

Supporting Information

Unprecedentedly Ultrafast Dynamics of Excited States of C=C Photo-switching Molecules in Nanocrystals/Microcrystals

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Experimental and Computational Methods

Materials: TS, DPE, SP, acetone and acetonitrile are purchased from J&K. All the materials were used without further purification.

Preparation of the nanocrystal/microcrystal suspension:

The nanocrystal/microcrystal was fabricated by reprecipitation method. Inject 100 μ l 20 mM high-concentration acetone solution of DPE/SP/TS into 100 ml water with sonicating for 10-15 min. For DPE and SP, the large particles were filtered out with a 220 nm water filter membrane to obtain a clear colorless nanocrystal suspension. For TS, the sizes of particles are large, so the filtration membrane filtration is not required to obtain an ivory-white microcrystal. The absorption spectra of solutions and nanocrystal/microcrystal are measured by Lambda 950 UV/Vis Spectrometer. Dynamic light scattering (DLS) data was obtained from Malvern Zetasizer Nano ZS90. DLS and scanning electron microscope (SEM) was used to measure the size of nanocrystal/microcrystal suspension.

Femtosecond transient absorption (fs-TA) experiments. The fs-TA measurements were performed with an apparatus and methods detailed previously.^[1,2] Fs-TA spectra were recorded by employing the harmonic (300 nm light) for the pump pulse and white-light continuum (350-750 nm light) for the probe pulse generated from the 800 nm output of a femtosecond regenerative amplified Ti:sapphire laser system. In this paper, the single-wavelength fitting is completed based on equation 1. The t is referred to delay time, and t_0 means zero time. The t_p , and A represent the instrument response value and the proportion of species respectively.

$$S(t) = e^{-\frac{(t-t_0)^2}{t_p}} * \sum_i A_i e^{-\frac{t-t_0}{t_i}} \quad (1)$$

Structural Characterization: The structure of the single crystals of DPE, SP and TS are given by a Rigaku OD (Enhance Cu X-ray source, $K\alpha$, $\lambda = 1.54184 \text{ \AA}$) using a CCD Plate (XtaLAB Pro: Kappa single) at 100 K. The structure of the crystal is solved by direct method in Olex2. The detailed structure information of the crystals is shown in table S1.

Theoretical calculations: The theoretical calculations are run in Gaussian16 software packages.^[2] DFT and TD-DFT calculations with B3LYP and 6-31G* being selected as function and basis set to perform the PES scanning for DPE, SP and TS.

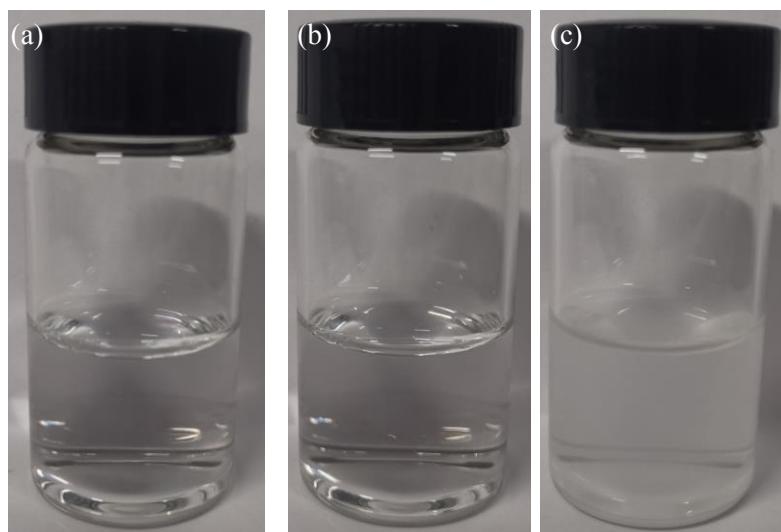


Figure S1. (a) DPE nanocrystal suspension, (b) SP nanocrystal suspension and (c) TS microcrystal suspension.

Table S1. Dynamic light scattering results of DPE, SP and TS nanocrystals/microcrystal suspensions.

Dynamic light scattering			
	Z-Average(d.nm)	PdI	St Dev(d.nm)
DPE nanocrystal	1 98	0.246	19.85
	2 95	0.271	21.90
	3 94	0.263	20.58
SP nanocrystal	1 162	0.416	10.62
	2 147	0.428	11.61
	3 151	0.534	12.33
TS microcrystal	1 2414	1.000	51.0
	2 2381	1.000	31.16
	3 2496	1.000	72.31

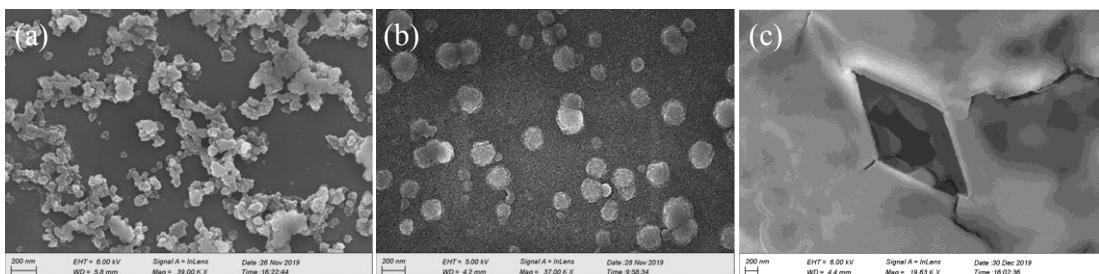


Figure S2. (a-b) SEM images of DPE and SP nanocrystal prepared by the reprecipitation method with 220 nm water system membrane filtration. (c) SEM images of TS microcrystal without filter by 220 nm water system membrane.

