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Syntheses, structures and theoretical calculations of stable triarylarsine radical cations

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Supporting Information

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1. Experimental Section

All experiments were carried out under a nitrogen atmosphere by using standard Schlenk techniques or in an argon-filled glovebox. Solvents were dried prior to use. $AgSbF_6$, $Na[BAr^F_4]$ (Ar^F =C_6H_3-3,5-$(CF_3)_2$)) was purchased from Alfa Aesar and used upon arrival**,** 1-Bromo-2,6-diisopropylbenzene[S1], tris(2,4,6-diisopropylphenyl)arsine **1** and tris(2,6-diisopropylphenyl)arsine **2**[S2] were synthesized according to the methods reported in the literature. Cyclic voltammetry was performed on an IM6ex electrochemical workstation, with platinum as the working and counter electrodes, Ag/Ag^+ as the reference electrode and 0.1 M $^nBu_4NPF_6$ as the supporting electrolyte. UV-vis spectra were recorded on the Lambda 750 spectrometer. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. X-ray crystal structures were obtained by using Bruker D8 Venture detectors. The structures were solved by direct methods and all refined on F^2 with the SHELX-2014 software package. The positions of the H atoms were calculated and considered isotropically according to a riding model. In the crystal structures, disorders at the As atom, CF_3 groups of the anion and the *i*Pr groups (only in $\mathbf{1}^{\bullet+}$), were observed and treated.

Syntheses of $\mathbf{1}^{\bullet+}$•$[BAr^F_4]^-$: Under anaerobic and anhydrous conditions, the solution of $AgSbF_6$ (0.157 g, 0.46 mmol) in CH_2Cl_2 (15 mL) was added dropwise to the mixture of **1** (0.308 g, 0.45 mmol) and $Na[BAr^F_4]$ (0.396 g, 0.45 mmol) in CH_2Cl_2 (~ 30 ml) at room temperature.The resultant solution was stirred overnight at room temperature and then filtered to remove the gray precipitate (Ag metal). The filtrate was concentrated and stored at around –30 °C for one day to afford purple crystals. Yield: 0.542 g, 77.8 %; m.p. 211-213 °C; UV-Vis (CH_2Cl_2): λ_{max} = 518 nm; elemental analysis (%) calcd: C 59.74, H 5.27; found: C 59.65, H 5.15.

Syntheses of $\mathbf{2}^{\bullet+}$•$[BAr^F_4]^-$: Under anaerobic and anhydrous conditions, the solution of $AgSbF_6$ (0.153 g, 0.45 mmol) in CH_2Cl_2 (15 mL) was added dropwise to the mixture of **2** (0.251 g, 0.45 mmol) and $Na[BAr^F_4]$ (0.401 g, 0.45 mmol) in CH_2Cl_2 (~ 30 ml). The resultant solution was stirred overnight at room temperature and then filtered to remove the gray precipitate (Ag metal). The filtrate was concentrated and stored at around –30 °C for one day to afford red crystals. Yield: 0.511 g, 80.1 %; m.p. 193-195 °C; UV-Vis (CH_2Cl_2): λ_{max} = 486 nm; elemental analysis (%) calcd: C 57.44, H 4.47; found: C 57.04, H 4.58.

Table S1. Crystal Data and Structure Refinement for $\mathbf{1}^{\bullet+}[BAr^{F}_{4}]^{-}$ and $\mathbf{2}^{\bullet+}[BAr^{F}_{4}]^{-}$

	$\mathbf{1}^{\bullet+}[BAr^{F}_{4}]^{-}$	$\mathbf{2}^{\bullet+}[BAr^{F}_{4}]^{-}$
formula	$C_{77}H_{81}AsBF_{24}$	$C_{68}H_{63}AsBF_{24}$
*M*r [g mol^{-1}]	1548.15	1421.91
crystal system	triclinic	Monoclinic
space group	*P* -1	*C*2/*c*
Z	2	4
Temp. (K)	153(2)	153(2)
μ (mm^{-1})	0.536	0.606
a (Å)	14.3468(12)	19.0845(17)
b (Å)	16.7636(14)	19.3689(16)
c (Å)	18.1282(16)	19.0896(19)
α	73.207(3)	
β	87.244(2)	105.786(3)
γ	68.719(2)	
V [Å^3]	3881.5(6)	6790.3(11)
*R*1 (*I*>2σ(*I*))	0.0527	0.0489
*wR*2 (*I*>2σ(*I*))	0.1368	0.1299

$R_1 = \Sigma||F_o| - |F_c||/\Sigma F_o|$, $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

