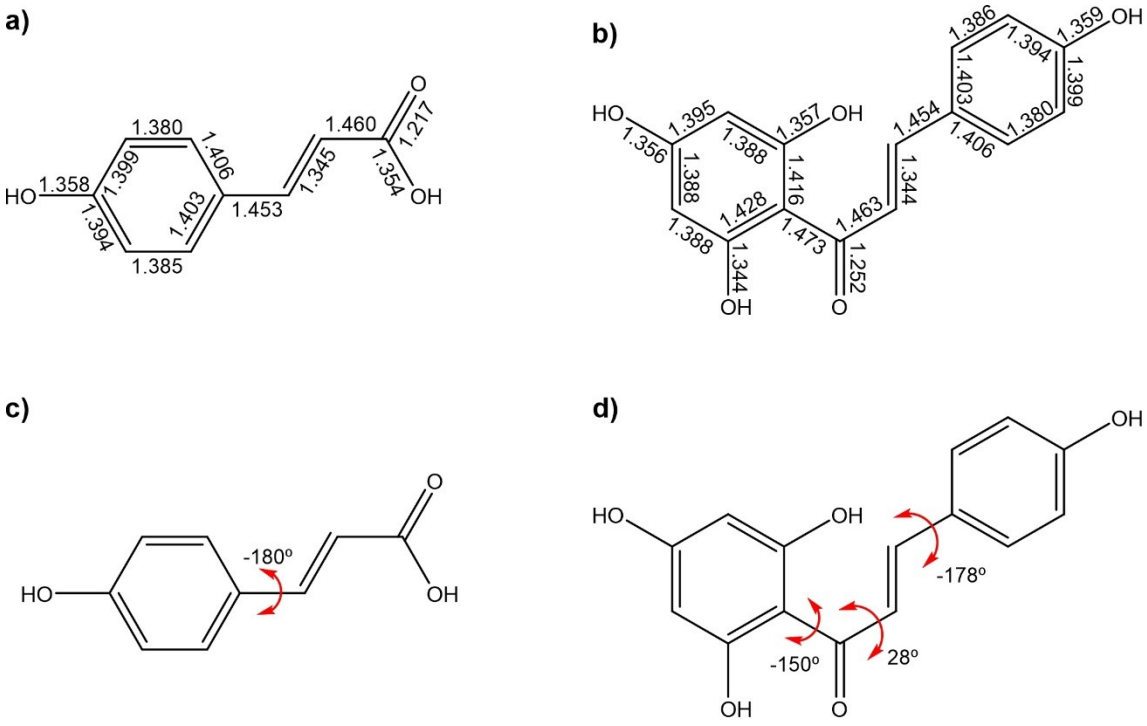


Fig S5. Left: theoretical UV-Vis spectra of **nch** computed at TD-B3LYP(PCM, ethanol)/def2TZVP//B3LYP(PCM,ethanol)/def2TZVP level and the assignment of its more relevant transitions (in nm). Right: Frontier orbitals of **nch** implied in the main transitions computed at B3LYP(PCM, ethanol)/def2TZVP. Red and blue display occupied orbitals and green and yellow unoccupied orbitals.



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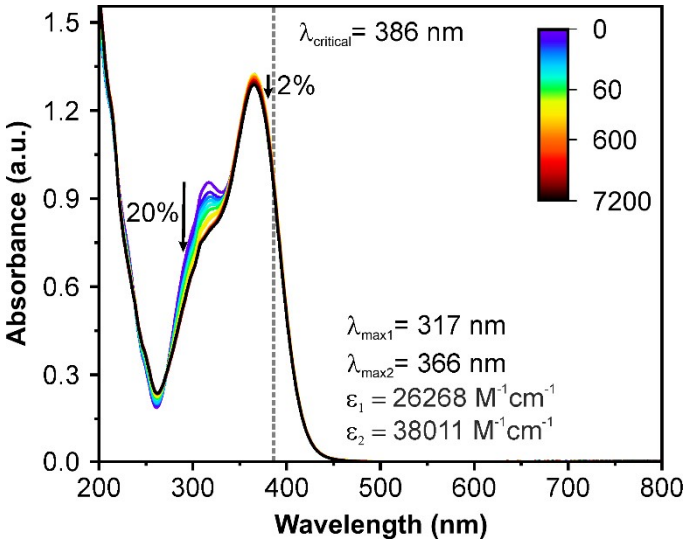

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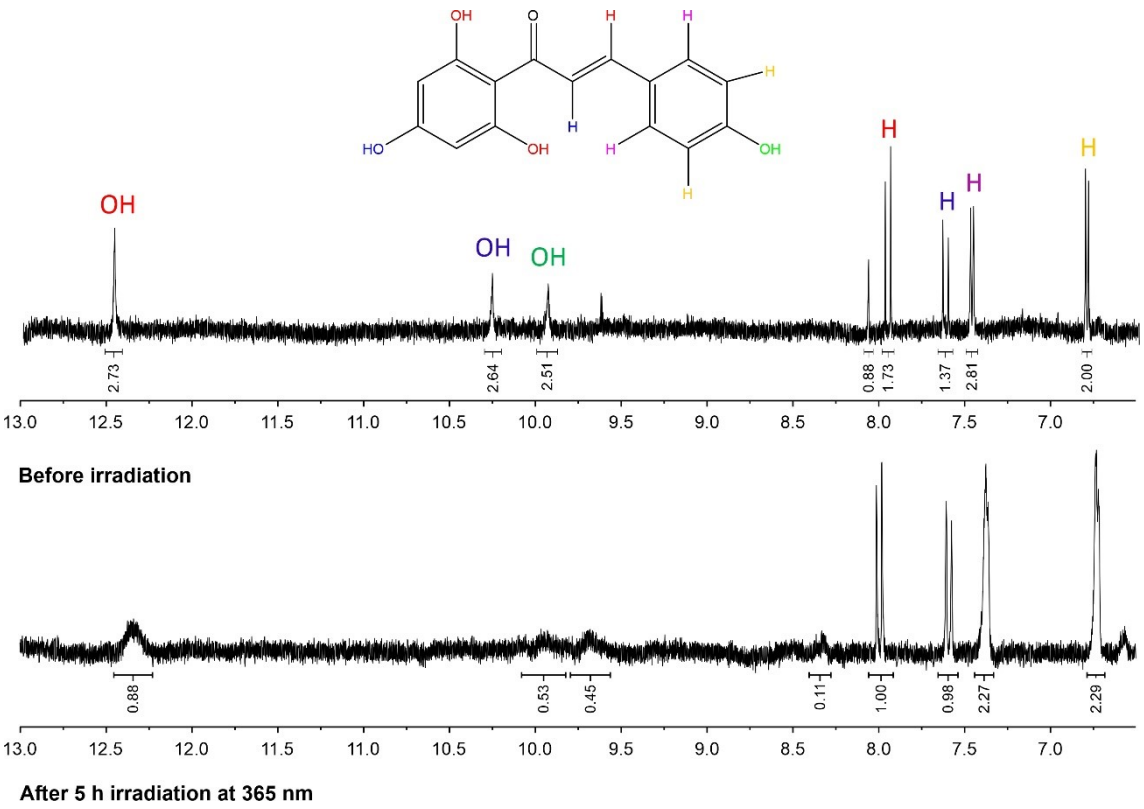

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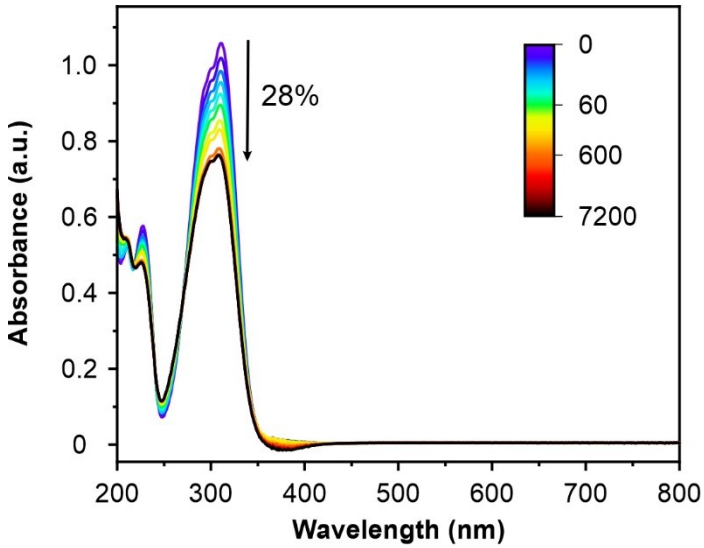


Fig S9. Photostability of a 1:1 mixture of **pca** and **nch** in ethanol after subtracting **nch** UV-Vis spectrum. The downwards arrow represents the absorbance difference before and after two hours of irradiation.

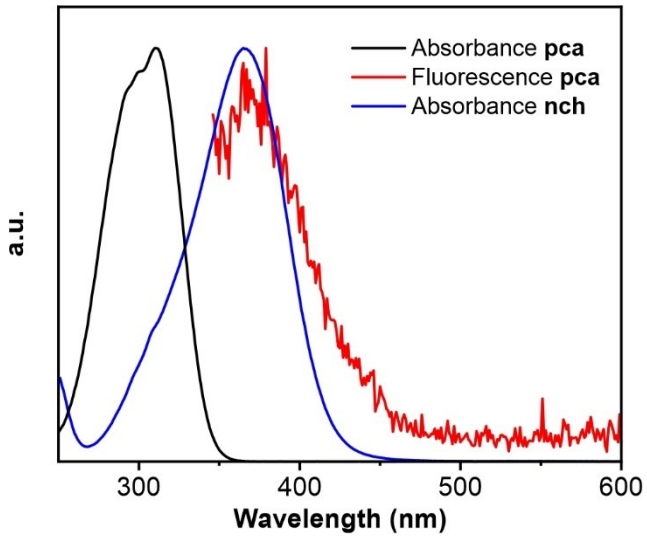


Fig S10. Absorbance spectra of **pca** (black line) and **nch** (blue line) and fluorescence spectrum of **pca** (red line) in ethanol.

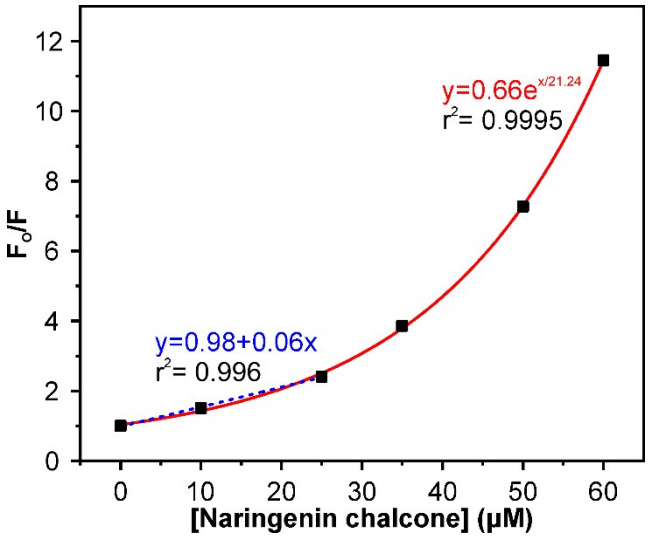


Fig S11. Stern-Volmer plot of the **pca** quenching by increasing concentrations of **nch**, where F_0 and F are fluorescence emission intensities in absence and presence of the quencher (**nch**). At low concentrations a linear fit was reached, corresponding the slope of the line to K_{SV} (Stern-Volmer constant). At higher concentrations, data deviates from a linear to an exponential fit.