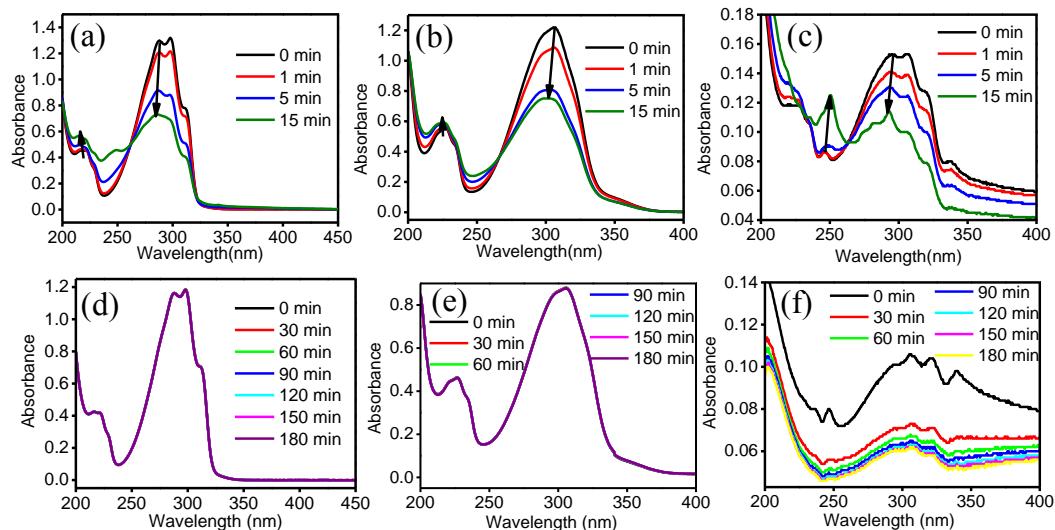


Figure S3. UV-vis spectra of the isomerization process of (a) DPE, (b) SP and (c) TS nanocrystal/microcrystal suspensions after irradiation by 254 nm from trans to cis isomers; (d-f) DPE, SP and TS nanocrystal/microcrystal suspension stability test.

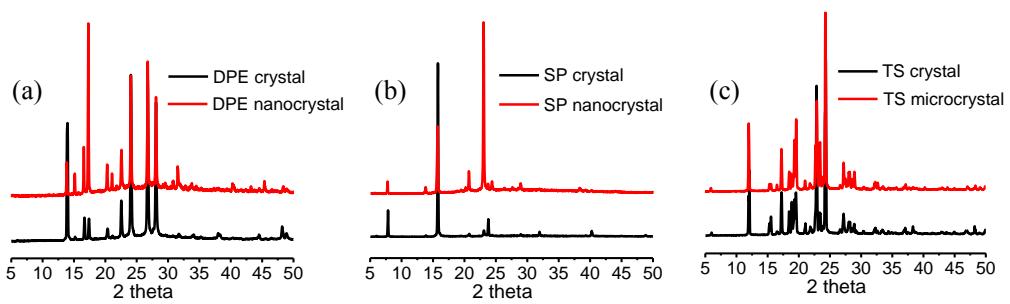


Figure S4. The comparison of PXRD from the nanocrystals/microcrystals and the single crystals for DPE (a), SP (b) and TS (c).

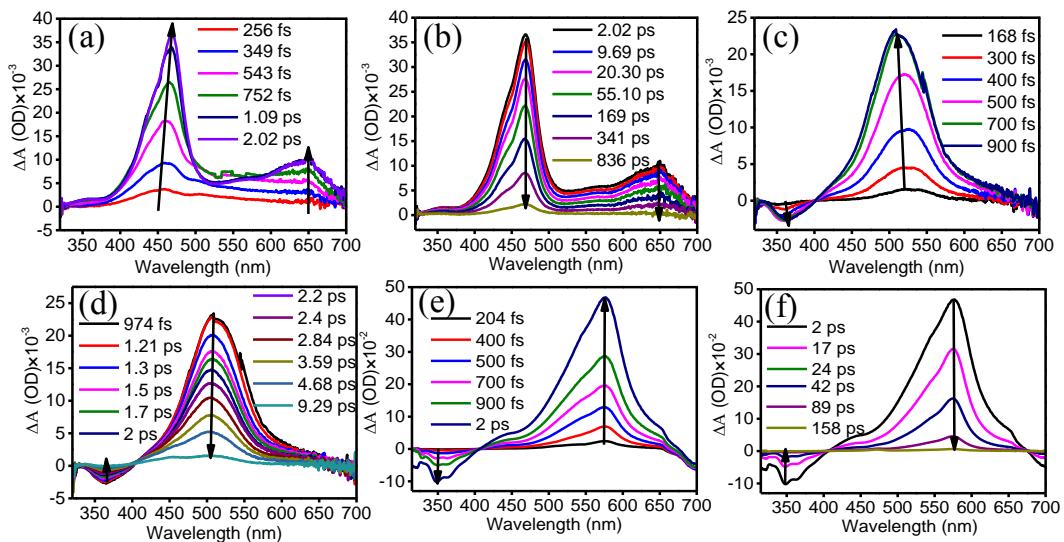


Figure S5. Fs-TA spectra of DPE (a-b), SP (c-d) and TS (e-f) in MeCN. .

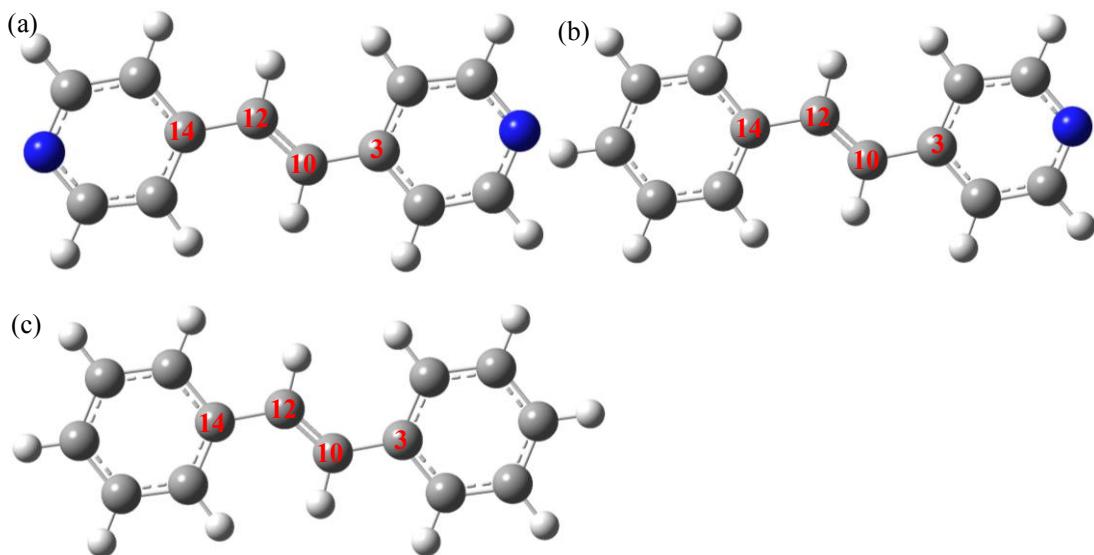
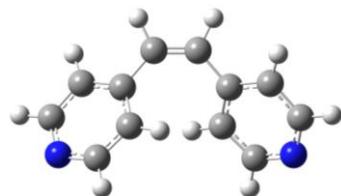


Figure S6. The structure of the trans isomer for (a) DPE, (b) SP and (c) TS.