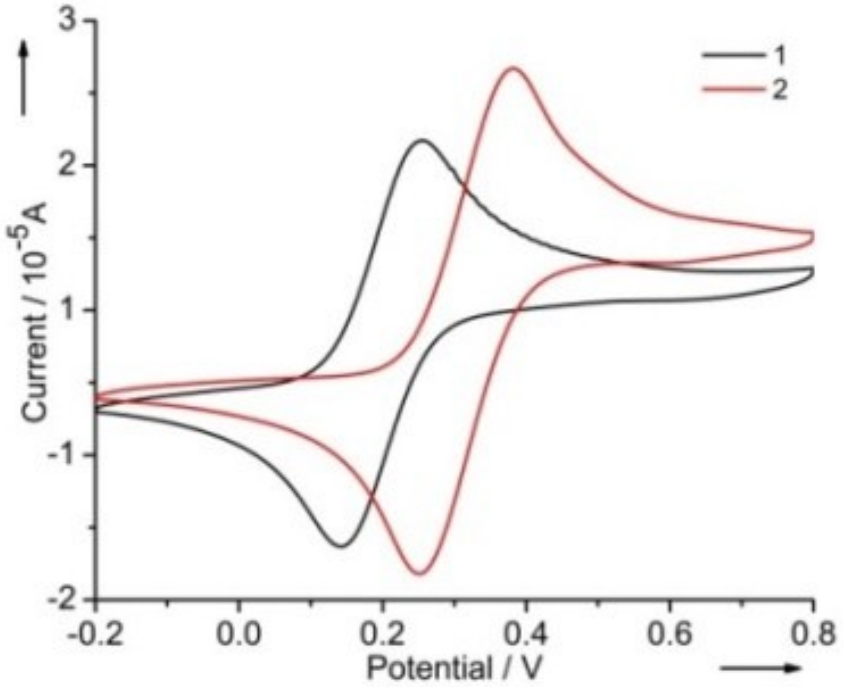


Figure S1. The cyclic voltammograms of **1** and **2** (1×10^{-3} M) in CH_2Cl_2 at 298 K, containing 0.1 M nBu$_4$NPF$_6$, scan rate: 100 mV s^{-1}.

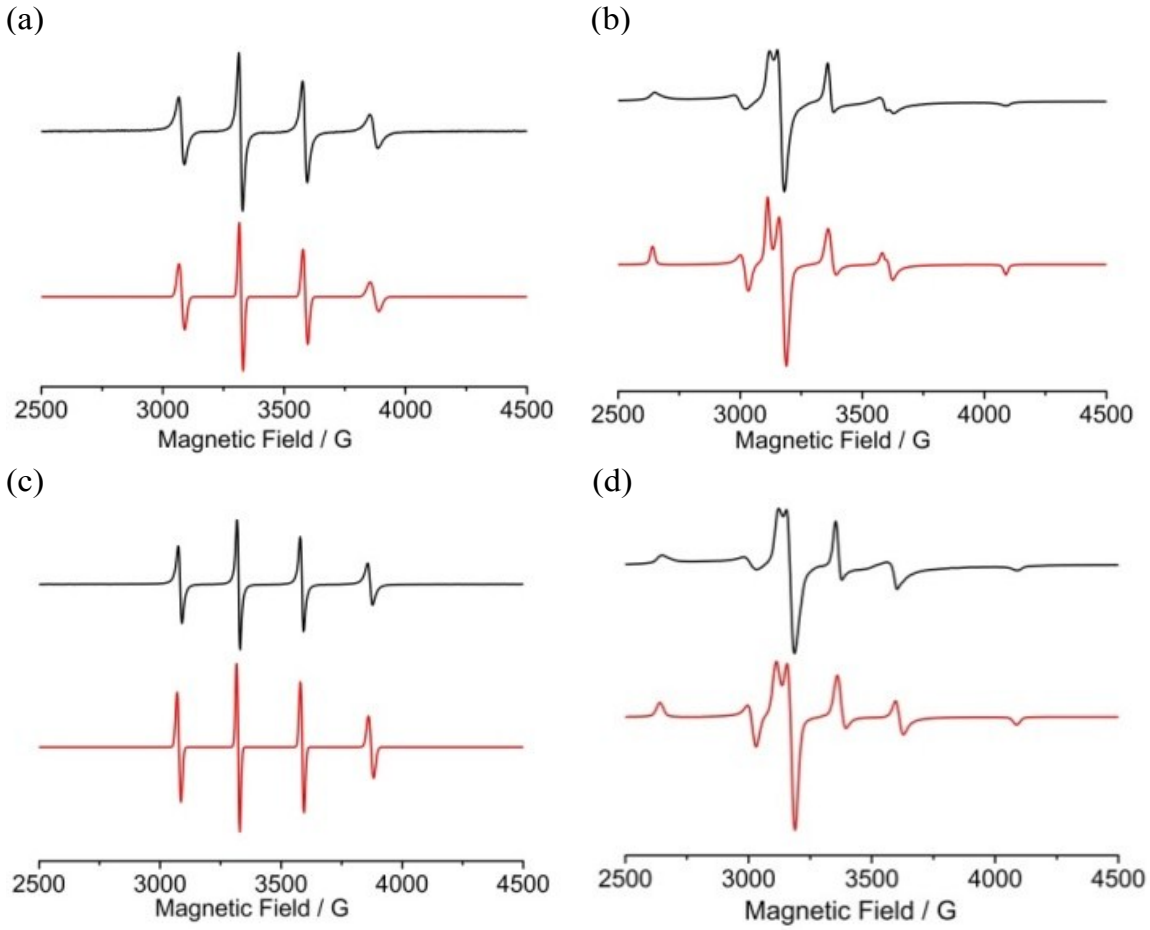


Figure S2. Experimental (black) and simulated (red) EPR spectra of $\mathbf{1}^{\bullet+}[BAr^{F}_{4}]^{-}$ (a, b) and $\mathbf{2}^{\bullet+}[BAr^{F}_{4}]^{-}$ (c, d) in THF solution at 298 (a, c) and 86 K (b, d).