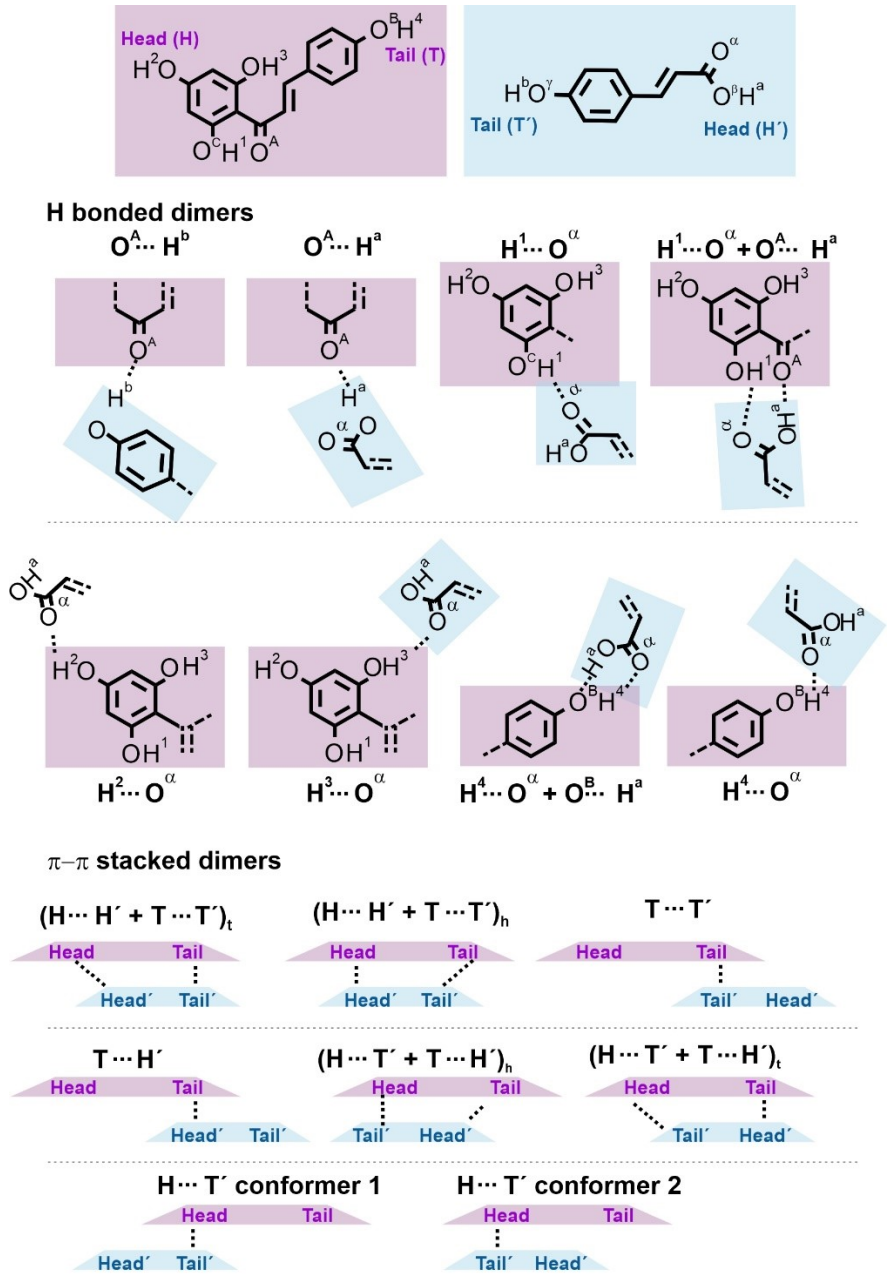
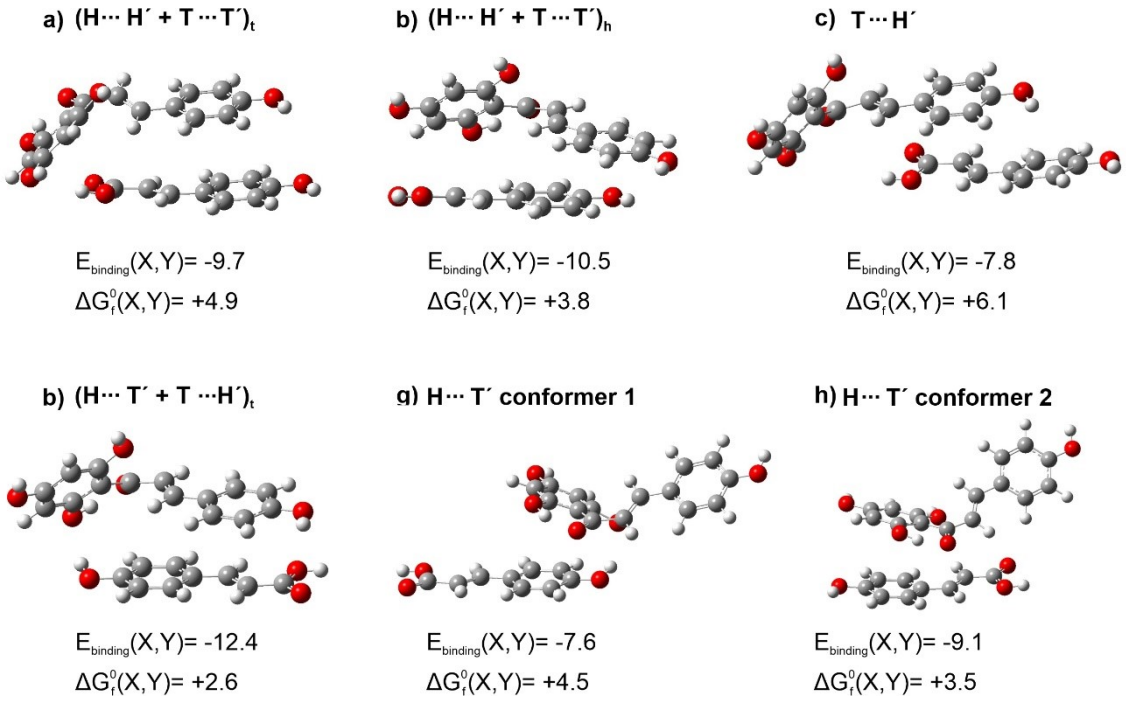


Fig S12. Schematic representation of all the **pca-nch** H-bonded and π-π stacked heterodimers analysed.



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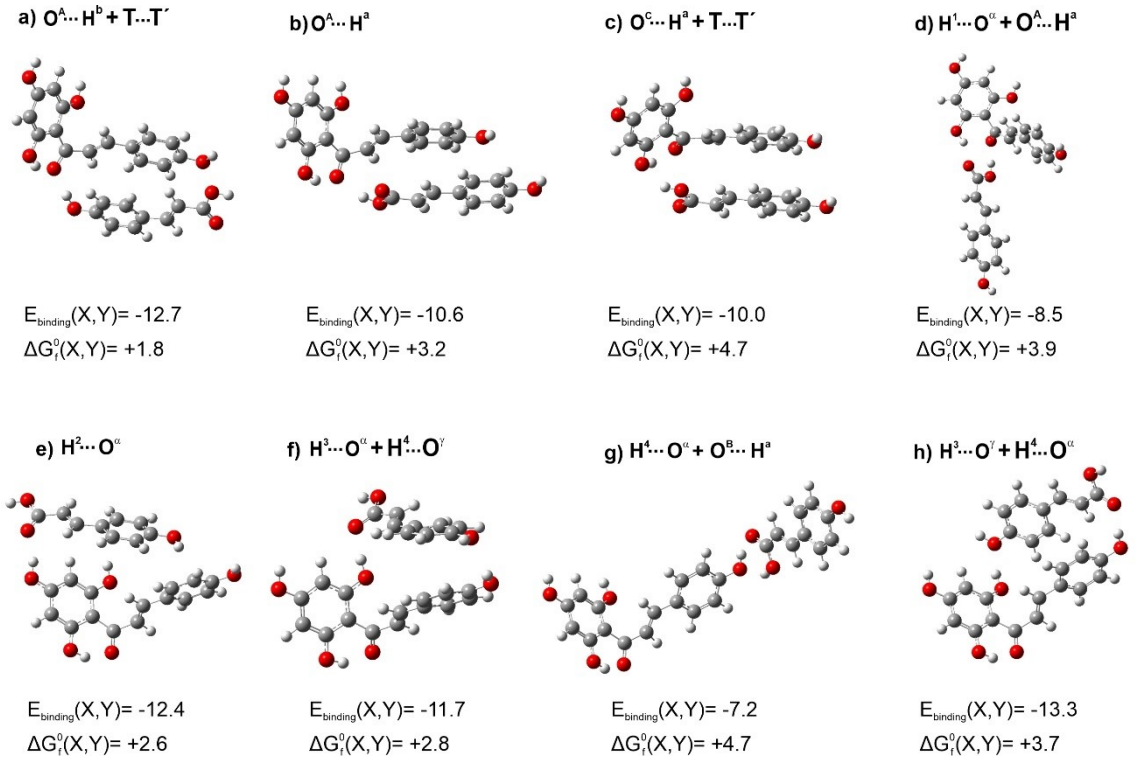

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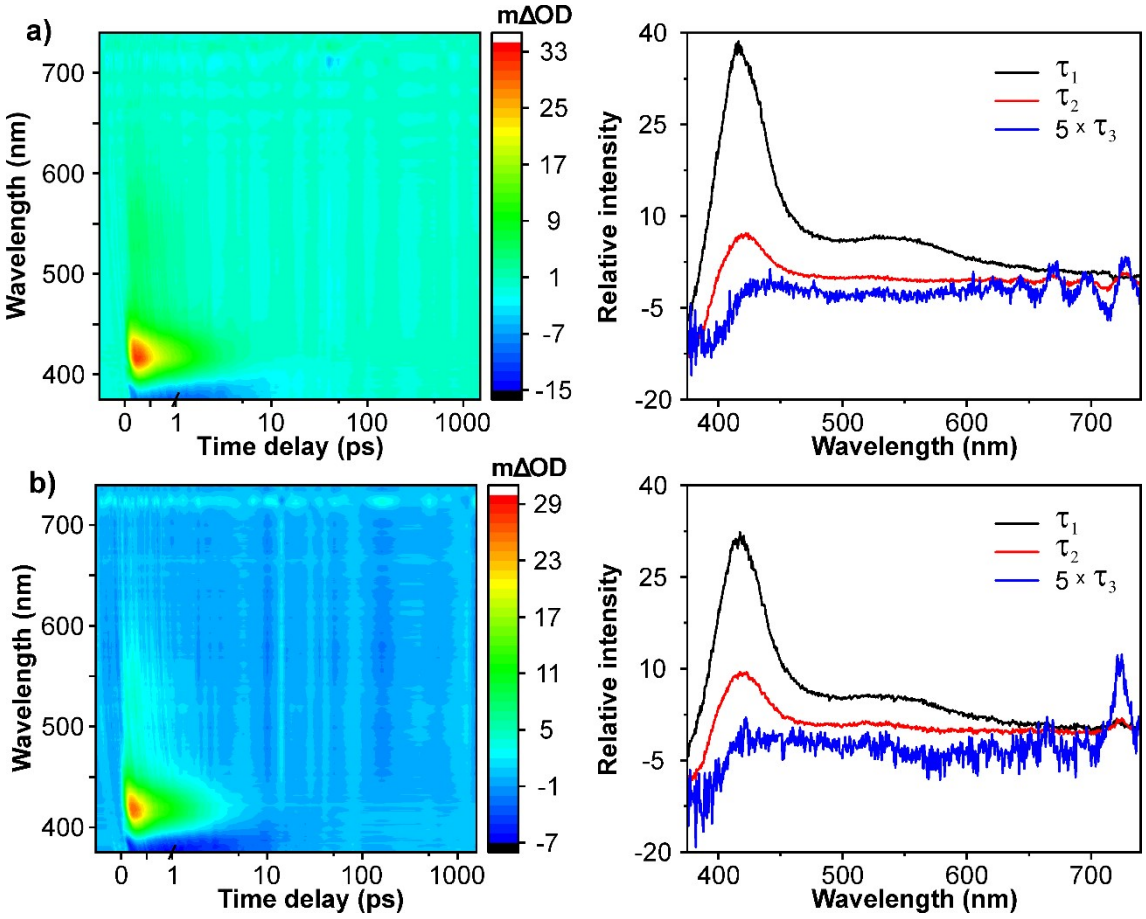