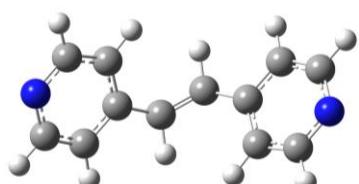
XYZ coordinates of selected optimized structures

Optimized DPE-cis-S₀



C	-2.40924500	-1.42947800	0.84668100
C	-1.41493700	-0.45482800	0.80830000
C	-1.63289100	0.71845400	0.06770600
C	-2.87672800	0.83610900	-0.57309200
C	-3.80007500	-0.20349000	-0.47758300
H	-2.25306700	-2.34095200	1.42154100
H	-0.49182000	-0.59979800	1.35865500
H	-3.11846300	1.72768600	-1.14583400
H	-4.76273900	-0.12575600	-0.98068700
C	-0.67411900	1.83675100	0.00099100
H	-1.14844700	2.81709800	-0.03771000
C	0.67411900	1.83675100	-0.00099100
H	1.14844700	2.81709800	0.03771000
C	1.63289100	0.71845400	-0.06770600
C	2.87672800	0.83610900	0.57309200
C	1.41493700	-0.45482800	-0.80830000
C	3.80007500	-0.20349000	0.47758300
H	3.11846300	1.72768600	1.14583400
C	2.40924500	-1.42947800	-0.84668100
H	0.49182000	-0.59979800	-1.35865500
H	4.76274000	-0.12575600	0.98068600
H	2.25306700	-2.34095200	-1.42154100
N	3.58790800	-1.32848300	-0.21614200
N	-3.58790800	-1.32848300	0.21614200

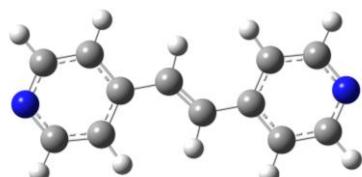
Optimized DPE-IC-S₀



C	-3.18165400	1.24550800	0.83632200
C	-2.06705600	1.14252000	0.01156800
C	-1.79512100	-0.08286700	-0.62847400
C	-2.70975800	-1.12714800	-0.40245300
C	-3.79078500	-0.91649600	0.44987900
H	-3.39526900	2.18416900	1.34509400

H	-1.40334400	1.99284200	-0.10998500
H	-2.56689700	-2.09527600	-0.87458600
H	-4.49561500	-1.72413200	0.64142900
C	-0.59772200	-0.33367300	-1.43112100
H	-0.46858600	-1.42404500	-1.49803000
C	0.59772300	0.33367500	-1.43112100
H	0.46858600	1.42404600	-1.49802900
C	1.79512100	0.08286700	-0.62847400
C	2.70975800	1.12714900	-0.40245200
C	2.06705600	-1.14252000	0.01156800
C	3.79078500	0.91649600	0.44988100
H	2.56689700	2.09527700	-0.87458400
C	3.18165400	-1.24550900	0.83632200
H	1.40334400	-1.99284200	-0.10998700
H	4.49561500	1.72413100	0.64143200
H	3.39526900	-2.18417000	1.34509300
N	4.04363900	-0.24370100	1.06882000
N	-4.04363900	0.24370000	1.06881900

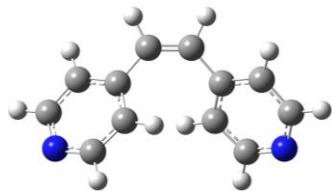
Optimized DPE-trans-S₀



C	3.88362400	1.23898500	0.00000100
C	2.49916200	1.10109500	0.00000200
C	1.93505100	-0.18743500	0.00000000
C	2.83747700	-1.26381300	-0.00000100
C	4.20917400	-1.01537200	-0.00000200
H	4.32932300	2.23251500	0.00000300
H	1.87593900	1.98986500	0.00000300
H	2.47075800	-2.28716800	-0.00000200
H	4.91332100	-1.84609000	-0.00000300
C	0.49415200	-0.45801600	0.00000000
H	0.23614800	-1.51566400	0.00000100
C	-0.49415200	0.45801600	0.00000000
H	-0.23614800	1.51566400	-0.00000100
C	-1.93505100	0.18743500	0.00000000
C	-2.83747700	1.26381300	-0.00000200
C	-2.49916200	-1.10109500	0.00000200
C	-4.20917400	1.01537200	-0.00000100
H	-2.47075800	2.28716800	-0.00000300
C	-3.88362400	-1.23898500	0.00000100
H	-1.87593900	-1.98986500	0.00000300

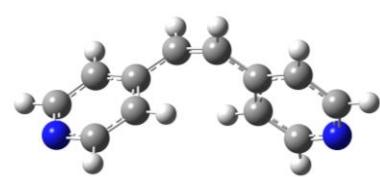
H	-4.91332100	1.84609000	-0.00000300
H	-4.32932300	-2.23251500	0.00000300
N	-4.74484900	-0.21056000	0.00000000
N	4.74484900	0.21056000	0.00000000

Optimized DPE-cis-S₁



C	-0.84880300	2.34280200	-1.38072400
C	-0.84880300	1.39878200	-0.36700600
C	-0.02895800	1.59467200	0.74260300
C	0.73291700	2.76088500	0.76773300
C	0.66735100	3.63891600	-0.30281100
H	-1.48462500	2.20600200	-2.25009100
H	-1.48762300	0.52857100	-0.43727100
H	1.37703800	2.98099200	1.61093000
H	1.26387900	4.54623800	-0.30121200
C	0.00849900	0.66686600	1.88894500
H	0.04510700	1.15567400	2.85840500
C	-0.00849900	-0.66686600	1.88894500
H	-0.04510700	-1.15567400	2.85840500
C	0.02895800	-1.59467200	0.74260300
C	-0.73291700	-2.76088500	0.76773300
C	0.84880300	-1.39878200	-0.36700600
C	-0.66735100	-3.63891600	-0.30281100
H	-1.37703800	-2.98099200	1.61093000
C	0.84880300	-2.34280200	-1.38072400
H	1.48762300	-0.52857100	-0.43727100
H	-1.26387900	-4.54623800	-0.30121200
H	1.48462500	-2.20600200	-2.25009100
N	0.10503300	-3.44660300	-1.36760000
N	-0.10503300	3.44660300	-1.36760000