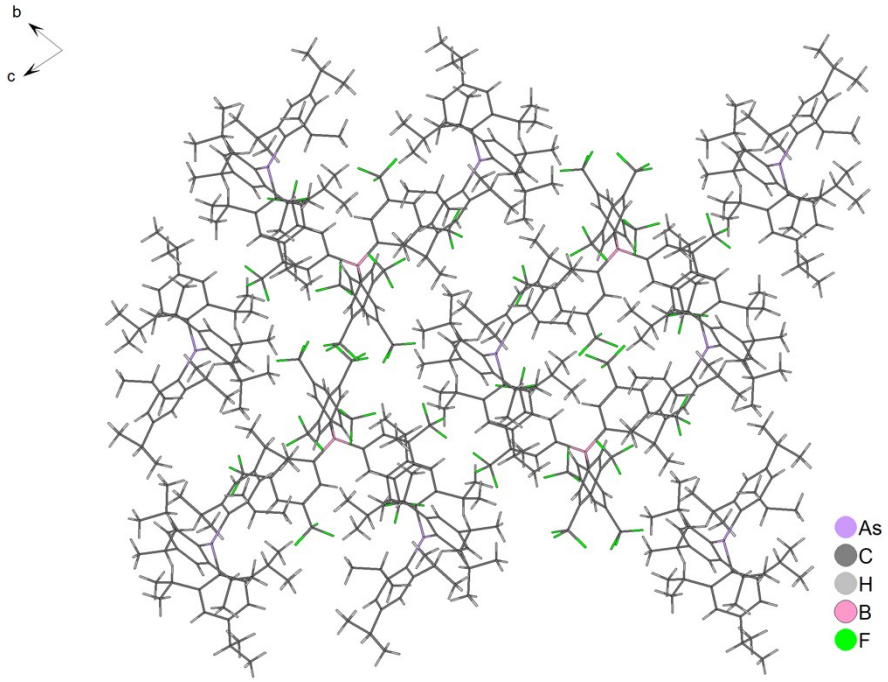


Figure S3. Crystal packing of $\mathbf{1}^{\bullet+}[BAr^{F}{}_{4}]^{-}$.

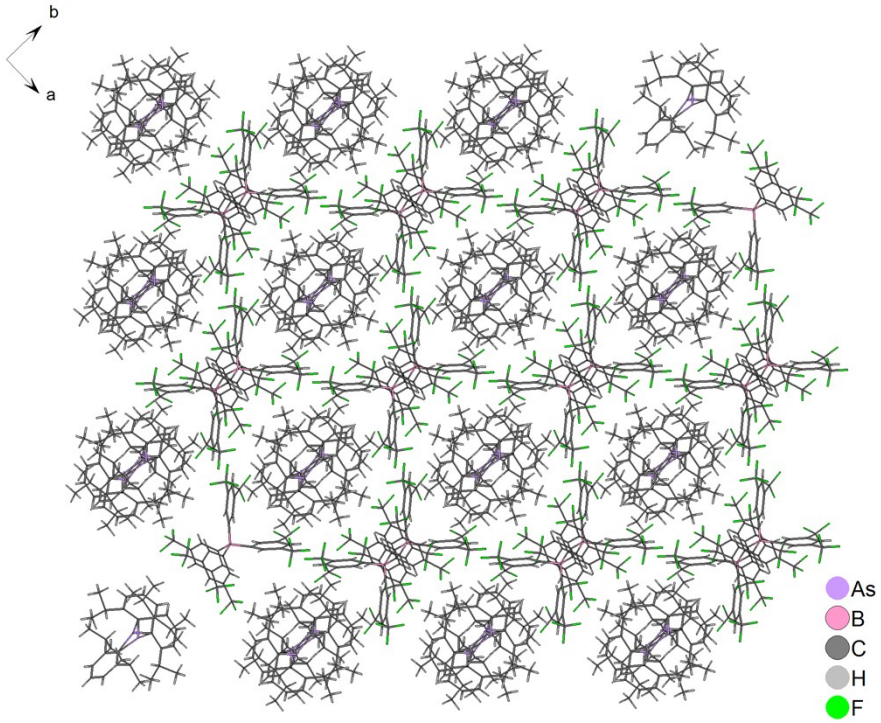


Figure S4. Crystal packing of $\mathbf{2}^{\bullet+}[BAr^{F}{}_{4}]^{-}$.

2. Theoretical calculation details

All calculations were performed with the Gaussian 09 program suite.[S3] The geometry optimizations were carried out at the UCAM-B3LYP/6-31(d) level of theory. The obtained stationary points were characterized by frequency calculations, and no imaginary frequency was found. Natural bond orbital (NBO) analyses were carried out by using the NBO 3.1 program implemented in Gaussian 09 program.[S4] The UV-vis absorption spectra were calculated by using time-dependent DFT (TD-DFT) method at the UPBE1PBE/6-31(d) level. In consideration of the solvent effects, dichloromethane was taken into account in the calculations of UV-vis absorption spectra by the Polarizable Continuum Model (PCM) model.[S5]

Table S2. Mulliken spin density, NBO charge and Mayer bond order (BO) of mainly selected atoms

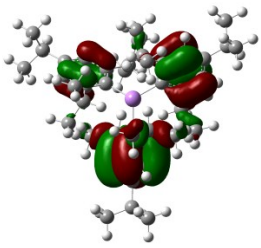
	$1^{\bullet+}$ (calc.)	$2^{\bullet+}$ (calc.)
MSD (As-total)/a.u	0.84	0.86
MSD (As-S)/a.u	0.01	0.01
MSD (As-P)/a.u	0.81	0.83
MSD (As-D)/a.u	0.02	0.02
MSD (As-5s)/a.u	0.03	0.03
MSD (As-4p)/a.u	0.46	0.47
MSD (As-5p)/a.u	0.35	0.35
MSD (As-6d)/a.u	0.02	0.02
MSD (C2)/a.u	-0.051	-0.054
MSD (C3)/a.u	-0.050	-0.054
MSD (C6)/a.u	-0.051	-0.054
q (As)/e	1.08	1.09
q (C2)/e	-0.22	-0.21
q (C3)/e	-0.22	-0.21
q (C6)/e	-0.22	-0.21
BO (As-C2)	0.95	0.94
BO (As-C3)	0.94	0.94
BO (As-C6)	0.95	0.94
SOMO (α)/eV	-9.79	-10.12
LUMO (α)/eV	-2.31	-2.57
HOMO (β)/eV	-10.69	-10.92
LUMO (β)/eV	-5.17	-5.38
ΔE(α)/eV	7.48	7.55
ΔE(β)/eV	5.52	5.54

Table S3. Calculated UV-Vis absorption properties.