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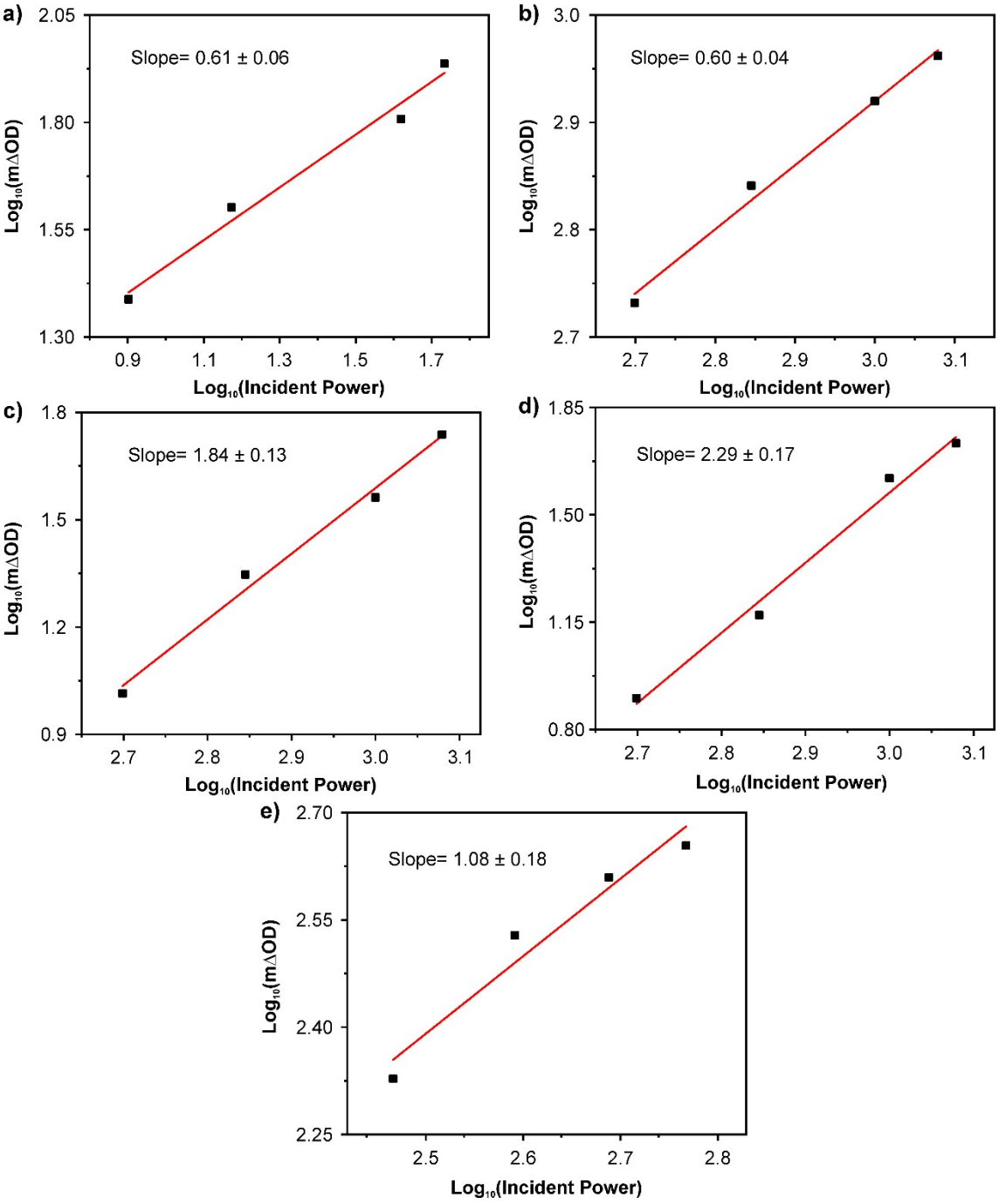

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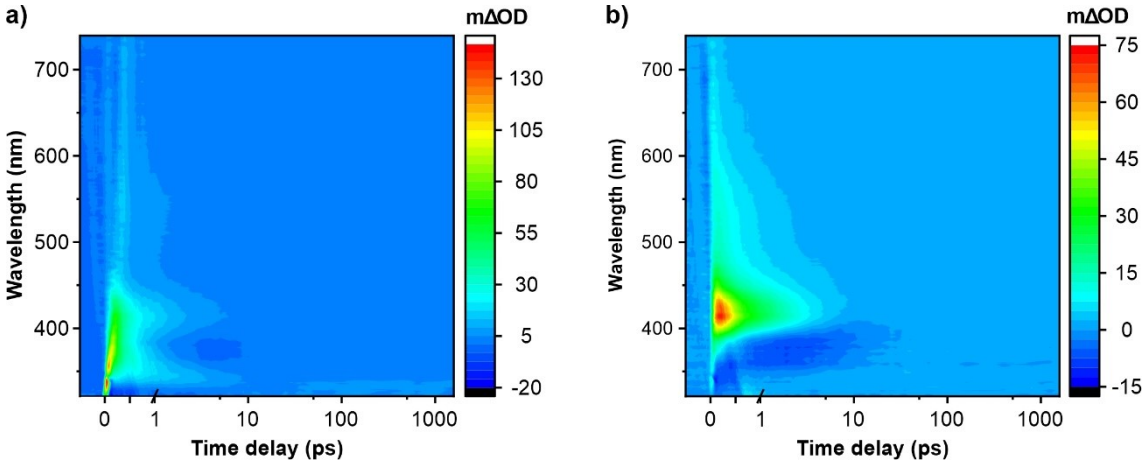

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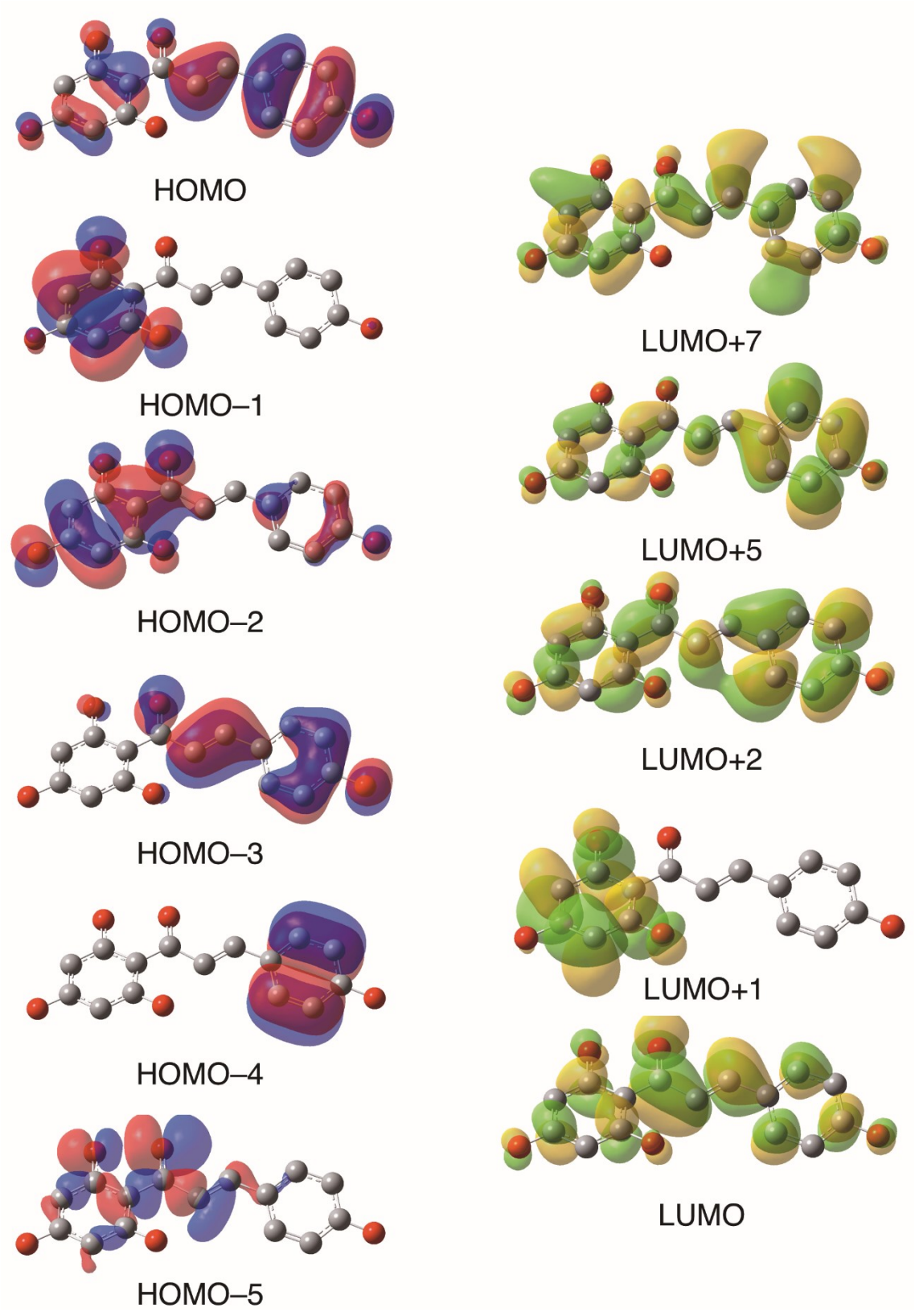

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Cartesian coordinates (optimized at the B3LYP (PCM,ethanol)/def2-TZVP level) of all the stationary points collected in the main text associated with the absorption spectra calculation.