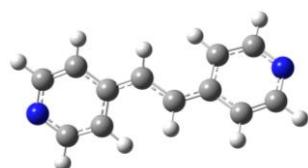
Optimized DPE-IC-S₁



C	2.88331400	-1.12073600	-1.13520600
C	1.73646000	-0.34404400	-0.93305300
C	1.72239600	0.57633700	0.12979400
C	2.86812100	0.67495800	0.94403400

C	3.96324800	-0.13988900	0.66182900
H	2.94144300	-1.85458900	-1.94879800
H	0.87066400	-0.45365800	-1.58131000
H	2.89753200	1.37285100	1.77441800
H	4.87994500	-0.10321300	1.26253600
C	0.56711500	1.37656900	0.38760700
H	0.59658700	2.03862800	1.26186400
C	-0.56673100	1.37107700	-0.40821800
H	-0.59640100	2.02029500	-1.29188500
C	-1.72228300	0.57518000	-0.13817800
C	-1.73865900	-0.32539100	0.94146600
C	-2.86589400	0.65791600	-0.95719400
C	-2.88565800	-1.09879800	1.15500500
H	-0.87463100	-0.42240600	1.59403400
C	-3.96117100	-0.15246100	-0.66305100
H	-2.89345700	1.34029200	-1.80042400
H	-2.94555200	-1.81736900	1.98199200
H	-4.87619100	-0.12771500	-1.26690900
N	-3.97605300	-1.01795000	0.37349000
N	3.97584000	-1.02453900	-0.35842100

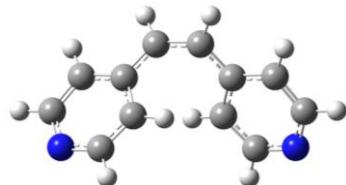
Optimized DPE-ts1-S₁



C	-1.20987500	3.55581700	-0.66110400
C	-1.02437700	2.24060500	-0.26266600
C	0.22890900	1.85097000	0.30741600
C	1.20987500	2.88208400	0.42011800
C	0.90477700	4.16139400	-0.00595100
H	-2.15859000	3.86292000	-1.09925300
H	-1.81730800	1.50665500	-0.38170200
H	2.18575700	2.65833800	0.84408900
H	1.64401300	4.95646000	0.07688300
C	0.48518800	0.52798300	0.72946700
H	1.48786700	0.31329900	1.11005800
C	-0.48518800	-0.52798300	0.72946700
H	-1.48786700	-0.31329900	1.11005800
C	-0.22890900	-1.85097000	0.30741600
C	-1.20987500	-2.88208400	0.42011800
C	1.02437700	-2.24060500	-0.26266600
C	-0.90477700	-4.16139400	-0.00595100
H	-2.18575700	-2.65833800	0.84408900

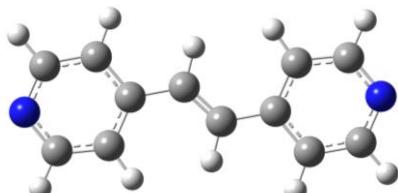
C	1.20987500	-3.55581700	-0.66110400
H	1.81730800	-1.50665500	-0.38170200
H	-1.64401300	-4.95646000	0.07688300
H	2.15859000	-3.86292000	-1.09925300
N	0.28620000	-4.52350300	-0.53053600
N	-0.28620000	4.52350300	-0.53053600

Optimized DPE-ts2-S₁



C	2.33811100	-1.36477800	-0.92841300
C	1.36123100	-0.38124700	-0.79777000
C	1.62951300	0.76075300	0.02529800
C	2.91718600	0.79578100	0.64007800
C	3.79904800	-0.24777900	0.43558500
H	2.14419400	-2.23444600	-1.55524000
H	0.42269300	-0.46332400	-1.33382600
H	3.19107400	1.63253000	1.27757700
H	4.77893600	-0.23412500	0.90995800
C	0.66808800	1.76799000	0.26269600
H	0.98542500	2.61686300	0.87659300
C	-0.66808800	1.76799000	-0.26269600
H	-0.98542500	2.61686200	-0.87659400
C	-1.62951300	0.76075300	-0.02529800
C	-2.91718600	0.79578100	-0.64007800
C	-1.36123100	-0.38124700	0.79777000
C	-3.79904700	-0.24777900	-0.43558500
H	-3.19107400	1.63253000	-1.27757700
C	-2.33811100	-1.36477800	0.92841300
H	-0.42269300	-0.46332400	1.33382600
H	-4.77893600	-0.23412500	-0.90995800
H	-2.14419400	-2.23444600	1.55524000
N	-3.53770000	-1.32883100	0.33448800
N	3.53770000	-1.32883100	-0.33448900

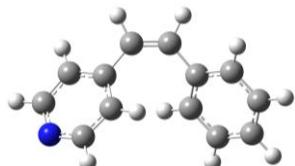
Optimized DPE-trans-S₁



C	3.86108800	1.23244200	0.00000200
C	2.48540200	1.09326500	0.00000200

C	1.92838100	-0.18683300	0.00000000
C	2.82245600	-1.25574700	-0.00000200
C	4.18637500	-1.00943100	-0.00000200
H	4.30586600	2.22279300	0.00000300
H	1.86533300	1.97982600	0.00000300
H	2.45782600	-2.27609300	-0.00000300
H	4.88962400	-1.83662300	-0.00000400
C	0.48642200	-0.45631800	0.00000100
H	0.22535200	-1.50957300	0.00000100
C	-0.48642200	0.45631800	0.00000000
H	-0.22535200	1.50957300	-0.00000100
C	-1.92838100	0.18683300	0.00000000
C	-2.82245600	1.25574700	-0.00000200
C	-2.48540200	-1.09326500	0.00000200
C	-4.18637500	1.00943100	-0.00000200
H	-2.45782600	2.27609300	-0.00000300
C	-3.86108800	-1.23244200	0.00000200
H	-1.86533300	-1.97982600	0.00000300
H	-4.88962400	1.83662300	-0.00000300
H	-4.30586600	-2.22279300	0.00000300
N	-4.71476900	-0.20938700	0.00000000
N	4.71476900	0.20938700	-0.00000100