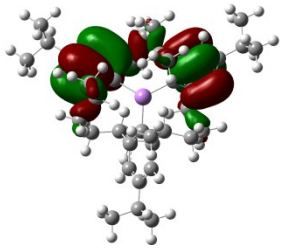
	Excited state	λ_{abs}	f	Transition nature	
$\mathbf{1}^{\bullet+}$	S_1	509.6	0.004	HOMO(β) → LUMO(β)	89.1%
	S_2	508.3	0.003	HOMO-1(β) → LUMO(β)	89.4%
	S_3	503.6	0.005	HOMO-2(β) →LUMO(β)	97.8%
	S_4	480.2	0.064	HOMO-3(β) →LUMO(β)	96.1%
	S_5	478.4	0.055	HOMO-4(β) → LUMO(β)	95.8%
$\mathbf{2}^{\bullet+}$	S_1	507.0	0.003	HOMO(β) → LUMO(β)	98.8%
	S_2	506.8	0.003	HOMO-1(β) → LUMO(β)	98.8%
	S_3	500.7	0.004	HOMO-2(β) → LUMO(β)	98.8%
	S_4	445.7	0.035	HOMO-4(β) → LUMO(β)	91.2%
	S_5	445.7	0.035	HOMO-3(β) → LUMO(β)	91.2%

Table S4. Main contour surfaces of the frontier molecular orbitals for **1**$^{\bullet+}$ and **2**$^{\bullet+}$.

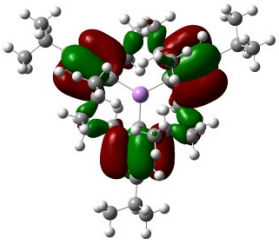
1$^{\bullet+}$



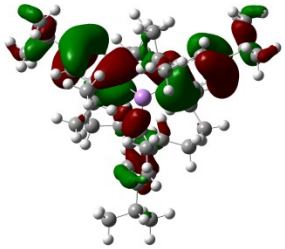
HOMO(β)



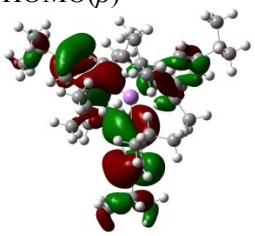
HOMO-1(β)



HOMO-2(β)



HOMO-3(β)



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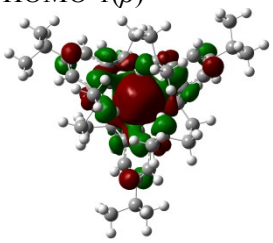
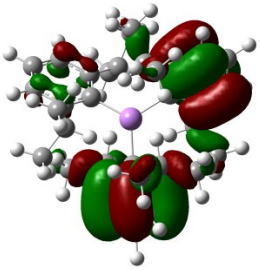


LUMO(β)

2$^{\bullet+}$



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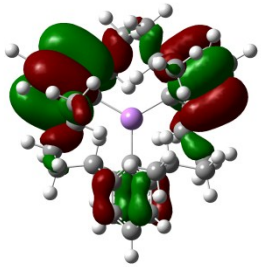

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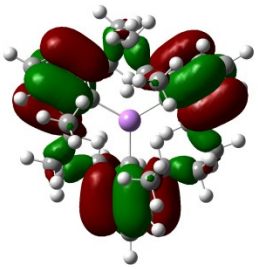

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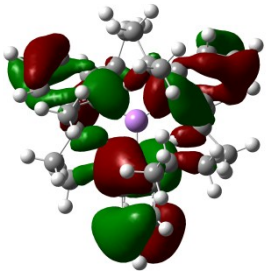

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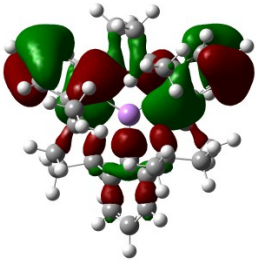

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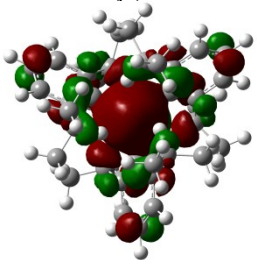

LUMO(β)