pca

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.959497	-1.074653	-0.000285
2	6	0	2.330439	-1.232156	-0.000085
3	6	0	3.162777	-0.107910	0.000259
4	6	0	2.605242	1.169843	0.000375
5	6	0	1.227371	1.313862	0.000163
6	6	0	0.371269	0.202895	-0.000149
7	6	0	-1.064547	0.425452	-0.000303
8	6	0	-2.037918	-0.503053	-0.000282
9	8	0	4.503051	-0.324450	0.000432
10	6	0	-3.464663	-0.191635	-0.000496
11	8	0	-4.343042	-1.034624	0.000108
12	8	0	-3.755538	1.130903	-0.000032
13	1	0	0.336814	-1.959377	-0.000564
14	1	0	2.777309	-2.217613	-0.000196
15	1	0	3.247449	2.042578	0.000623
16	1	0	0.801369	2.309781	0.000248
17	1	0	-1.366966	1.467176	-0.000448
18	1	0	-1.826034	-1.563599	-0.000095
19	1	0	4.979332	0.516088	0.000883
20	1	0	-4.721850	1.214462	0.000313

nch

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.070173	-1.387579	-0.196443
2	6	0	-4.233442	-0.127045	-0.752853
3	6	0	-3.274151	0.848053	-0.515503
4	6	0	-2.081892	0.568821	0.218861
5	6	0	-1.997839	-0.710187	0.820207
6	6	0	-2.969404	-1.678414	0.609680
7	8	0	-5.037328	-2.305100	-0.442292
8	8	0	-3.501263	2.070846	-1.023643
9	8	0	-0.965695	-0.963251	1.664329
10	6	0	-1.063709	1.628989	0.317571
11	6	0	0.373997	1.383429	0.434022
12	6	0	1.014162	0.305155	-0.050924
13	6	0	2.926427	-1.098279	-0.698567
14	6	0	2.449243	0.078450	-0.102942
15	6	0	3.398827	0.974683	0.419728
16	6	0	4.751414	0.708209	0.350451
17	6	0	5.201400	-0.472227	-0.249720
18	6	0	4.281432	-1.377724	-0.775427
19	8	0	6.543290	-0.680585	-0.289885
20	8	0	-1.418087	2.825468	0.214928
21	1	0	-5.111166	0.109942	-1.337026
22	1	0	-2.881865	-2.646705	1.088982
23	1	0	-4.832366	-3.138428	0.001055
24	1	0	-2.804953	2.662859	-0.633293
25	1	0	-1.050627	-1.855067	2.025152
26	1	0	0.922593	2.241287	0.805044
27	1	0	0.417138	-0.494547	-0.474285
28	1	0	2.218257	-1.807384	-1.109789
29	1	0	3.075845	1.894107	0.889538
30	1	0	5.476158	1.402187	0.755525
31	1	0	4.625737	-2.293671	-1.240664
32	1	0	6.740159	-1.519609	-0.726597

Cartesian coordinates (optimized at the ωB97XD(PCM,ethanol)/6-31+G(d,p) level) of all the stationary points collected in the main text associated with the S_0 and S_1 surface exploration for **nch**.

s-trans-S_0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.282215	0.800096	0.162081
2	6	0	3.975556	1.265737	0.249774
3	6	0	2.878138	0.417971	0.041891
4	6	0	3.137332	-0.931097	-0.260741
5	6	0	4.433390	-1.409323	-0.351047
6	6	0	5.512339	-0.543108	-0.139650
7	6	0	1.530030	0.971663	0.148341
8	6	0	0.367734	0.306256	0.006519
9	6	0	-0.912478	1.023643	0.118040
10	8	0	-0.902031	2.276154	0.169265
11	8	0	6.758860	-1.069223	-0.242793
12	6	0	-2.204509	0.319043	0.098346
13	6	0	-3.391597	1.079831	-0.148962
14	6	0	-4.639491	0.478145	-0.281767
15	6	0	-4.747622	-0.897469	-0.131353
16	6	0	-3.628021	-1.681848	0.163623
17	6	0	-2.383527	-1.078257	0.284059
18	8	0	-5.978792	-1.437811	-0.262967
19	8	0	-3.345421	2.409768	-0.278659
20	8	0	-1.308360	-1.827804	0.620059
21	1	0	-5.512761	1.085438	-0.486043
22	1	0	-3.731348	-2.752114	0.316589
23	1	0	-5.951066	-2.392580	-0.134192
24	1	0	-2.400729	2.671170	-0.098799
25	1	0	-1.560444	-2.753000	0.715145
26	1	0	0.339279	-0.754551	-0.193445
27	1	0	1.473200	2.035459	0.372420
28	1	0	3.804374	2.312492	0.484591
29	1	0	2.317231	-1.621297	-0.429957
30	1	0	4.628533	-2.450335	-0.585247
31	1	0	6.116408	1.475963	0.326805
32	1	0	7.426335	-0.393031	-0.082023

TS-S_0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.606130	-1.132563	0.213171
2	6	0	-1.978353	0.127743	0.227373
3	6	0	-2.785461	1.235115	-0.168226
4	6	0	-4.125818	1.079055	-0.534950
5	6	0	-4.693751	-0.185994	-0.522223
6	6	0	-3.942924	-1.301057	-0.152622
7	6	0	-0.557257	0.387511	0.626490
8	8	0	-0.127549	1.621159	0.474475
9	8	0	-2.272176	2.469264	-0.198389
10	8	0	-6.001802	-0.290619	-0.886158
11	8	0	-1.877686	-2.227786	0.566381
12	6	0	0.290233	-0.557591	1.138280
13	6	0	1.624027	-0.125095	1.542455
14	6	0	2.755764	-0.137889	0.748045
15	6	0	4.011180	0.297297	1.279467
16	6	0	5.138232	0.305967	0.504176
17	6	0	5.045873	-0.122696	-0.840809
18	6	0	3.819279	-0.555990	-1.398548
19	6	0	2.698887	-0.563075	-0.617982
20	8	0	6.096505	-0.142286	-1.645385
21	1	0	-4.706588	1.946263	-0.827590

22	1	0	-4.388372	-2.292384	-0.149691
23	1	0	-6.289262	-1.208663	-0.839677
24	1	0	-1.269163	2.317350	0.077856
25	1	0	-2.427660	-3.016811	0.517062
26	1	0	0.008446	-1.583185	1.336136
27	1	0	1.776422	0.230470	2.567595
28	1	0	4.061817	0.624349	2.313289
29	1	0	1.741456	-0.886429	-1.012728
30	1	0	3.800357	-0.871176	-2.434959
31	1	0	6.091877	0.634724	0.903261
32	1	0	6.899652	0.163214	-1.202534

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.685336	2.528799	0.543895
2	6	0	1.491383	2.233129	-0.549116
3	6	0	1.987676	0.941824	-0.690868
4	6	0	1.641334	-0.096300	0.221349
5	6	0	0.879246	0.274701	1.356837
6	6	0	0.397194	1.565928	1.517511
7	8	0	0.222366	3.794375	0.640188
8	8	0	2.770823	0.700463	-1.752243
9	8	0	0.669205	-0.658404	2.308518
10	6	0	1.984661	-1.475988	-0.134058
11	6	0	1.203748	-2.655909	0.317325
12	6	0	-0.130681	-2.788599	0.320810
13	6	0	-2.267414	-1.591871	0.720969
14	6	0	-1.132671	-1.782268	-0.075487
15	6	0	-0.988871	-0.987164	-1.220787
16	6	0	-1.916719	-0.004616	-1.537074
17	6	0	-3.019995	0.197405	-0.705787
18	6	0	-3.201252	-0.605097	0.422564
19	8	0	-3.893780	1.181427	-1.053228
20	8	0	2.936609	-1.703048	-0.907298
21	1	0	1.741104	2.995326	-1.276956
22	1	0	-0.178682	1.828522	2.400121
23	1	0	-0.327549	3.899820	1.424679
24	1	0	3.093720	-0.227695	-1.667320
25	1	0	0.097086	-0.307667	2.999946
26	1	0	1.820506	-3.513263	0.573591
27	1	0	-0.528876	-3.740538	0.668535
28	1	0	-2.412478	-2.207935	1.603898
29	1	0	-0.143041	-1.144246	-1.883161
30	1	0	-1.797744	0.608380	-2.424156
31	1	0	-4.066452	-0.461212	1.063545
32	1	0	-4.617222	1.228169	-0.418705

s-trans-S_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.290273	0.814239	-0.038500
2	6	0	4.023234	1.330986	0.017841
3	6	0	2.858812	0.485784	0.019124
4	6	0	3.086326	-0.936318	-0.027653
5	6	0	4.356185	-1.452351	-0.085341
6	6	0	5.470104	-0.588017	-0.096617
7	6	0	1.581646	1.067458	0.063062
8	6	0	0.367434	0.339487	0.071868
9	6	0	-0.889484	1.002641	0.137052
10	8	0	-0.901530	2.302011	0.193209
11	8	0	6.680628	-1.152793	-0.163431
12	6	0	-2.172960	0.291903	0.083829
13	6	0	-3.370890	1.082954	-0.072841
14	6	0	-4.633760	0.504639	-0.185781
15	6	0	-4.755990	-0.875638	-0.126253

16	6	0	-3.629339	-1.690554	0.054694
17	6	0	-2.371316	-1.115031	0.163535
18	8	0	-5.999584	-1.397335	-0.239647
19	8	0	-3.279706	2.406994	-0.120392
20	8	0	-1.288459	-1.909637	0.364650
21	1	0	-5.505139	1.135960	-0.312430
22	1	0	-3.738909	-2.769758	0.119845
23	1	0	-5.975311	-2.359081	-0.183442
24	1	0	-2.260616	2.600381	0.019099
25	1	0	-1.554399	-2.835131	0.395500
26	1	0	0.378412	-0.738436	0.019454
27	1	0	1.513765	2.150483	0.099303
28	1	0	3.883564	2.406627	0.060137
29	1	0	2.244208	-1.618330	-0.020285
30	1	0	4.526103	-2.522738	-0.124634
31	1	0	6.155610	1.470166	-0.038854
32	1	0	7.380272	-0.487155	-0.176915

TS-S_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.395970	-1.106275	0.233305
2	6	0	-2.095812	0.263511	0.012348
3	6	0	-3.208668	1.102627	-0.325865
4	6	0	-4.514248	0.618043	-0.370400
5	6	0	-4.749146	-0.724673	-0.108575
6	6	0	-3.694700	-1.596072	0.185304
7	6	0	-0.761744	0.880874	0.105250
8	8	0	-0.608230	2.089732	-0.324701
9	8	0	-3.015820	2.394601	-0.600040
10	8	0	-6.031951	-1.154113	-0.165119
11	8	0	-1.368922	-1.956931	0.481873
12	6	0	0.337927	0.242519	0.731792
13	6	0	1.591093	0.939151	0.892364
14	6	0	2.823347	0.426400	0.480721
15	6	0	4.023258	1.196913	0.627969
16	6	0	5.237464	0.715268	0.207548
17	6	0	5.313508	-0.561073	-0.391647
18	6	0	4.157192	-1.345909	-0.553694
19	6	0	2.941319	-0.868663	-0.126205
20	8	0	6.472388	-1.086091	-0.816245
21	1	0	-5.329998	1.287044	-0.617022
22	1	0	-3.884423	-2.652061	0.356759
23	1	0	-6.085477	-2.095959	0.031619
24	1	0	-2.002273	2.519071	-0.567441
25	1	0	-1.703270	-2.847863	0.633013
26	1	0	0.215094	-0.752443	1.144916
27	1	0	1.570518	1.949209	1.303395
28	1	0	3.962187	2.181512	1.081498
29	1	0	2.051183	-1.479161	-0.241354
30	1	0	4.249025	-2.327150	-1.006450
31	1	0	6.138549	1.308912	0.330262
32	1	0	7.210236	-0.484535	-0.656631

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.308871	-1.014896	0.473089
2	6	0	-1.969830	0.303243	0.086446
3	6	0	-2.993531	1.068274	-0.543361
4	6	0	-4.289053	0.580907	-0.687673
5	6	0	-4.581111	-0.704352	-0.249023
6	6	0	-3.595088	-1.517015	0.318098
7	6	0	-0.646000	0.924257	0.299603
8	8	0	-0.336667	1.961989	-0.336869
9	8	0	-2.750719	2.301327	-1.010462
10	8	0	-5.851414	-1.137373	-0.414839

11	8	0	-1.329005	-1.803459	0.976119
12	6	0	0.295047	0.428267	1.280249
13	6	0	1.616287	0.993038	1.375364
14	6	0	2.742410	0.430576	0.690380
15	6	0	4.028742	0.994855	0.833966
16	6	0	5.124198	0.468584	0.170778
17	6	0	4.966997	-0.647078	-0.661304
18	6	0	3.709174	-1.224957	-0.821856
19	6	0	2.612887	-0.692589	-0.156003
20	8	0	6.009517	-1.207551	-1.335852
21	1	0	-5.050093	1.194563	-1.153934
22	1	0	-3.823453	-2.535318	0.618606
23	1	0	-5.953962	-2.035857	-0.081834
24	1	0	-1.777586	2.454234	-0.913430
25	1	0	-1.679338	-2.671692	1.203965
26	1	0	-0.031645	-0.341614	1.973207
27	1	0	1.780229	1.860148	2.014231
28	1	0	4.161223	1.859686	1.477122
29	1	0	1.638731	-1.152881	-0.290703
30	1	0	3.599601	-2.088412	-1.469322
31	1	0	6.104166	0.920486	0.295710
32	1	0	6.824881	-0.729482	-1.150916

Cartesian coordinates of conical intersection computed at CASSCF(12,11)(PCM,ethanol)/6-31+G(d,p) level of theory for **nch**.