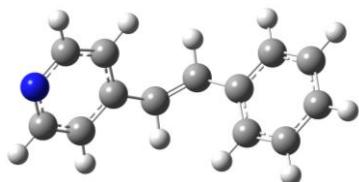
Optimized SP-cis-S₀



C	2.35470200	-1.42857000	-0.91064600
C	1.40002500	-0.41947700	-0.85247200
C	1.62170900	0.73458600	-0.08456100
C	2.84372100	0.85356600	0.59592200
C	3.79418100	-0.16130700	0.54696800
H	2.16725300	-2.30906800	-1.51501400
H	0.48136000	-0.51665800	-1.41725400
H	3.04243800	1.74940200	1.17522800
H	4.72661700	-0.05292100	1.08954900
C	0.65993000	1.85070000	-0.02509200
H	1.12724700	2.83287000	0.00049100
C	-0.68465400	1.84479100	-0.01713000
H	-1.16720900	2.81834900	-0.06278900
C	-1.63157400	0.71841600	0.06333700
C	-2.87106500	0.80568200	-0.58522000
C	-1.40451800	-0.43514600	0.82729500

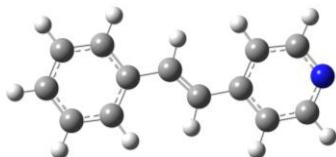
C	-3.78118800	-0.24059800	-0.47306800
H	-3.12070000	1.67950300	-1.17731000
C	-2.38512600	-1.41862700	0.88239900
H	-0.48320800	-0.55905900	1.38136400
H	-4.73983000	-0.18554800	-0.98219000
H	-2.22159200	-2.31396400	1.47620600
N	-3.55929900	-1.34550600	0.24436900
C	3.55196000	-1.30852300	-0.20545000
H	4.29409800	-2.09731500	-0.25255000

Optimized SP-IC-S₀



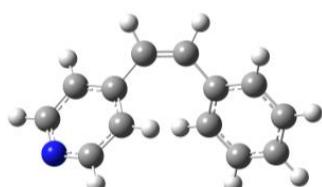
C	3.11921300	-1.35403100	0.77853100
C	2.01087000	-1.13370200	-0.02664500
C	1.78777800	0.12669400	-0.61617400
C	2.73632500	1.14146500	-0.39042400
C	3.84040000	0.91905500	0.42280100
H	3.26436400	-2.32542200	1.23781400
H	1.29128100	-1.92941600	-0.17814000
H	2.58823700	2.11371300	-0.84799100
H	4.54948500	1.72048900	0.59683100
C	0.58717600	0.43667100	-1.38880400
H	0.46372800	1.52811900	-1.38304100
C	-0.60874300	-0.22124700	-1.45146200
H	-0.48110900	-1.30278100	-1.59337500
C	-1.80170300	-0.03040200	-0.63028400
C	-2.73434900	-1.07317200	-0.50144500
C	-2.05590000	1.13068700	0.12303600
C	-3.81186200	-0.92587100	0.36335400
H	-2.60779200	-1.99356600	-1.06048200
C	-3.16885200	1.17543500	0.95079200
H	-1.37947400	1.97591300	0.08595100
H	-4.52906200	-1.73454500	0.47708700
H	-3.36687100	2.06412400	1.54421900
N	-4.04670800	0.17321700	1.08759300
C	4.03903100	-0.32946700	1.01000000
H	4.89786800	-0.50184400	1.64831000

Optimized SP-trans-S₀



C	-3.86516900	-1.29234400	0.00000200
C	-2.48900800	-1.11154800	0.00000200
C	-1.93035800	0.17941000	0.00000000
C	-2.81012000	1.27477700	-0.00000100
C	-4.18935400	1.09417400	-0.00000200
H	-4.27375400	-2.29669000	0.00000300
H	-1.84395100	-1.98209300	0.00000300
H	-2.40053600	2.27970500	-0.00000300
H	-4.84579100	1.95698100	-0.00000300
C	-0.48861300	0.43749900	0.00000000
H	-0.22561400	1.49207300	0.00000000
C	0.50197600	-0.47184100	0.00000000
H	0.25023900	-1.52865900	-0.00000100
C	1.93924800	-0.19337600	0.00000000
C	2.84912400	-1.26118000	-0.00000200
C	2.49806200	1.09556200	0.00000200
C	4.21643100	-1.00618000	-0.00000200
H	2.49077000	-2.28497000	-0.00000300
C	3.87823400	1.24189400	0.00000100
H	1.87325100	1.98026400	0.00000300
H	4.92376400	-1.83133900	-0.00000300
H	4.31701100	2.23611600	0.00000300
N	4.74459000	0.22047700	0.00000000
C	-4.72374300	-0.19137900	0.00000000
H	-5.79778700	-0.33752700	0.00000000

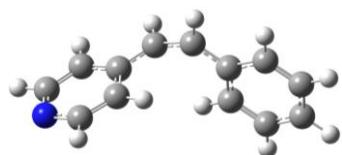
Optimized SP-cis-S1



C	-2.35470200	-1.42857000	0.91064600
C	-1.40002500	-0.41947700	0.85247200
C	-1.62170900	0.73458600	0.08456100
C	-2.84372100	0.85356600	-0.59592200
C	-3.79418100	-0.16130700	-0.54696800
H	-2.16725300	-2.30906800	1.51501400
H	-0.48136000	-0.51665800	1.41725400
H	-3.04243800	1.74940200	-1.17522800
H	-4.72661700	-0.05292100	-1.08954900

C	-0.65993000	1.85070000	0.02509200
H	-1.12724700	2.83287000	-0.00049100
C	0.68465400	1.84479100	0.01713000
H	1.16720900	2.81834900	0.06278900
C	1.63157400	0.71841600	-0.06333700
C	2.87106500	0.80568200	0.58522000
C	1.40451800	-0.43514600	-0.82729500
C	3.78118800	-0.24059800	0.47306800
H	3.12070000	1.67950300	1.17731000
C	2.38512600	-1.41862700	-0.88239900
H	0.48320800	-0.55905900	-1.38136400
H	4.73983000	-0.18554800	0.98219000
H	2.22159200	-2.31396400	-1.47620600
N	3.55929900	-1.34550600	-0.24436900
C	-3.55196000	-1.30852300	0.20545000
H	-4.29409800	-2.09731500	0.25255000