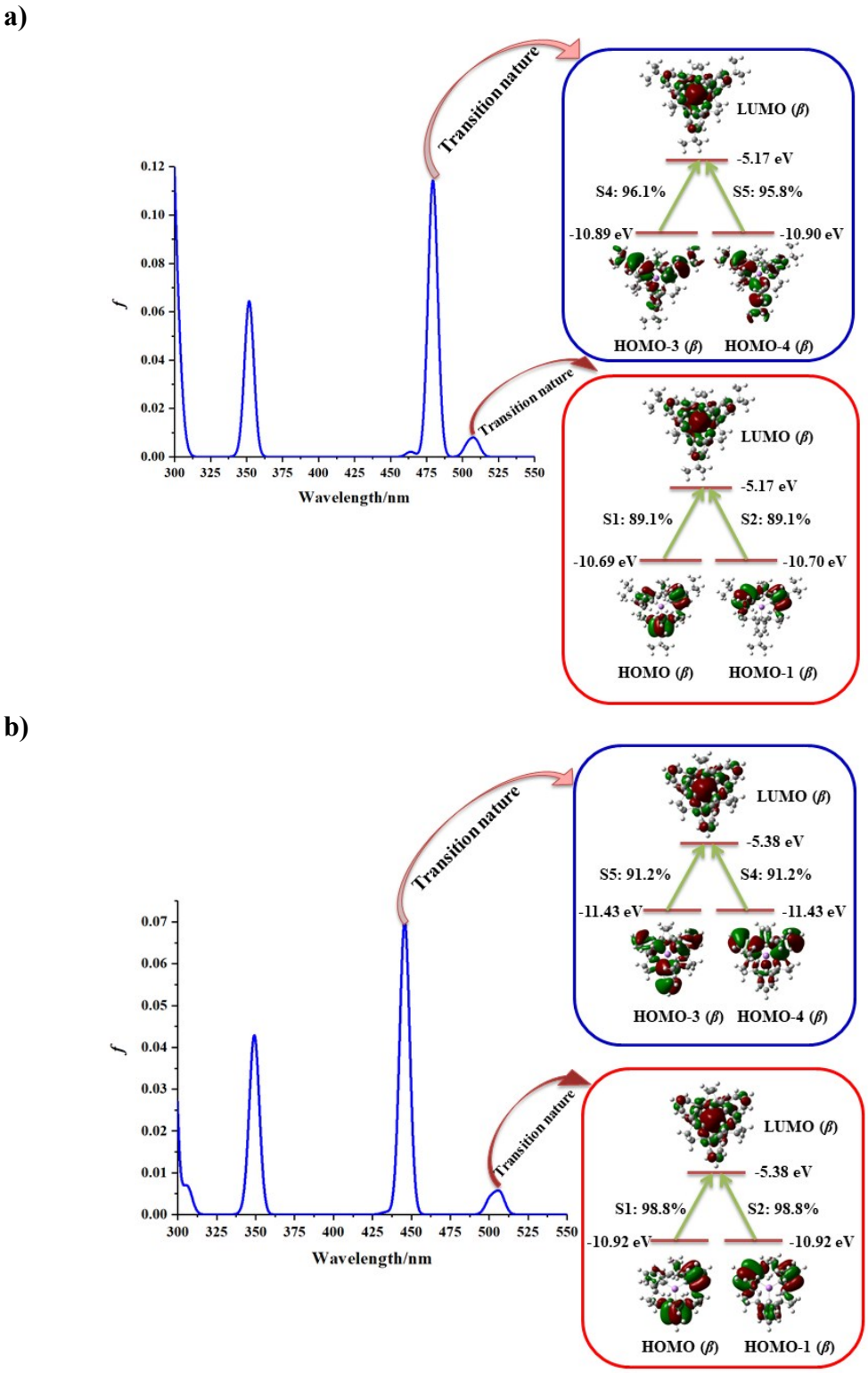

Figure S5. Calculated UV-Vis absorption spectra of $\mathbf{1}^{\bullet+}$ and $\mathbf{2}^{\bullet+}$ in CH_2Cl_2 at room temperature and the main contour surfaces of the frontier molecular orbitals related to electron transitions.

Optimized coordinates for the studied compounds

Compound 1

As	0.06591500	0.00453600	0.77769500
C	1.83227900	-0.54092900	0.05537000
C	-0.42924300	1.78225800	0.05389500
C	0.15076000	2.46746700	-1.02831600
C	-1.59197700	-2.28049300	1.28489000
C	-1.35783900	-1.29434000	0.29082100
C	-1.36888600	2.46560200	0.86825900
C	2.10903400	-1.50951800	-0.92532500
C	-2.21105900	-1.25584100	-0.83268900
C	-0.16637000	3.81480700	-1.22875200
H	0.29883800	4.34383100	-2.05629900
C	-2.11526300	-0.20943900	-1.93258300
H	-1.15738200	0.29612500	-1.82230500
C	-1.66167900	3.79968300	0.61395000
H	-2.38164000	4.30884300	1.24612800
C	-3.22510500	-2.20413700	-0.95872600
H	-3.87600100	-2.15561100	-1.82630000
C	-2.60437000	-3.21945600	1.09240200
H	-2.76837000	-3.98349100	1.84466400
C	1.08561600	1.82807400	-2.04443300
H	1.11718900	0.75993000	-1.83827600
C	-1.05595300	4.50492300	-0.42302400
C	2.91474100	0.01538300	0.78655100
C	-0.77850100	-2.35487600	2.57632900
H	-0.56085700	-1.32250800	2.86538100
C	1.06068500	-2.10208500	-1.85350600
H	0.13938500	-1.54491800	-1.70222100
C	-2.05935600	1.77923100	2.04529700
H	-2.11350500	0.71043700	1.82175500
C	0.58038000	2.00743000	-3.48284000
H	-0.45436900	1.67280000	-3.59500400
H	1.20103600	1.42899900	-4.17539000
H	0.62725100	3.05326300	-3.80183100
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C	3.42581900	-1.94569000	-1.10069200
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H	-1.45775600	-1.63685600	-3.46069500
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H	1.67391700	-0.90391700	-3.57922400
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H	-5.06945400	-5.87502200	-1.52692700
H	-3.32339300	-5.57786300	-1.43309300
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C	4.48844400	-1.43431900	-0.37546000
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H	-2.50750000	-2.56243600	3.90129100
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H	-1.63581200	-4.08083100	3.62773300
C	-1.23145700	1.94198900	3.32518700
H	-0.21781200	1.56692600	3.17568400
H	-1.68378900	1.37883100	4.14916200
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H	5.84772500	-2.72749700	-1.35633500
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H	-3.97525100	1.58994500	3.02463600
H	-4.09762900	2.17746500	1.35884000
H	-3.56051800	3.25949100	2.65425600
C	2.70260900	1.07151600	1.87002800
H	1.79327700	1.62835100	1.62632800
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H	-4.47439700	-4.91279000	0.67409700
C	0.56760700	-3.05307200	2.35104500
H	0.41885500	-4.10236800	2.07139300
H	1.17048800	-3.02931300	3.26545800
H	1.14204600	-2.57060100	1.55892300
C	2.49238200	0.39738900	3.23148000
H	1.68458800	-0.33451500	3.18262300
H	2.23397500	1.14086800	3.99358700
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H	4.75252700	1.68594100	2.35408200
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H	5.87548800	-3.35163600	1.05486300
H	6.60044900	-1.79103900	1.46100900
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H	-1.16342900	7.90328100	0.29367600
H	0.07961800	6.72912000	0.76447600
H	-1.56184400	6.58769500	1.40590800
H	-6.03926800	-2.93139100	-1.05958800
H	-6.69600500	-4.37034200	-0.26945400
H	-6.09102300	-3.01807000	0.70556600