CI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.962635	-0.823104	-0.171231
2	6	0	2.847466	0.447823	0.430825
3	6	0	4.027365	1.204807	0.604256
4	6	0	5.258566	0.719744	0.199354
5	6	0	5.345541	-0.548743	-0.388282
6	6	0	4.197703	-1.316910	-0.572956
7	6	0	1.598208	0.900171	1.018499
8	6	0	0.334166	0.253844	0.874599
9	6	0	-0.774760	0.854382	0.013550
10	8	0	-0.579091	1.986899	-0.493839
11	8	0	6.532457	-1.089876	-0.778184
12	6	0	-2.127915	0.259181	-0.040674
13	6	0	-2.411800	-1.105184	0.192258
14	6	0	-3.711324	-1.599313	0.172231
15	6	0	-4.770351	-0.723933	-0.084892
16	6	0	-4.544992	0.626744	-0.322355
17	6	0	-3.238862	1.107403	-0.314570
18	8	0	-1.367881	-1.939574	0.412462
19	8	0	-3.065495	2.414468	-0.560003
20	8	0	-6.053281	-1.150776	-0.127678
21	1	0	-5.368763	1.297804	-0.533386
22	1	0	-3.896663	-2.656878	0.335644
23	1	0	-6.105564	-2.099073	0.036931
24	1	0	-2.087946	2.558226	-0.620027
25	1	0	-1.686671	-2.834700	0.575484
26	1	0	0.037972	-0.516843	1.583876
27	1	0	1.671187	1.691289	1.765726
28	1	0	3.970876	2.179722	1.080347
29	1	0	2.083069	-1.452645	-0.268321
30	1	0	4.288107	-2.311108	-0.998511
31	1	0	6.156072	1.313245	0.352766
32	1	0	7.254785	-0.479632	-0.596273

Cartesian coordinates (optimized at the ωB97XD(PCM, ethanol)/def2-TZVP level) of all the stationary points associated to **pca**-**nch** heterodimers.

pca

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.955425	-1.068962	-0.000335
2	6	0	2.323693	-1.228586	-0.000219
3	6	0	3.155166	-0.109003	0.000170
4	6	0	2.600127	1.165578	0.000412
5	6	0	1.224668	1.310248	0.000282
6	6	0	0.373721	0.204333	-0.000069
7	6	0	-1.067216	0.426772	-0.000131
8	6	0	-2.027979	-0.502903	0.000035
9	8	0	4.488251	-0.324639	0.000263
10	6	0	-3.459099	-0.188680	-0.000029
11	8	0	-4.330513	-1.030224	0.000027
12	8	0	-3.743230	1.122432	-0.000404
13	1	0	0.331992	-1.953704	-0.000661
14	1	0	2.768043	-2.215213	-0.000435
15	1	0	3.241682	2.038764	0.000694
16	1	0	0.800290	2.307196	0.000466
17	1	0	-1.372953	1.468132	-0.000298
18	1	0	-1.814131	-1.563394	0.000248
19	1	0	4.961996	0.511497	0.000701
20	1	0	-4.704018	1.213400	-0.000495

nch

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.966594	-1.438891	-0.185037
2	6	0	-4.149159	-0.209192	-0.794614
3	6	0	-3.234170	0.803702	-0.558661
4	6	0	-2.073497	0.591183	0.230270
5	6	0	-1.966540	-0.654527	0.882357
6	6	0	-2.892863	-1.662069	0.672333
7	8	0	-4.885834	-2.391924	-0.431481
8	8	0	-3.477227	1.990163	-1.126040
9	8	0	-0.963760	-0.832156	1.765195
10	6	0	-1.083784	1.678930	0.319777
11	6	0	0.358299	1.439141	0.439044
12	6	0	0.970099	0.360752	-0.058502
13	6	0	2.853925	-1.073399	-0.712059
14	6	0	2.404407	0.103683	-0.112713
15	6	0	3.363902	0.975413	0.415238
16	6	0	4.708885	0.683836	0.346883
17	6	0	5.135360	-0.498112	-0.257606
18	6	0	4.200831	-1.379229	-0.788790
19	8	0	6.465538	-0.732837	-0.296776
20	8	0	-1.454021	2.854752	0.199516
21	1	0	-5.009282	-0.025925	-1.422635
22	1	0	-2.793162	-2.608211	1.191352
23	1	0	-4.672045	-3.197533	0.046791
24	1	0	-2.835886	2.625138	-0.737919
25	1	0	-1.014131	-1.712753	2.146197
26	1	0	0.913123	2.285493	0.826656
27	1	0	0.352775	-0.422537	-0.487253
28	1	0	2.132297	-1.766330	-1.128369
29	1	0	3.058415	1.898644	0.890419
30	1	0	5.445601	1.361705	0.757704
31	1	0	4.525802	-2.299407	-1.259536
32	1	0	6.644322	-1.569614	-0.734242

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.187360	1.979578	0.298380
2	6	0	-1.895797	2.332097	0.624036
3	6	0	-1.152964	1.530449	1.488287
4	6	0	-1.729346	0.395126	2.045799
5	6	0	-3.021016	0.045976	1.701854
6	6	0	-3.775567	0.822181	0.820861
7	6	0	-5.125416	0.387507	0.484958
8	6	0	-5.985814	0.988751	-0.343473
9	8	0	0.124204	1.893533	1.742215
10	6	0	-7.328003	0.476771	-0.628849
11	8	0	-8.108371	1.021270	-1.378992
12	8	0	-7.640951	-0.660561	0.010725
13	1	0	-3.738920	2.610284	-0.386837
14	1	0	-1.434263	3.211341	0.195249
15	1	0	-1.158668	-0.222254	2.728055
16	1	0	-3.454731	-0.853265	2.123007
17	1	0	-5.446951	-0.529593	0.968099
18	1	0	-5.747382	1.904607	-0.867522
19	1	0	0.624470	1.133891	2.069430
20	1	0	-8.537920	-0.903775	-0.249315
21	6	0	-1.022893	-2.908314	0.029115
22	6	0	-1.396591	-2.173877	-1.081476
23	6	0	-0.749793	-0.978605	-1.352786
24	6	0	0.336445	-0.521448	-0.559821
25	6	0	0.612333	-1.258396	0.609001
26	6	0	-0.031428	-2.446437	0.892013
27	8	0	-1.685123	-4.056359	0.263938
28	8	0	-1.179798	-0.276687	-2.402841
29	8	0	1.465346	-0.725707	1.519741
30	6	0	1.053628	0.689369	-0.988229
31	6	0	2.467749	0.933769	-0.680711
32	6	0	3.377438	-0.035786	-0.557350
33	6	0	5.620026	-1.017822	-0.340384
34	6	0	4.817447	0.122419	-0.385939
35	6	0	5.443099	1.367270	-0.252968
36	6	0	6.807059	1.467237	-0.084731
37	6	0	7.590073	0.314345	-0.045174
38	6	0	6.990906	-0.933228	-0.173326
39	8	0	8.922014	0.471894	0.120949
40	8	0	0.485439	1.516806	-1.714368
41	1	0	-2.204171	-2.506397	-1.717885
42	1	0	0.191846	-2.982104	1.807136
43	1	0	-1.358779	-4.476319	1.064396
44	1	0	-0.712857	0.591174	-2.368050
45	1	0	1.592407	-1.338381	2.249799
46	1	0	2.746668	1.980229	-0.715077
47	1	0	3.035442	-1.065433	-0.597081
48	1	0	5.161029	-1.994505	-0.439083
49	1	0	4.856663	2.276725	-0.277671
50	1	0	7.284558	2.432804	0.018790
51	1	0	7.594121	-1.832892	-0.141905
52	1	0	9.360069	-0.383239	0.130987

H ⋯ T´ conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.790500	1.168267	-1.381114
2	6	0	3.987944	0.489841	-1.399394
3	6	0	4.847697	0.569570	-0.305653
4	6	0	4.504262	1.350107	0.791290
5	6	0	3.299582	2.028675	0.794207
6	6	0	2.414313	1.945008	-0.279876
7	6	0	1.123190	2.610731	-0.178422
8	6	0	0.082937	2.463815	-1.005522
9	8	0	5.999988	-0.134344	-0.367588

10	6	0	-1.215503	3.104576	-0.797548
11	8	0	-2.165441	2.955071	-1.535433
12	8	0	-1.291956	3.873674	0.300372
13	1	0	2.130903	1.080042	-2.234673
14	1	0	4.267730	-0.121759	-2.246917
15	1	0	5.170444	1.414243	1.643439
16	1	0	3.028917	2.620778	1.660058
17	1	0	0.998128	3.251687	0.687821
18	1	0	0.114360	1.811116	-1.866457
19	1	0	6.504555	-0.016729	0.441621
20	1	0	-2.185511	4.236218	0.339864
21	6	0	2.717219	-2.782498	-0.559196
22	6	0	2.938768	-2.355184	0.736732
23	6	0	2.068606	-1.439700	1.304959
24	6	0	0.909432	-0.976466	0.619811
25	6	0	0.763957	-1.397399	-0.721402
26	6	0	1.641095	-2.299174	-1.296752
27	8	0	3.601962	-3.651620	-1.084328
28	8	0	2.355512	-1.018142	2.537541
29	8	0	-0.217652	-0.860378	-1.472003
30	6	0	0.003266	-0.064839	1.329304
31	6	0	-1.418929	0.099759	1.003432
32	6	0	-2.210234	-0.881334	0.566521
33	6	0	-4.350280	-1.978105	0.048636
34	6	0	-3.651098	-0.808475	0.346161
35	6	0	-4.374146	0.388324	0.403454
36	6	0	-5.734617	0.412564	0.184113
37	6	0	-6.414917	-0.770238	-0.101218
38	6	0	-5.716545	-1.969796	-0.170480
39	8	0	-7.748998	-0.688442	-0.306046
40	8	0	0.416087	0.575621	2.309668
41	1	0	3.802395	-2.693171	1.291268
42	1	0	1.509421	-2.595362	-2.330949
43	1	0	3.366184	-3.865458	-1.991103
44	1	0	1.733708	-0.273300	2.724536
45	1	0	-0.177612	-1.217191	-2.363152
46	1	0	-1.818939	1.060597	1.306183
47	1	0	-1.763651	-1.847810	0.356207
48	1	0	-3.813177	-2.917503	-0.009584
49	1	0	-3.866050	1.321485	0.610560
50	1	0	-6.287101	1.342204	0.224935
51	1	0	-6.238980	-2.891669	-0.397098
52	1	0	-8.110724	-1.558107	-0.496265