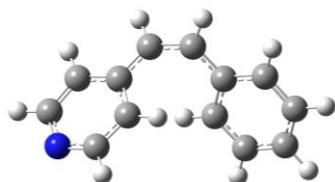
Optimized SP-IC-S₁



C	2.95794700	-1.21969300	-1.05298000
C	1.80941100	-0.46854600	-0.88447400
C	1.75183500	0.55773700	0.10310000
C	2.91806000	0.78927400	0.89091900
C	4.05936700	0.03732000	0.70339400
H	2.98394900	-2.00067000	-1.80457000
H	0.93143400	-0.64429000	-1.49443800
H	2.89544200	1.57457500	1.63909700
H	4.93799100	0.22848200	1.30915700
C	0.59766000	1.34040900	0.27864100
H	0.66362700	2.11704800	1.04737200
C	-0.60879700	1.28476100	-0.51522900
H	-0.67767500	1.95204900	-1.37613200
C	-1.75843600	0.53264200	-0.19639400
C	-2.94600300	0.61347100	-0.97825500
C	-1.82371000	-0.33985400	0.92663100
C	-4.05359900	-0.12850000	-0.62087700
H	-2.97857800	1.25993200	-1.84888200
C	-2.99418600	-1.03363700	1.18477400
H	-0.96316200	-0.45406100	1.57569300
H	-4.96111600	-0.06890600	-1.21631300
H	-3.04804400	-1.69820000	2.04332900
N	-4.10809200	-0.95080300	0.44252500

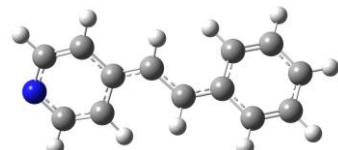
C	4.08777200	-0.97406400	-0.26598200
H	4.98885900	-1.55825400	-0.41159900

Optimized SP-ts₁-S₁



C	2.29681800	-1.39104700	-0.95106100
C	1.34602400	-0.38931200	-0.79777200
C	1.62525500	0.76095800	0.01779800
C	2.91172300	0.83495200	0.64031500
C	3.83982400	-0.17380500	0.47769800
H	2.06984400	-2.25285600	-1.57345500
H	0.39523300	-0.44754400	-1.31517300
H	3.14148900	1.69952000	1.25882700
H	4.80831200	-0.10186100	0.96568000
C	0.66172300	1.76894200	0.23518400
H	0.98053600	2.63032900	0.83149600
C	-0.67588000	1.76112000	-0.29138200
H	-0.99357000	2.60349300	-0.91333000
C	-1.63642700	0.75861700	-0.03670800
C	-2.92601100	0.77974000	-0.65063200
C	-1.37141600	-0.37039100	0.80650300
C	-3.80732800	-0.26001300	-0.42864200
H	-3.20141900	1.60543000	-1.30215500
C	-2.34726000	-1.35195400	0.95211700
H	-0.43468100	-0.44259100	1.34738700
H	-4.78778600	-0.25235900	-0.90279200
H	-2.15159800	-2.21070900	1.59408200
N	-3.54768400	-1.33032300	0.35798800
C	3.53863300	-1.29915800	-0.31672900
H	4.27334300	-2.09049100	-0.43661100

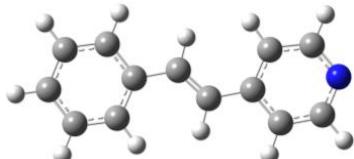
Optimized SP-ts₂-S₁



C	2.29723000	-1.39089300	-0.95119700
C	1.34627300	-0.38936800	-0.79773200
C	1.62529500	0.76078000	0.01801500
C	2.91171100	0.83486900	0.64059500
C	3.83998000	-0.17366900	0.47779500
H	2.07040400	-2.25263600	-1.57370300

H	0.39545200	-0.44773500	-1.31504400
H	3.14131000	1.69934500	1.25926400
H	4.80843500	-0.10164900	0.96578800
C	0.66169000	1.76864700	0.23532300
H	0.98026900	2.62990200	0.83192900
C	-0.67578800	1.76080900	-0.29150800
H	-0.99324800	2.60303200	-0.91375600
C	-1.63641800	0.75839100	-0.03694800
C	-2.92594000	0.77964400	-0.65096500
C	-1.37168300	-0.37046500	0.80647800
C	-3.80749600	-0.25982600	-0.42875800
H	-3.20113000	1.60523000	-1.30268100
C	-2.34775100	-1.35175500	0.95230100
H	-0.43495100	-0.44282000	1.34732400
H	-4.78792200	-0.25206600	-0.90292800
H	-2.15229800	-2.21040900	1.59443600
N	-3.54812200	-1.32997100	0.35815300
C	3.53901000	-1.29889200	-0.31686300
H	4.27386100	-2.09004300	-0.43691400

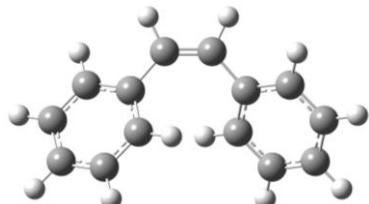
Optimized SP-trans-S₁



C	-3.86516900	-1.29234400	0.00000200
C	-2.48900800	-1.11154800	0.00000200
C	-1.93035800	0.17941000	0.00000000
C	-2.81012000	1.27477700	-0.00000100
C	-4.18935400	1.09417400	-0.00000200
H	-4.27375400	-2.29669000	0.00000300
H	-1.84395100	-1.98209300	0.00000300
H	-2.40053600	2.27970500	-0.00000300
H	-4.84579100	1.95698100	-0.00000300
C	-0.48861300	0.43749900	0.00000000
H	-0.22561400	1.49207300	0.00000000
C	0.50197600	-0.47184100	0.00000000
H	0.25023900	-1.52865900	-0.00000100
C	1.93924800	-0.19337600	0.00000000
C	2.84912400	-1.26118000	-0.00000200
C	2.49806200	1.09556200	0.00000200
C	4.21643100	-1.00618000	-0.00000200
H	2.49077000	-2.28497000	-0.00000300
C	3.87823400	1.24189400	0.00000100
H	1.87325100	1.98026400	0.00000300

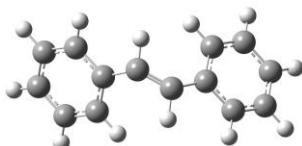
H	4.92376400	-1.83133900	-0.00000300
H	4.31701100	2.23611600	0.00000300
N	4.74459000	0.22047700	0.00000000
C	-4.72374300	-0.19137900	0.00000000
H	-5.79778700	-0.33752700	0.00000000