Compound 2

As	0.00084600	0.00103000	-0.66572900
C	1.87464000	0.07229500	-0.00812700
C	-0.87422300	-1.65891600	-0.01218300
C	-0.43097600	-2.51233900	1.01656400
C	-0.80970000	2.73200700	-0.82434000
C	-1.00074400	1.58678300	-0.00998700
C	-1.95948200	-2.06579800	-0.82945800
C	2.39005300	0.88337300	1.02132200
C	-1.96504300	1.62577500	1.01566400
C	-1.02431200	-3.76989700	1.15981600
H	-0.66929600	-4.43589700	1.94010200
C	-2.17434800	0.51229500	2.02975900
H	-1.39297600	-0.22803400	1.87048900
C	-2.53261500	-3.31958600	-0.63680000
H	-3.36111100	-3.63227700	-1.26256400
C	-2.76048300	2.76643600	1.15804500
H	-3.51771700	2.78897500	1.93556200
C	-1.61191500	3.85315000	-0.63239900
H	-1.46815800	4.72847000	-1.25607900
C	0.63654000	-2.13770600	2.03252400
H	0.88792800	-1.09091400	1.87417200
C	-2.05761200	-4.18082600	0.33999200
C	2.77122000	-0.66344700	-0.82420800
C	0.23278100	2.76697000	-1.93967600
H	1.03564100	2.07410200	-1.67102800
C	1.52962100	1.61874000	2.03668500
H	0.49814100	1.31127200	1.87680100
C	-2.50434700	-1.18220700	-1.94941400
H	-2.30576700	-0.14019200	-1.68203000
C	0.12684800	-2.27818900	3.47352400
H	-0.80009400	-1.72021500	3.63196200
H	0.87476100	-1.89928100	4.17781000
H	-0.06479500	-3.32323100	3.73588000
C	-2.59903800	3.86849600	0.34066600
C	3.77559700	0.99943800	1.16622000
H	4.17352300	1.64013000	1.94700400
C	-2.04165900	1.02192900	3.47144000
H	-1.09466600	1.54476900	3.63089500

H	-2.08833000	0.18382900	4.17455500
H	-2.85057200	1.71056100	3.73431100
C	1.90543700	1.24729400	3.47778600
H	1.88848200	0.16537000	3.63516700
H	1.20126800	1.70302400	4.18166500
H	2.90501200	1.60644300	3.74143200
C	4.14319500	-0.53181200	-0.62980600
H	4.82939900	-1.09240200	-1.25489300
C	-3.52390300	-0.18918100	1.84436700
H	-4.35459400	0.50681200	2.00488300
H	-3.63082600	-1.01052900	2.56077500
H	-3.62076000	-0.60704100	0.84045600
C	4.64969100	0.31071200	0.34740500
C	1.59522300	3.13860300	1.85381400
H	2.61342700	3.51030000	2.01270800
H	0.93867900	3.64005000	2.57266800
H	1.27924900	3.43287100	0.85118400
C	1.91848300	-2.95638200	1.84806800
H	2.68252800	-2.63999700	2.56596900
H	2.33010000	-2.83037700	0.84484800
H	1.72970600	-4.02380100	2.00677400
C	-0.38274400	2.28392000	-3.25783800
H	-0.81437000	1.28879800	-3.13915100
H	0.37894600	2.23298200	-4.04363600
H	-1.17001700	2.96916100	-3.59041000
C	-1.77116700	-1.47779400	-3.26284000
H	-0.69386900	-1.35712600	-3.13779200
H	-2.10088300	-0.79276000	-4.05167200
H	-1.97202600	-2.50208300	-3.59520300
C	-4.01952900	-1.28651000	-2.14887600
H	-4.34884600	-0.51954700	-2.85674200
H	-4.56588500	-1.13835900	-1.21278300
H	-4.31668300	-2.25456600	-2.56424900
C	2.28138900	-1.57818000	-1.94460600
H	1.27851400	-1.92614400	-1.68034500
C	0.89889800	4.13304400	-2.13145300
H	0.21008600	4.87442200	-2.54845700
H	1.73173900	4.03816600	-2.83512200
H	1.29464300	4.53025800	-1.19214700
C	2.17669900	-0.79792400	-3.25999100
H	1.53339600	0.07535800	-3.14020400
H	1.75194700	-1.42761400	-4.04948600
H	3.16578500	-0.46067000	-3.58855500
C	3.12930600	-2.83911400	-2.13881300
H	4.11738000	-2.61396100	-2.55238400
H	2.63118400	-3.50935300	-2.84625100
H	3.27172700	-3.38420400	-1.20113400
H	-3.22803700	4.74439300	0.46904400
H	-2.50418700	-5.16223700	0.46928800
H	5.72267100	0.41558700	0.47789100