$(H \cdots H' + T \cdots T')_h$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.205661	2.118502	1.172611
2	6	0	0.972574	2.191352	1.882569
3	6	0	2.190957	2.217856	1.206995
4	6	0	2.214321	2.189829	-0.181195
5	6	0	1.025704	2.105212	-0.880864
6	6	0	-0.205189	2.067781	-0.225422
7	6	0	-1.422973	1.957731	-1.018996
8	6	0	-2.679173	2.052936	-0.574121
9	8	0	3.318977	2.250588	1.952200
10	6	0	-3.856448	1.912413	-1.433313
11	8	0	-4.992656	2.088452	-1.051638
12	8	0	-3.584544	1.565020	-2.700928
13	1	0	-1.139128	2.067238	1.718169
14	1	0	0.968247	2.200205	2.964496
15	1	0	3.159915	2.193485	-0.710501
16	1	0	1.054041	2.055767	-1.963030
17	1	0	-1.271564	1.782636	-2.079267
18	1	0	-2.915109	2.244102	0.464152
19	1	0	4.092137	2.187340	1.384232
20	1	0	-4.424461	1.508118	-3.172743
21	6	0	-3.810517	-1.667509	-0.540992
22	6	0	-3.827466	-0.830296	0.559674
23	6	0	-2.713164	-0.769518	1.379497
24	6	0	-1.532098	-1.502577	1.093277

25	6	0	-1.593764	-2.402622	0.008907
26	6	0	-2.707507	-2.472737	-0.810461
27	8	0	-4.910766	-1.690923	-1.318145
28	8	0	-2.787868	0.036831	2.444832
29	8	0	-0.558763	-3.244042	-0.187538
30	6	0	-0.354431	-1.287373	1.952853
31	6	0	1.028580	-1.373689	1.476712
32	6	0	1.403788	-1.156316	0.214201
33	6	0	2.977778	-0.921921	-1.656219
34	6	0	2.768007	-1.017749	-0.281119
35	6	0	3.881269	-0.915537	0.558614
36	6	0	5.147201	-0.723351	0.047110
37	6	0	5.334416	-0.634349	-1.331198
38	6	0	4.242091	-0.737287	-2.185282
39	8	0	6.595706	-0.442572	-1.778125
40	8	0	-0.518200	-0.918339	3.124887
41	1	0	-4.695743	-0.227387	0.782379
42	1	0	-2.730764	-3.173500	-1.636845
43	1	0	-4.793177	-2.305960	-2.047142
44	1	0	-1.996431	-0.156647	2.996314
45	1	0	-0.737680	-3.814146	-0.939870
46	1	0	1.753752	-1.457623	2.277624
47	1	0	0.633357	-1.031848	-0.538641
48	1	0	2.128942	-0.981282	-2.327076
49	1	0	3.758715	-0.960249	1.632908
50	1	0	6.003722	-0.635558	0.702760
51	1	0	4.380949	-0.665121	-3.257550
52	1	0	6.605423	-0.394402	-2.737751

$(H \cdots H' + T \cdots T')_t$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.223608	-1.016013	-1.331682
2	6	0	4.578837	-0.864178	-1.142595
3	6	0	5.201090	-1.471829	-0.053537
4	6	0	4.453982	-2.238847	0.832528
5	6	0	3.093305	-2.381078	0.630294
6	6	0	2.449408	-1.774785	-0.447586
7	6	0	1.002909	-1.901546	-0.565353
8	6	0	0.233394	-1.415611	-1.543459
9	8	0	6.529937	-1.273001	0.095069
10	6	0	-1.227784	-1.507739	-1.553278
11	8	0	-1.914750	-1.085346	-2.456869
12	8	0	-1.761008	-2.082851	-0.465228
13	1	0	2.758991	-0.512854	-2.169474
14	1	0	5.170274	-0.261214	-1.818859
15	1	0	4.933652	-2.713144	1.680499
16	1	0	2.514126	-2.967318	1.333878
17	1	0	0.515163	-2.425531	0.250496
18	1	0	0.640607	-0.888141	-2.395538
19	1	0	6.852376	-1.742265	0.869195
20	1	0	-2.725934	-2.026030	-0.542103
21	6	0	-4.722591	-1.247326	1.352370
22	6	0	-4.994057	-0.997509	0.015806
23	6	0	-4.408023	0.100171	-0.601411
24	6	0	-3.438171	0.893470	0.066010
25	6	0	-3.258092	0.649255	1.442215
26	6	0	-3.880015	-0.411830	2.079095
27	8	0	-5.333581	-2.304924	1.917154
28	8	0	-4.778336	0.361679	-1.853780
29	8	0	-2.499598	1.509169	2.149239
30	6	0	-2.688750	1.881557	-0.732743
31	6	0	-1.282335	2.218053	-0.488964
32	6	0	-0.411562	1.437429	0.157810
33	6	0	1.715833	0.948796	1.282914
34	6	0	1.022205	1.659016	0.303081
35	6	0	1.747556	2.543126	-0.501583
36	6	0	3.105722	2.710816	-0.332151
37	6	0	3.775578	1.996423	0.658719
38	6	0	3.073178	1.119847	1.475671
39	8	0	5.110595	2.182622	0.768388

40	8	0	-3.223487	2.388205	-1.728617
41	1	0	-5.704270	-1.605696	-0.526165
42	1	0	-3.727308	-0.573191	3.139716
43	1	0	-5.080090	-2.387461	2.840531
44	1	0	-4.337380	1.203430	-2.109057
45	1	0	-2.460098	1.234150	3.069067
46	1	0	-0.959876	3.116757	-1.002505
47	1	0	-0.779332	0.537981	0.638505
48	1	0	1.180032	0.241072	1.904479
49	1	0	1.248842	3.091457	-1.290704
50	1	0	3.666817	3.380140	-0.971075
51	1	0	3.592910	0.549950	2.236291
52	1	0	5.470967	1.605485	1.446957

T ⋯ H´

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.016057	1.190238	0.120395
2	6	0	-6.287863	0.661148	0.075218
3	6	0	-6.617785	-0.426373	0.881485
4	6	0	-5.665205	-0.964785	1.740329
5	6	0	-4.396304	-0.414554	1.782703
6	6	0	-4.039811	0.661304	0.970353
7	6	0	-2.665744	1.149943	1.012180
8	6	0	-2.104744	2.019586	0.168372
9	8	0	-7.875285	-0.912085	0.790469
10	6	0	-0.698525	2.423303	0.229438
11	8	0	-0.175709	3.150161	-0.586985
12	8	0	-0.014730	1.922805	1.268884
13	1	0	-4.783198	2.032808	-0.517797
14	1	0	-7.039134	1.076630	-0.583439
15	1	0	-5.918337	-1.804536	2.376675
16	1	0	-3.659286	-0.840431	2.453110
17	1	0	-2.044732	0.726359	1.794313
18	1	0	-2.646709	2.456574	-0.659492
19	1	0	-7.991228	-1.652847	1.391498
20	1	0	0.901367	2.213390	1.178544
21	6	0	6.043221	-1.304098	1.308533
22	6	0	5.997865	0.073078	1.445542
23	6	0	5.172893	0.807366	0.609340
24	6	0	4.316743	0.179931	-0.332163
25	6	0	4.445633	-1.216098	-0.479068
26	6	0	5.288860	-1.953087	0.335378
27	8	0	6.868246	-1.979662	2.131648
28	8	0	5.197664	2.138452	0.741607
29	8	0	3.764869	-1.821995	-1.472197
30	6	0	3.374745	1.024765	-1.088028
31	6	0	2.040056	0.569209	-1.486386
32	6	0	1.338160	-0.337586	-0.800597
33	6	0	-0.662292	-1.570435	-0.092896
34	6	0	-0.048146	-0.728182	-1.020212
35	6	0	-0.808277	-0.290263	-2.109690
36	6	0	-2.126699	-0.664805	-2.257319
37	6	0	-2.724950	-1.490213	-1.308356
38	6	0	-1.983599	-1.951913	-0.227140
39	8	0	-4.025129	-1.810931	-1.487682
40	8	0	3.665452	2.205785	-1.321967
41	1	0	6.619546	0.577254	2.171622
42	1	0	5.375991	-3.024530	0.198779
43	1	0	6.836060	-2.921222	1.941649
44	1	0	4.695356	2.506636	-0.017930
45	1	0	3.952067	-2.764413	-1.471235
46	1	0	1.593770	1.153877	-2.281640
47	1	0	1.820559	-0.829865	0.037993
48	1	0	-0.094261	-1.926400	0.758453
49	1	0	-0.366933	0.359336	-2.854516
50	1	0	-2.713049	-0.314483	-3.096595
51	1	0	-2.444367	-2.597832	0.510531
52	1	0	-4.369547	-2.251423	-0.705214

$(H \cdots T' + T \cdots H')_t$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.779818	1.911962	1.417574
2	6	0	0.555366	2.175839	1.631593
3	6	0	1.375779	2.536974	0.562887
4	6	0	0.840045	2.624831	-0.716806
5	6	0	-0.499966	2.348332	-0.918036
6	6	0	-1.338997	1.994566	0.137661
7	6	0	-2.742318	1.711313	-0.137368
8	6	0	-3.689119	1.428045	0.761775
9	8	0	2.672924	2.803405	0.827519
10	6	0	-5.079871	1.131057	0.419485
11	8	0	-5.927488	0.856162	1.241718
12	8	0	-5.361165	1.186526	-0.890683
13	1	0	-1.392148	1.623047	2.261990
14	1	0	0.984925	2.100939	2.622077
15	1	0	1.469938	2.906447	-1.550913
16	1	0	-0.905108	2.407320	-1.921241
17	1	0	-3.025450	1.734491	-1.184614
18	1	0	-3.486110	1.383751	1.823116
19	1	0	3.196440	2.725881	0.016640
20	1	0	-6.293589	0.961972	-0.997349
21	6	0	5.021159	-0.925630	1.225964
22	6	0	4.982428	0.222515	0.449834
23	6	0	4.035472	0.321320	-0.550510
24	6	0	3.063207	-0.682701	-0.770870
25	6	0	3.179432	-1.856361	0.000036
26	6	0	4.136997	-1.973713	0.994557
27	8	0	5.964018	-0.989302	2.184428
28	8	0	4.044865	1.445533	-1.296352
29	8	0	2.367424	-2.893137	-0.282140
30	6	0	2.032705	-0.444505	-1.799617
31	6	0	0.661527	-0.938102	-1.681408
32	6	0	0.046362	-1.123444	-0.509823
33	6	0	-1.822983	-1.608526	1.007118
34	6	0	-1.356452	-1.452871	-0.297627
35	6	0	-2.271568	-1.615394	-1.343397
36	6	0	-3.590266	-1.926724	-1.096545
37	6	0	-4.034711	-2.078903	0.214944
38	6	0	-3.144994	-1.917081	1.270850
39	8	0	-5.339547	-2.378866	0.397293
40	8	0	2.303032	0.275548	-2.770828
41	1	0	5.692272	1.021776	0.607689
42	1	0	4.206699	-2.887589	1.573038
43	1	0	5.919045	-1.830526	2.647140
44	1	0	3.469605	1.263521	-2.075082
45	1	0	2.566225	-3.633265	0.297280
46	1	0	0.125781	-0.978379	-2.622281
47	1	0	0.626612	-0.996162	0.398715
48	1	0	-1.136190	-1.476331	1.834794
49	1	0	-1.952530	-1.493889	-2.370392
50	1	0	-4.295021	-2.045566	-1.908880
51	1	0	-3.488291	-2.027539	2.292717
52	1	0	-5.552095	-2.383634	1.334282

$O^A \cdots H^a$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.194833	-0.848828	1.211507
2	6	0	5.929613	0.509800	1.236888
3	6	0	4.919370	1.015739	0.436931
4	6	0	4.104204	0.165483	-0.363168
5	6	0	4.451240	-1.206192	-0.396663
6	6	0	5.474811	-1.708930	0.384792
7	8	0	7.191046	-1.295749	1.995539
8	8	0	4.724688	2.334647	0.464789
9	8	0	3.793942	-2.012011	-1.248909