Optimized TS-cis-S₀



C	-2.38919600	-1.45753000	0.87017100
C	-1.41677300	-0.46290000	0.79771300
C	-1.64574200	0.71705300	0.06596700
C	-2.89463100	0.87211600	-0.56259900
C	-3.86478300	-0.12667300	-0.49782100
H	-2.19269300	-2.35807000	1.44634800
H	-0.47549700	-0.59071400	1.32181200
H	-3.09924300	1.78741800	-1.11355000
H	-4.81819300	0.01373700	-1.00052000
C	-0.67481700	1.82561200	-0.00136300
H	-1.14233100	2.80971600	-0.04401300
C	0.67481700	1.82561200	0.00136300
H	1.14233100	2.80971600	0.04401300
C	1.64574200	0.71705300	-0.06596700
C	2.89463100	0.87211600	0.56259900
C	1.41677300	-0.46290000	-0.79771300
C	3.86478300	-0.12667300	0.49782100
H	3.09924300	1.78741800	1.11355000
C	2.38919600	-1.45753000	-0.87017100
H	0.47549700	-0.59071400	-1.32181200
H	4.81819300	0.01373700	1.00052000
H	2.19269300	-2.35807000	-1.44634800
C	-3.61492800	-1.29860800	0.21787300
H	-4.37143700	-2.07650500	0.27692500
C	3.61492800	-1.29860800	-0.21787300
H	4.37143700	-2.07650500	-0.27692500

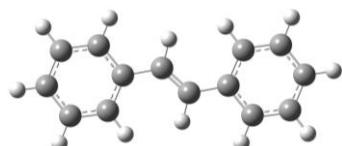
Optimized TS-IC-S₀



C	-3.13774000	-1.29394500	-0.89070000
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C	-2.02144700	-1.13077100	-0.07758000
C	-1.80235200	0.07873200	0.61681100
C	-2.76336300	1.10154400	0.48165300
C	-3.87437600	0.93823700	-0.34070300
H	-3.27775400	-2.22789900	-1.42894400
H	-1.29062900	-1.93026700	0.00087500
H	-2.61948200	2.03545100	1.01958900
H	-4.59210700	1.74823700	-0.44131800
C	-0.60111600	0.32915300	1.41339000
H	-0.47633800	1.42078800	1.48685300
C	0.60111600	-0.32915300	1.41339000
H	0.47633800	-1.42078800	1.48685300
C	1.80235200	-0.07873200	0.61681100
C	2.76336300	-1.10154400	0.48165300
C	2.02144700	1.13077100	-0.07758000
C	3.87437600	-0.93823700	-0.34070300
H	2.61948200	-2.03545100	1.01958900
C	3.13774000	1.29394500	-0.89070000
H	1.29062900	1.93026700	0.00087500
H	4.59210700	-1.74823700	-0.44131800
H	3.27775400	2.22789900	-1.42894500
C	-4.07023700	-0.26086200	-1.02985200
H	-4.93515800	-0.38702800	-1.67517500
C	4.07023700	0.26086200	-1.02985200
H	4.93515800	0.38702800	-1.67517500

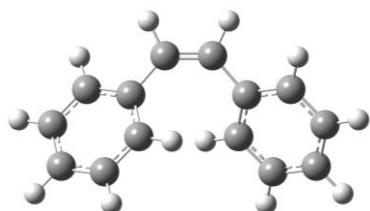
Optimized TS-trans-S₀



C	3.87178100	1.29934500	0.00000200
C	2.49361000	1.10988400	0.00000200
C	1.94014500	-0.18601000	0.00000000
C	2.82921000	-1.27720900	-0.00000100
C	4.20994900	-1.08859300	-0.00000200
H	4.27328600	2.30943900	0.00000300
H	1.84129900	1.97815100	0.00000300
H	2.42432500	-2.28682300	-0.00000300
H	4.87135800	-1.95101600	-0.00000300
C	0.49864400	-0.45383400	0.00000000
H	0.24326200	-1.51259900	0.00000000
C	-0.49864400	0.45383400	0.00000000
H	-0.24326200	1.51259900	-0.00000100
C	-1.94014500	0.18601000	0.00000000

C	-2.82921000	1.27720900	-0.00000200
C	-2.49361000	-1.10988400	0.00000200
C	-4.20994900	1.08859300	-0.00000200
H	-2.42432500	2.28682300	-0.00000300
C	-3.87178100	-1.29934500	0.00000200
H	-1.84129900	-1.97815100	0.00000300
H	-4.87135800	1.95101600	-0.00000300
H	-4.27328600	-2.30943900	0.00000300
C	4.73921200	0.20229200	0.00000000
H	5.81503100	0.35490800	0.00000000
C	-4.73921200	-0.20229200	0.00000000
H	-5.81503100	-0.35490800	0.00000000

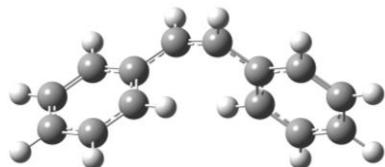
Optimized TS-cis-S₁



C	-0.80334500	2.41248700	-1.45753000
C	-0.75797700	1.43842400	-0.46290000
C	-0.02014200	1.64694000	0.71705300
C	0.64293600	2.87785300	0.87211600
C	0.60518100	3.84943200	-0.12667300
H	-1.38476700	2.23209400	-2.35807000
H	-1.30806700	0.51209800	-0.59071400
H	1.19936800	3.06705400	1.78741800
H	1.13421800	4.78848300	0.01373700
C	0.02014200	0.67451800	1.82561200
H	0.07578600	1.14066400	2.80971600
C	-0.02014200	-0.67451800	1.82561200
H	-0.07578600	-1.14066400	2.80971600
C	0.02014200	-1.64694000	0.71705300
C	-0.64293600	-2.87785300	0.87211600
C	0.75797700	-1.43842400	-0.46290000
C	-0.60518100	-3.84943200	-0.12667300
H	-1.19936800	-3.06705400	1.78741800
C	0.80334500	-2.41248700	-1.45753000
H	1.30806700	-0.51209800	-0.59071400
H	-1.13421800	-4.78848300	0.01373700
H	1.38476700	-2.23209400	-2.35807000
C	-0.11718900	3.61959100	-1.29860800
H	-0.15516500	4.37745000	-2.07650500
C	0.11718900	-3.61959100	-1.29860800