Compound $1^{\bullet+}$

As	0.07107800	0.00983900	0.20191700

C	1.95620700	-0.13944200	-0.05188900
C	-0.80227400	1.68977400	-0.02744400
C	-0.52118600	2.52178600	-1.12611600
C	-0.78980800	-2.53078400	1.15150600
C	-1.00508600	-1.56495200	0.14853500
C	-1.74179000	2.06123500	0.95784000
C	2.49250800	-0.97025300	-1.05328200
C	-2.00074000	-1.73811200	-0.83540700
C	-1.20001200	3.73405800	-1.20955800
H	-0.99396400	4.39368900	-2.04692500
C	-2.23253200	-0.76093300	-1.97858200
H	-1.43376600	-0.01435400	-1.95081500
C	-2.40299100	3.27333800	0.80197700
H	-3.13317900	3.56758700	1.54917400
C	-2.78251500	-2.88515500	-0.77149800
H	-3.55538700	-3.02824500	-1.51986200
C	-1.59233500	-3.66805100	1.14435600
H	-1.43916300	-4.42381100	1.90910600
C	0.46834000	2.15498500	-2.22057200
H	0.74703400	1.10586200	-2.08224800
C	-2.14667200	4.12782200	-0.26882500
C	2.79037900	0.58067500	0.83197100
C	0.23360200	-2.36775900	2.26611800
H	0.74668700	-1.41085100	2.11549000
C	1.64619800	-1.71215600	-2.07620300
H	0.60574700	-1.40413700	-1.94013300
C	-2.03099400	1.22254600	2.19538900
H	-1.35335100	0.36001400	2.18473100
C	-0.14265400	2.27175000	-3.62170000
H	-1.07348800	1.70287200	-3.70600400
H	0.55892600	1.88951300	-4.36918700
H	-0.36091500	3.31099400	-3.88310200
C	-2.59697900	-3.86452300	0.20326900
C	3.87826300	-1.07918500	-1.13008800
H	4.31129800	-1.71789400	-1.89402000
C	-2.14452800	-1.45229000	-3.34524000
H	-1.20936600	-2.00874200	-3.45871900
H	-2.19792100	-0.70863900	-4.14609000
H	-2.96994000	-2.15367700	-3.49679500
C	2.03638600	-1.33815600	-3.51210500
H	2.01162300	-0.25562300	-3.66923200
H	1.34461700	-1.80128900	-4.22212400
H	3.04232200	-1.68816500	-3.76031700
C	-3.26291100	-5.95997200	-1.02656700
H	-3.84320500	-6.88450500	-0.95527500
H	-2.21236200	-6.22875900	-1.17040600
H	-3.60004000	-5.42604400	-1.92122600
C	4.16495700	0.44058300	0.68914400
H	4.81624400	0.98704300	1.36370500
C	-3.55980500	-0.00885700	-1.83275800
H	-4.40733800	-0.70130100	-1.82388000
H	-3.70014300	0.67877000	-2.67241300
H	-3.58799800	0.57628800	-0.91032100

C	4.73256000	-0.38819700	-0.27730400
C	1.69810600	-3.22980600	-1.87239400
H	2.72046100	-3.60794500	-1.96924600
H	1.08328600	-3.73494300	-2.62357500
H	1.32261000	-3.51091400	-0.88542700
C	1.75456800	2.98005400	-2.10940900
H	2.46117100	2.69536400	-2.89493100
H	2.23951200	2.81971600	-1.14355100
H	1.54768000	4.04960800	-2.21469700
C	-2.87510700	5.44970600	-0.40923700
H	-2.49835400	5.93018400	-1.31970900
C	-0.44838400	-2.29381900	3.63814900
H	-1.20308500	-1.50205500	3.67144900
H	0.29110500	-2.09341100	4.41938200
H	-0.94446600	-3.23671700	3.88628300
C	-1.72490600	1.99851400	3.48210700
H	-0.69893800	2.37958500	3.48672900
H	-1.85249000	1.34991100	4.35394900
H	-2.39799100	2.85196000	3.60503100
C	6.23618100	-0.52866000	-0.40617600
H	6.42497400	-1.24299700	-1.21609100
C	-3.45966300	0.67067900	2.20228900
H	-3.63086000	0.07380200	3.10336300
H	-3.64404100	0.03227200	1.33420900
H	-4.19860200	1.47787100	2.19400200
C	2.25809000	1.44296500	1.96913300
H	1.16790200	1.49812200	1.87238600
C	-3.45756600	-5.11164700	0.23639900
H	-3.12580100	-5.70969800	1.09327200
C	1.30759500	-3.45965000	2.24141100
H	0.87077900	-4.45387600	2.37497200
H	2.02431500	-3.30188900	3.05298800
H	1.86073200	-3.45672600	1.29849300
C	2.56162000	0.79875600	3.32855400
H	2.17354900	-0.22219600	3.39181400
H	2.11268900	1.38461400	4.13638800
H	3.64005500	0.75431500	3.50838500
C	6.88938500	0.80299300	-0.79719600
H	6.75336400	1.55786700	-0.01565200
H	6.46701900	1.19945000	-1.72511500
H	7.96507600	0.66895500	-0.94382500
C	2.78093600	2.88221800	1.92412000
H	3.86713000	2.92019500	2.04877600
H	2.33820100	3.46548900	2.73694500
H	2.53259100	3.37636400	0.98130500
C	-4.93706800	-4.77024400	0.45117000
C	-4.38480400	5.24193300	-0.58207500
H	-4.82880000	4.78345600	0.30777100
H	-4.60508600	4.59772300	-1.43827600
H	-4.88332200	6.20231100	-0.74216100
C	6.86319500	-1.09801700	0.87210300
H	7.93689100	-1.25120200	0.73026400
H	6.41619400	-2.05857200	1.14416400