10	6	0	2.973495	0.745959	-1.076155
11	6	0	1.756653	0.004018	-1.418818
12	6	0	1.154882	-0.807272	-0.546548
13	6	0	-0.814485	-1.811990	0.521442
14	6	0	-0.217045	-1.295006	-0.627657
15	6	0	-0.999467	-1.188530	-1.781619
16	6	0	-2.327484	-1.557306	-1.780339
17	6	0	-2.913191	-2.038879	-0.611959
18	6	0	-2.147547	-2.178933	0.539016
19	8	0	-4.225729	-2.357189	-0.656161
20	8	0	2.957338	1.969141	-1.331247
21	1	0	6.516147	1.175898	1.853188
22	1	0	5.728637	-2.761495	0.336983
23	1	0	7.298933	-2.245586	1.895691
24	1	0	4.055431	2.539519	-0.226645
25	1	0	4.136971	-2.907469	-1.185525
26	1	0	1.240920	0.375274	-2.295540
27	1	0	1.686218	-1.066812	0.364422
28	1	0	-0.228780	-1.906404	1.428190
29	1	0	-0.568763	-0.802701	-2.696832
30	1	0	-2.931814	-1.462347	-2.672985
31	1	0	-2.598556	-2.559586	1.447736
32	1	0	-4.554510	-2.530189	0.230466
33	6	0	-4.681991	1.273983	-0.371335
34	6	0	-5.986932	0.830942	-0.356296
35	6	0	-6.461397	0.102226	0.732428
36	6	0	-5.618049	-0.166797	1.804796
37	6	0	-4.312482	0.290680	1.777363
38	6	0	-3.814168	1.012973	0.693802
39	6	0	-2.415490	1.424360	0.706677
40	6	0	-1.738008	2.029451	-0.270975
41	8	0	-7.745795	-0.317273	0.690694
42	6	0	-0.296884	2.289666	-0.130750
43	8	0	0.355414	2.125199	0.877462
44	8	0	0.243025	2.715533	-1.276595
45	1	0	-4.334797	1.832005	-1.231375
46	1	0	-6.652625	1.035546	-1.184514
47	1	0	-5.982606	-0.727872	2.657208
48	1	0	-3.659684	0.072114	2.614052
49	1	0	-1.862246	1.177825	1.608293
50	1	0	-2.185028	2.287651	-1.221660
51	1	0	-7.962902	-0.807562	1.488122
52	1	0	1.220727	2.664107	-1.214002

$O^{A} \cdots H^{b} + T \cdots T'$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.912085	1.428909	-0.880159
2	6	0	5.657791	0.193456	-1.451891
3	6	0	4.648654	-0.597761	-0.930707
4	6	0	3.819977	-0.144255	0.133313
5	6	0	4.156556	1.097786	0.720179
6	6	0	5.181023	1.878174	0.217264
7	8	0	6.909146	2.158328	-1.410141
8	8	0	4.467901	-1.796878	-1.489393
9	8	0	3.488992	1.486791	1.820995
10	6	0	2.689438	-0.970692	0.545771
11	6	0	1.446237	-0.430929	1.094140
12	6	0	0.892910	0.701664	0.649954
13	6	0	-0.932468	2.281828	0.208679
14	6	0	-0.465926	1.161487	0.897268
15	6	0	-1.356200	0.500665	1.751328
16	6	0	-2.652314	0.937471	1.906900
17	6	0	-3.100934	2.051019	1.199056
18	6	0	-2.234182	2.727722	0.349759
19	8	0	-4.389982	2.419074	1.367622
20	8	0	2.716284	-2.202093	0.333127
21	1	0	6.254443	-0.166114	-2.277878
22	1	0	5.426436	2.821793	0.690376
23	1	0	7.011314	2.987531	-0.934847
24	1	0	3.818992	-2.279334	-0.933555

25	1	0	3.827792	2.331530	2.129235
26	1	0	0.890707	-1.129649	1.707178
27	1	0	1.475178	1.327353	-0.019817
28	1	0	-0.264431	2.809459	-0.461804
29	1	0	-1.040755	-0.382524	2.291586
30	1	0	-3.340552	0.412887	2.556393
31	1	0	-2.579844	3.591882	-0.204983
32	1	0	-4.597200	3.171196	0.806239
33	6	0	-1.774651	-1.480522	-1.076345
34	6	0	-0.625304	-2.150155	-0.716090
35	6	0	-0.659307	-3.099015	0.308074
36	6	0	-1.875348	-3.414930	0.907318
37	6	0	-3.024848	-2.753457	0.519506
38	6	0	-2.995750	-1.753007	-0.454083
39	6	0	-4.210379	-1.001686	-0.732896
40	6	0	-4.294254	0.170266	-1.368746
41	8	0	0.449239	-3.727864	0.741587
42	6	0	-5.582758	0.853226	-1.509508
43	8	0	-6.666207	0.424701	-1.181467
44	8	0	-5.439567	2.073363	-2.056394
45	1	0	-1.718081	-0.732045	-1.856490
46	1	0	0.312873	-1.928779	-1.208133
47	1	0	-1.901010	-4.164700	1.687356
48	1	0	-3.963510	-2.993858	1.004948
49	1	0	-5.132295	-1.420176	-0.338666
50	1	0	-3.424258	0.690339	-1.746535
51	1	0	1.253584	-3.227661	0.490960
52	1	0	-6.316143	2.473910	-2.117551

$O^{c} \cdots H^{a} + T \cdots T'$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.300569	1.071554	-1.309765
2	6	0	5.129374	-0.281788	-1.056698
3	6	0	4.238598	-0.669199	-0.074673
4	6	0	3.448762	0.263329	0.630805
5	6	0	3.691952	1.624020	0.382040
6	6	0	4.603678	2.028562	-0.581162
7	8	0	6.186725	1.411415	-2.265903
8	8	0	4.112007	-1.995987	0.155598
9	8	0	3.044324	2.533741	1.137532
10	6	0	2.436060	-0.257202	1.577804
11	6	0	1.091056	0.305226	1.674897
12	6	0	0.515947	1.005783	0.691436
13	6	0	-1.237540	2.323800	-0.407710
14	6	0	-0.864567	1.460820	0.623348
15	6	0	-1.849118	1.067329	1.536710
16	6	0	-3.143691	1.523374	1.430567
17	6	0	-3.491214	2.393323	0.399158
18	6	0	-2.531601	2.796029	-0.522064
19	8	0	-4.777867	2.800229	0.335906
20	8	0	2.695828	-1.271315	2.233546
21	1	0	5.700228	-1.022677	-1.597866
22	1	0	4.781857	3.084033	-0.750890
23	1	0	6.237752	2.367174	-2.352299
24	1	0	3.672439	-2.093538	1.026187
25	1	0	3.299622	3.422216	0.876046
26	1	0	0.536613	-0.019034	2.547594
27	1	0	1.121507	1.263324	-0.171623
28	1	0	-0.496451	2.633140	-1.135294
29	1	0	-1.606306	0.374829	2.332274
30	1	0	-3.905878	1.200696	2.127258
31	1	0	-2.800396	3.463579	-1.332246
32	1	0	-4.906598	3.382726	-0.417301
33	6	0	-3.586886	-1.989588	0.215355
34	6	0	-4.912118	-1.613808	0.220814
35	6	0	-5.372298	-0.677034	-0.703054
36	6	0	-4.494499	-0.129781	-1.629783
37	6	0	-3.165246	-0.509686	-1.617158
38	6	0	-2.682829	-1.444715	-0.702709
39	6	0	-1.267053	-1.790676	-0.730130

40	6	0	-0.657009	-2.740021	-0.014056
41	8	0	-6.678916	-0.334609	-0.645363
42	6	0	0.781370	-3.009986	-0.079926
43	8	0	1.332228	-3.852734	0.596205
44	8	0	1.457956	-2.250257	-0.950654
45	1	0	-3.249440	-2.707686	0.951575
46	1	0	-5.604908	-2.029181	0.940916
47	1	0	-4.846196	0.605751	-2.343697
48	1	0	-2.482216	-0.062184	-2.328889
49	1	0	-0.659580	-1.200574	-1.408736
50	1	0	-1.189267	-3.376347	0.680461
51	1	0	-6.876245	0.331599	-1.308962
52	1	0	2.404998	-2.439709	-0.833716

$H^{1} \cdots O^{\alpha} + O^{A} \cdots H^{a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.703687	2.210205	0.884076
2	6	0	4.481865	2.771519	1.215660
3	6	0	3.331021	2.345256	0.565726
4	6	0	3.392708	1.340170	-0.415300
5	6	0	4.642787	0.792985	-0.722863
6	6	0	5.798155	1.218460	-0.086311
7	8	0	6.791709	2.666080	1.542972
8	8	0	2.186118	2.927061	0.953426
9	8	0	4.685527	-0.141497	-1.699589
10	6	0	2.163056	0.947008	-1.153029
11	6	0	1.657787	-0.414626	-1.106160
12	6	0	2.109195	-1.326656	-0.232270
13	6	0	2.235517	-3.487132	0.920508
14	6	0	1.630231	-2.685365	-0.049560
15	6	0	0.584644	-3.238705	-0.800011
16	6	0	0.164941	-4.532778	-0.590472
17	6	0	0.784686	-5.316042	0.383824
18	6	0	1.825150	-4.788169	1.141205
19	8	0	0.331838	-6.575864	0.546548
20	8	0	1.535617	1.819896	-1.759692
21	1	0	4.416666	3.530648	1.982336
22	1	0	6.758645	0.794045	-0.354555
23	1	0	7.580343	2.208866	1.239776
24	1	0	1.376782	2.523559	0.585263
25	1	0	5.589607	-0.435935	-1.835191
26	1	0	0.837356	-0.623617	-1.782417
27	1	0	2.918973	-1.030826	0.428375
28	1	0	3.045577	-3.081191	1.514535
29	1	0	0.087538	-2.649476	-1.559486
30	1	0	-0.643801	-4.956376	-1.171132
31	1	0	2.308448	-5.393459	1.898741
32	1	0	0.823326	-7.021625	1.241866
33	6	0	-5.537612	1.086421	1.163469
34	6	0	-6.867130	0.868516	1.451220
35	6	0	-7.763304	0.578232	0.422951
36	6	0	-7.311931	0.509840	-0.890042
37	6	0	-5.974235	0.730116	-1.163589
38	6	0	-5.059834	1.022115	-0.150782
39	6	0	-3.663746	1.242585	-0.507786
40	6	0	-2.653996	1.536790	0.317326
41	8	0	-9.054408	0.373209	0.762087
42	6	0	-1.275662	1.733956	-0.140464
43	8	0	-0.369520	1.984014	0.641602
44	8	0	-1.086889	1.620070	-1.443475
45	1	0	-4.861968	1.309768	1.979010
46	1	0	-7.230845	0.918953	2.469113
47	1	0	-8.004422	0.286099	-1.692738
48	1	0	-5.630359	0.674454	-2.189627
49	1	0	-3.437564	1.153126	-1.565531
50	1	0	-2.784120	1.645517	1.385743
51	1	0	-9.578497	0.182409	-0.020511
52	1	0	-0.119499	1.713089	-1.648564