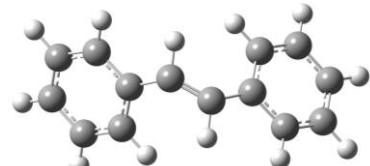
H 0.15516500 -4.37745000 -2.07650500

Optimized TS-IC-S₁



C	-2.85134500	-1.10841400	1.18743300
C	-1.73125300	-0.32063300	0.94359200
C	-1.72066900	0.58323200	-0.13713300
C	-2.86111100	0.67380900	-0.96327300
C	-3.97150100	-0.11532000	-0.70902000
H	-2.85003700	-1.80612800	2.02354900
H	-0.85184400	-0.40148100	1.58270500
H	-2.86305500	1.36810200	-1.80032400
H	-4.85012600	-0.04228400	-1.34763200
C	-0.56722000	1.37710500	-0.40053400
H	-0.59069800	2.02837300	-1.27996500
C	0.56724900	1.37727500	0.40014200
H	0.59072000	2.02867700	1.27944500
C	1.72069800	0.58331100	0.13691900
C	1.73122700	-0.32095500	-0.94347300
C	2.86116000	0.67416000	0.96299600
C	2.85129300	-1.10886600	-1.18704000
H	0.85175400	-0.40211100	-1.58247000
C	3.97152600	-0.11506800	0.70900200
H	2.86314600	1.36878900	1.79977000
H	2.84993000	-1.80693100	-2.02286300
H	4.85015300	-0.04184400	1.34758800
C	-3.97152600	-1.00973500	0.36621500
H	-4.84623300	-1.62642800	0.55806600
C	3.97149300	-1.00990200	-0.36588900
H	4.84616300	-1.62672800	-0.55749200

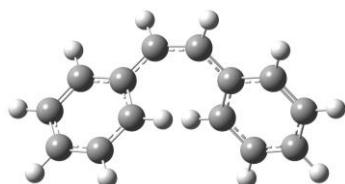
Optimized TS-ts₁-S₁



C	-2.33561700	-1.37084200	0.98339100
C	-1.37556000	-0.38145900	0.80894900
C	-1.63877700	0.75042600	-0.03604600
C	-2.92243800	0.81678800	-0.66545200
C	-3.86106500	-0.17902100	-0.48026800

H	-2.11744500	-2.21845900	1.62867900
H	-0.42634600	-0.43648100	1.33025100
H	-3.14314000	1.66714800	-1.30693700
H	-4.82727800	-0.10880700	-0.97370100
C	-0.66565700	1.74574100	-0.27249600
H	-0.97312700	2.59397300	-0.89309800
C	0.66565600	1.74574000	0.27249700
H	0.97312800	2.59397000	0.89310000
C	1.63877600	0.75042500	0.03604500
C	2.92243900	0.81679100	0.66544600
C	1.37555800	-0.38146500	-0.80894500
C	3.86106700	-0.17901800	0.48026300
H	3.14314200	1.66715300	1.30692700
C	2.33561600	-1.37084700	-0.98338500
H	0.42634200	-0.43649200	-1.33024300
H	4.82728100	-0.10879900	0.97369200
H	2.11744300	-2.21846700	-1.62866800
C	-3.57536900	-1.28653700	0.34327400
H	-4.31763600	-2.06792600	0.48111700
C	3.57537100	-1.28653700	-0.34327400
H	4.31763800	-2.06792500	-0.48111600

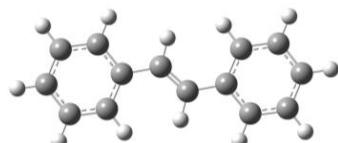
Optimized TS-ts₂-S₁



C	3.46395100	1.27997000	-0.73355300
C	2.18159900	1.04120400	-0.26636400
C	1.84456000	-0.20809500	0.34967500
C	2.88348800	-1.18503700	0.46418900
C	4.15992500	-0.92737300	0.00017100
H	3.69709100	2.23439600	-1.19964900
H	1.40395800	1.79435600	-0.36803400
H	2.65059200	-2.14087700	0.92865100
H	4.93382100	-1.68430700	0.10127500
C	0.54107800	-0.47200200	0.82833300
H	0.36829900	-1.46518100	1.25650900
C	-0.54107800	0.47200200	0.82833300
H	-0.36829900	1.46518000	1.25650900
C	-1.84456000	0.20809500	0.34967500
C	-2.88348800	1.18503700	0.46418900
C	-2.18159900	-1.04120400	-0.26636400
C	-4.15992500	0.92737300	0.00017100

H	-2.65059100	2.14087700	0.92865100
C	-3.46395100	-1.27997000	-0.73355300
H	-1.40395800	-1.79435600	-0.36803400
H	-4.93382100	1.68430700	0.10127500
H	-3.69709100	-2.23439600	-1.19964900
C	4.46483400	0.30683600	-0.60296600
H	5.47273900	0.50751700	-0.95565600
C	-4.46483400	-0.30683600	-0.60296600
H	-5.47273900	-0.50751700	-0.95565600

Optimized TS-trans-S₁



C	1.28990300	3.87493700	-0.00000200
C	1.10380200	2.49630800	-0.00000200
C	-0.19073900	1.93968600	0.00000000
C	-1.28410200	2.82608800	0.00000100
C	-1.09885200	4.20728300	0.00000200
H	2.29901500	4.27890300	-0.00000300
H	1.97365700	1.84611600	-0.00000300
H	-2.29272600	2.41874300	0.00000300
H	-1.96288500	4.86658800	0.00000300
C	-0.45504800	0.49753600	0.00000000
H	-1.51318700	0.23957400	0.00000000
C	0.45504800	-0.49753600	0.00000000
H	1.51318700	-0.23957400	0.00000000
C	0.19073900	-1.93968600	0.00000000
C	1.28410200	-2.82608800	0.00000100
C	-1.10380200	-2.49630800	-0.00000200
C	1.09885200	-4.20728300	0.00000200
H	2.29272600	-2.41874300	0.00000300
C	-1.28990300	-3.87493700	-0.00000200
H	-1.97365700	-1.84611600	-0.00000300
H	1.96288500	-4.86658800	0.00000300
H	-2.29901500	-4.27890300	-0.00000300
C	0.19073900	4.73969100	0.00000000
H	0.34073200	5.81587900	0.00000000
C	-0.19073900	-4.73969100	0.00000000
H	-0.34073200	-5.81587900	0.00000000

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