H	6.73697500	-0.41485900	1.71853300
C	-2.57715400	6.38548700	0.76876600
H	-3.06156800	7.35400000	0.61428700
H	-1.50288300	6.55737000	0.88241000
H	-2.95459900	5.97428900	1.71087700
H	-5.34006500	-4.19366700	-0.38803500
H	-5.52853900	-5.68646600	0.53574200
H	-5.08497800	-4.18537900	1.36364000

Compound $2^{\bullet+}$

As	0.00048100	-0.00138800	-0.16219700
C	1.75339400	-0.74463500	0.00572200
C	-1.52170900	-1.14601700	-0.00313300
C	-1.60176000	-2.10253100	1.02797500
C	0.40331700	2.69644100	-0.96672000
C	-0.23257200	1.88869200	-0.00090400
C	-2.53410800	-1.00143700	-0.97441400
C	2.61867300	-0.32720400	1.03613600
C	-1.02861200	2.43314500	1.02606300
C	-2.72284000	-2.92850000	1.05370500
H	-2.81158800	-3.67949300	1.83129900
C	-1.68503600	1.59947000	2.11527600
H	-1.32828100	0.57017600	2.01316900
C	-3.64267500	-1.83914600	-0.88291400
H	-4.43933400	-1.74938800	-1.61378200
C	-1.18814200	3.81645500	1.05196300
H	-1.79991000	4.26599900	1.82665500
C	0.22591000	4.07465200	-0.87584100
H	0.70413900	4.72186800	-1.60336600
C	-0.55459000	-2.25306700	2.12019300
H	0.15922400	-1.43011700	2.01791300
C	-3.73483700	-2.79729200	0.11476100
C	2.13950900	-1.69772200	-0.95992000
C	1.21772800	2.13896400	-2.12550100
H	1.22702600	1.04606200	-2.03905800
C	2.21922700	0.65471900	2.12632200
H	1.15026500	0.86160400	2.01847700
C	-2.44895800	-0.02484800	-2.13882900
H	-1.50088800	0.51977300	-2.05593800
C	-1.17040200	-2.13666400	3.52020500
H	-1.74934100	-1.21524100	3.63347100
H	-0.38154300	-2.13888300	4.27820400
H	-1.83479000	-2.97723800	3.73942300
C	-0.56623100	4.63006700	0.11700700
C	3.89728300	-0.87869500	1.06533600
H	4.58985800	-0.57341400	1.84232100
C	-1.28022200	2.07329700	3.51692000
H	-0.19310500	2.11497400	3.63296200
H	-1.67770600	1.38989800	4.27313600
H	-1.67766000	3.06820200	3.73634900
C	2.41821100	0.06118900	3.52675200
H	1.91023600	-0.90175900	3.63505700
H	2.02000800	0.74361200	4.28346300

H	3.47715400	-0.09294300	3.75240700
C	3.42223900	-2.23129500	-0.86536900
H	3.74724800	-2.96787800	-1.59251700
C	-3.20991300	1.56651800	1.96747200
H	-3.63540500	2.57265000	2.03299100
H	-3.65564400	0.96335500	2.76409900
H	-3.50711200	1.13271700	1.00963600
C	4.29547400	-1.82241600	0.13063100
C	2.95473400	1.99181300	1.98833500
H	4.03850800	1.85613000	2.05683100
H	2.65308200	2.67559800	2.78745200
H	2.73116100	2.47155200	1.03239200
C	0.23592500	-3.55771400	1.97600400
H	0.97981800	-3.64147600	2.77396800
H	0.76192900	-3.59934600	1.01916100
H	-0.42298800	-4.42906800	2.04136900
C	0.55997800	2.47148700	-3.47108600
H	-0.47664100	2.12310600	-3.51121300
H	1.11131000	1.99868100	-4.28931100
H	0.55552400	3.54986700	-3.65477600
C	-2.41560400	-0.76867600	-3.48026800
H	-1.60556900	-1.50370300	-3.51458700
H	-2.27012800	-0.06124400	-4.30204900
H	-3.35437400	-1.29962500	-3.66319500
C	-3.56906400	1.01958000	-2.11327500
H	-3.46852300	1.69988100	-2.96415900
H	-3.53995800	1.61756700	-1.19867100
H	-4.55537900	0.55073900	-2.18055100
C	1.25453800	-2.12330000	-2.12297100
H	0.29992200	-1.59129300	-2.03569200
C	2.67720600	2.60284400	-2.09439500
H	2.75283800	3.69165900	-2.17028000
H	3.22621700	2.17460400	-2.93825600
H	3.17818400	2.29174200	-1.17403500
C	1.87241100	-1.70875100	-3.46471500
H	2.08509400	-0.63581900	-3.49770000
H	1.18985800	-1.94703500	-4.28588900
H	2.81091800	-2.23945700	-3.64974600
C	0.93558000	-3.62137900	-2.10220100
H	1.84465700	-4.22537000	-2.17878500
H	0.29503000	-3.88110900	-2.95022000
H	0.41393500	-3.90924500	-1.18575500
H	-0.69983900	5.70596500	0.16321900
H	-4.60238500	-3.44747100	0.16121300
H	5.29468100	-2.24282100	0.17946600

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