$H^{2} \cdots O^{\alpha}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.276014	-1.761674	-0.492631
2	6	0	2.914815	-3.076434	-0.751609
3	6	0	1.698216	-3.549412	-0.290544
4	6	0	0.760099	-2.698670	0.357698
5	6	0	1.189049	-1.384046	0.643479
6	6	0	2.431935	-0.931258	0.243055
7	8	0	4.464654	-1.343069	-0.943550
8	8	0	1.420817	-4.839109	-0.507659
9	8	0	0.386107	-0.587283	1.376207
10	6	0	-0.553747	-3.244366	0.709420
11	6	0	-1.771833	-2.418687	0.781668
12	6	0	-2.045037	-1.443498	-0.084571
13	6	0	-3.671963	-0.089094	-1.358226
14	6	0	-3.299976	-0.694900	-0.159499
15	6	0	-4.152080	-0.547102	0.938669
16	6	0	-5.329103	0.165732	0.842966
17	6	0	-5.688862	0.756604	-0.366123
18	6	0	-4.850467	0.631900	-1.470674
19	8	0	-6.851611	1.442736	-0.405019
20	8	0	-0.697215	-4.462624	0.881674
21	1	0	3.586376	-3.738893	-1.279235
22	1	0	2.764331	0.054476	0.534163
23	1	0	4.620711	-0.395098	-0.770188
24	1	0	0.600350	-5.039755	-0.004017
25	1	0	0.747940	0.304733	1.410419
26	1	0	-2.517395	-2.780834	1.480493
27	1	0	-1.295503	-1.180649	-0.825984
28	1	0	-3.032915	-0.190313	-2.227242
29	1	0	-3.879757	-0.979663	1.893017
30	1	0	-5.977775	0.283493	1.700932
31	1	0	-5.122429	1.087169	-2.415681
32	1	0	-7.000598	1.801459	-1.283949
33	6	0	0.724553	3.011603	0.946716
34	6	0	-0.637920	3.101941	1.134546
35	6	0	-1.509428	2.645152	0.145453
36	6	0	-0.998292	2.108402	-1.032223
37	6	0	0.368032	2.007849	-1.201610
38	6	0	1.257610	2.457688	-0.224110
39	6	0	2.682743	2.258299	-0.432997
40	6	0	3.693692	2.674955	0.335964
41	8	0	-2.830407	2.749944	0.383979
42	6	0	5.055067	2.223649	0.046012
43	8	0	5.349763	1.276506	-0.661682
44	8	0	5.983618	2.948857	0.665202
45	1	0	1.382508	3.359557	1.732725
46	1	0	-1.046520	3.515048	2.047130
47	1	0	-1.669538	1.766862	-1.808705
48	1	0	0.756792	1.568100	-2.112108
49	1	0	2.940559	1.655737	-1.299305
50	1	0	3.562626	3.324331	1.190837
51	1	0	-3.335720	2.290603	-0.298113
52	1	0	6.851457	2.578181	0.456621

$H^{3} \cdots O^{\alpha} + H^{4} \cdots O^{\gamma}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.707740	-0.783375	1.578348
2	6	0	5.273382	0.468306	1.394482
3	6	0	4.692088	1.342448	0.491557
4	6	0	3.490668	1.019673	-0.191823
5	6	0	2.985720	-0.289307	-0.020867
6	6	0	3.581654	-1.176979	0.863602
7	8	0	5.312667	-1.608949	2.455601
8	8	0	5.299592	2.519851	0.301467
9	8	0	1.944492	-0.682326	-0.765089

10	6	0	2.876917	2.046132	-1.047332
11	6	0	1.425098	2.155273	-1.236788
12	6	0	0.542720	1.845685	-0.283791
13	6	0	-1.629867	1.913968	0.861884
14	6	0	-0.901511	2.047115	-0.320201
15	6	0	-1.604050	2.354008	-1.490240
16	6	0	-2.975695	2.499752	-1.482507
17	6	0	-3.684058	2.347847	-0.292414
18	6	0	-3.000870	2.081950	0.887405
19	8	0	-5.032224	2.452139	-0.341689
20	8	0	3.584016	2.919777	-1.569549
21	1	0	6.174504	0.750946	1.919820
22	1	0	3.179468	-2.177060	0.972121
23	1	0	4.850688	-2.450693	2.494211
24	1	0	4.861953	2.939935	-0.471457
25	1	0	1.778229	-1.638730	-0.650477
26	1	0	1.129376	2.664379	-2.146838
27	1	0	0.919762	1.412260	0.637853
28	1	0	-1.110683	1.673535	1.782103
29	1	0	-1.075418	2.454199	-2.429734
30	1	0	-3.517192	2.705930	-2.396541
31	1	0	-3.545480	1.979280	1.817350
32	1	0	-5.422508	2.094686	0.464612
33	6	0	-3.391318	-1.485396	-0.569372
34	6	0	-4.562678	-0.885863	-0.161988
35	6	0	-4.762474	-0.609133	1.186697
36	6	0	-3.803416	-0.965866	2.125550
37	6	0	-2.625223	-1.550780	1.701455
38	6	0	-2.395647	-1.822963	0.352642
39	6	0	-1.134244	-2.432040	-0.045931
40	6	0	-0.889564	-3.080211	-1.189419
41	8	0	-5.888841	0.071989	1.517504
42	6	0	0.433714	-3.641886	-1.453944
43	8	0	1.458019	-3.370088	-0.849348
44	8	0	0.429622	-4.516148	-2.456835
45	1	0	-3.235711	-1.664329	-1.625516
46	1	0	-5.315405	-0.588404	-0.879667
47	1	0	-3.958194	-0.746461	3.175183
48	1	0	-1.864631	-1.797790	2.432216
49	1	0	-0.326284	-2.365337	0.677542
50	1	0	-1.652618	-3.258699	-1.934841
51	1	0	-5.955356	0.167920	2.471816
52	1	0	1.332232	-4.835663	-2.588279

$H^{4} \cdots O^{\alpha} + O^{B} \cdots H^{a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.135916	2.625483	1.024250
2	6	0	7.270317	2.659043	-0.353403
3	6	0	6.843745	1.573042	-1.100046
4	6	0	6.202475	0.458983	-0.497544
5	6	0	6.148702	0.441733	0.911583
6	6	0	6.598950	1.512537	1.665154
7	8	0	7.575027	3.696325	1.713039
8	8	0	7.040691	1.626144	-2.421721
9	8	0	5.694693	-0.670153	1.523228
10	6	0	5.660299	-0.591110	-1.377223
11	6	0	4.453193	-1.359980	-1.056123
12	6	0	3.447289	-0.882812	-0.317848
13	6	0	1.245068	-0.870830	0.769935
14	6	0	2.158906	-1.517009	-0.063738
15	6	0	1.788689	-2.753427	-0.605079
16	6	0	0.563863	-3.318405	-0.322237
17	6	0	-0.331242	-2.658070	0.518054
18	6	0	0.013335	-1.426766	1.065138
19	8	0	-1.519438	-3.252386	0.767771
20	8	0	6.179089	-0.789973	-2.484364
21	1	0	7.730324	3.505268	-0.843424
22	1	0	6.554147	1.470550	2.747143
23	1	0	7.446766	3.566098	2.656520
24	1	0	6.833030	0.732456	-2.773683

25	1	0	5.721298	-0.554225	2.476670
26	1	0	4.373362	-2.295910	-1.596552
27	1	0	3.574801	0.087693	0.151391
28	1	0	1.506298	0.088990	1.199936
29	1	0	2.465553	-3.286004	-1.260656
30	1	0	0.282703	-4.274484	-0.744261
31	1	0	-0.681144	-0.909921	1.715803
32	1	0	-2.071313	-2.694532	1.357320
33	6	0	-7.722368	1.284768	0.853641
34	6	0	-8.836497	2.089673	0.772319
35	6	0	-9.529534	2.199070	-0.433300
36	6	0	-9.092285	1.496625	-1.550940
37	6	0	-7.971923	0.692135	-1.454272
38	6	0	-7.264430	0.566323	-0.257613
39	6	0	-6.094525	-0.299214	-0.221243
40	6	0	-5.305544	-0.544381	0.831623
41	8	0	-10.614831	3.000654	-0.453966
42	6	0	-4.148855	-1.431456	0.775655
43	8	0	-3.439226	-1.646131	1.747940
44	8	0	-3.917478	-1.994713	-0.408788
45	1	0	-7.201859	1.216492	1.800056
46	1	0	-9.186981	2.642741	1.633733
47	1	0	-9.626630	1.579532	-2.489930
48	1	0	-7.637567	0.147380	-2.329088
49	1	0	-5.852741	-0.790580	-1.158273
50	1	0	-5.471298	-0.100406	1.803721
51	1	0	-11.016091	2.998334	-1.327152
52	1	0	-3.132154	-2.563333	-0.344835

$H^{3} \cdots O^{\gamma} + H^{4} \cdots O^{\alpha}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.826555	1.558682	-1.156693
2	6	0	5.401580	0.347924	-1.508457
3	6	0	4.951203	-0.812192	-0.900652
4	6	0	3.868420	-0.797994	0.013549
5	6	0	3.367134	0.461965	0.400371
6	6	0	3.828321	1.628731	-0.189488
7	8	0	5.300674	2.664019	-1.764964
8	8	0	5.561884	-1.956977	-1.230288
9	8	0	2.473477	0.508986	1.399337
10	6	0	3.340400	-2.084507	0.492521
11	6	0	1.908558	-2.303269	0.738503
12	6	0	0.947860	-1.699656	0.033204
13	6	0	-1.306727	-1.543661	-0.948480
14	6	0	-0.483084	-1.983408	0.088397
15	6	0	-1.079343	-2.676250	1.146141
16	6	0	-2.438344	-2.912233	1.170048
17	6	0	-3.247042	-2.467747	0.123689
18	6	0	-2.667032	-1.793418	-0.948293
19	8	0	-4.571565	-2.700524	0.210271
20	8	0	4.093099	-3.061735	0.594897
21	1	0	6.209866	0.307375	-2.224634
22	1	0	3.433059	2.587232	0.123944
23	1	0	4.845839	3.445972	-1.440835
24	1	0	5.235726	-2.641968	-0.608657
25	1	0	2.188646	1.421406	1.572823
26	1	0	1.690549	-3.127967	1.407248
27	1	0	1.240493	-0.940542	-0.686698
28	1	0	-0.871528	-0.996875	-1.776701
29	1	0	-0.476841	-3.014620	1.979742
30	1	0	-2.896651	-3.426494	2.004826
31	1	0	-3.285557	-1.451122	-1.768229
32	1	0	-5.079329	-2.114215	-0.384785
33	6	0	-1.926794	1.186571	1.104494
34	6	0	-0.700742	1.470968	1.663314
35	6	0	-0.100178	2.700063	1.413234
36	6	0	-0.730838	3.643734	0.615636
37	6	0	-1.961456	3.343475	0.059294
38	6	0	-2.583032	2.115916	0.289769
39	6	0	-3.848862	1.822647	-0.372672

40	6	0	-4.587941	0.726424	-0.182873
41	8	0	1.127734	2.913076	1.963389
42	6	0	-5.721217	0.352231	-1.024154
43	8	0	-6.115731	-0.797844	-1.124020
44	8	0	-6.281976	1.345585	-1.706668
45	1	0	-2.359287	0.211735	1.287872
46	1	0	-0.190546	0.740321	2.276537
47	1	0	-0.258335	4.598277	0.418354
48	1	0	-2.445990	4.075427	-0.575479
49	1	0	-4.174011	2.545049	-1.114420
50	1	0	-4.310964	-0.027059	0.539710
51	1	0	1.435764	3.805233	1.779288
52	1	0	-6.976068	0.976167	-2.267969

References

1 S. A. Kovalenko, A. L. Dobryakov, J. Ruthmann and N. P. Ernsting, *Phys. Rev. A*, 1999, **59**, 2369–2384.