SUPPORTING INFORMATION

for

Regioselective Ultrafast Photoinduced Electron Transfer from Naphthols to Halocarbon Solvents

Subhajyoti Chaudhuri[†], *Atanu Acharya*[†], *Erik T J Nibbering*[‡], *and Victor S Batista*[†,*]

[†] Department of Chemistry, P.O. Box 208107, Yale University, New Haven, CT 06520, USA

[‡] Max Born Institut für Nichtlineare Optik and Kurzzeitspektroskopie, Max Born Strasse 2A, 12489 Berlin, Germany

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1. Computational Method

Figure S1 shows the energies (E_i, i=1,2...,6) and nuclear configurations (R_j, j=1,2,3) relevant for the PET process.

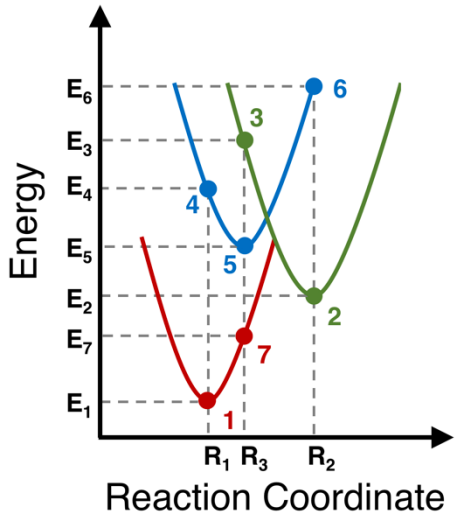


Figure S1. Relevant energies and configurations computed for PET rate calculations.

The energies (E_i) are computed as described below.

E_1: E_1 is obtained by ground state geometry optimization of the naphthol-$CHCl_3$ donor-acceptor complex in a dielectric continuum of $CHCl_3$.

E_4: We obtain the $E_{^1L_b \leftarrow S_0}$ (denoted in article as $\Delta E_{ex,G}$) excitation energy using EOM-CCSD on the naphthol molecule (since only the solute get photoexcited).

$$E_4 = E_1 + \Delta E_{Ex,G}$$

This accounts for the photoexcited naphthol and the solvent in the same nuclear configuration as the ground state.

E_5: To get an accurate estimate of ΔG^0, we need E_5. Performing excited state optimization on the naphthol-$CHCl_3$ complex poses a problem due to artificial crossing over of states, which makes it difficult to converge to the correct optimized excited state (which is critical for this PET since only the ^1L_b state is fluorescent). To circumvent this problem, we perform excited state optimization on the naphthol only (a valid approximation since solvent reorganization happens on timescales significantly slower than the adiabatic relaxation of the excited naphthol). This gives us $\Delta E_{^1L_b \leftarrow S_0}(R_3)$ (denoted in article as $\Delta E_{Ex,Ad}$).

To obtain E_5 we need the nuclear configuration R_3, for which we add the explicit $CHCl_3$ molecule from the R_1 configuration to the naphthol optimized at the ^1L_b excitation. A ground state single point energy calculation on this configuration gives us E_7.

$$E_5 = E_7 + \Delta E_{Ex,Ad}$$

The adiabatic correction to the excited state is thus obtained as:

$\Delta E_{corr} = E_5 - E_4$

E_3: E_3 is obtained using a single point energy calculation constraining an electron on the $CHCl_3$ molecule and a hole on the naphthol at the same nuclear configuration R_3 generated before using CDFT.

E_2: E_2 is obtained via CDFT optimization, constraining an electron on the $CHCl_3$ molecule and a hole on the naphthol, generating configuration R_2.

E_6: To obtain E_6, we compute the $E_{^1L_b \leftarrow S_0}$ (denoted in article as $\Delta E_{ex,CS}$) excitation energy using EOM-CCSD on the naphthol molecule from configuration R_2.

2. Level of Theory for Different Calculations

Table S1 shows the various levels of theory used for the different calculations. The naphthol and the electron accepting $CHCl_3$ molecule are optimized in a dielectric continuum solvent model at B3LYP-D/6-31+G(d,p) for ground and charge separated state calculations. Since only the naphthol gets photoexcited, for the excited state calculations, only the naphthol molecule is used in a dielectric continuum solvent model at EOM-CCSD/ 6-31+G(d,p).

A detailed account of why EOM-CCSD is used instead of the more commonly used TDDFT has been provided by Acharya et al[1].

Table S1. Level of theory used or the different types of computations

Type of Calculation	Method	Level of Theory
Ground State	DFT	B3LYP-D/6-31+G(d,p)
Excited State	EOM-CCSD	EOM-CCSD/6-31+G(d,p)
	TDDFT	B3LYP-D/6-31+G(d,p)
Charge Separated State	CDFT	B3LYP-D/6-31+G(d,p)
Electronic Coupling	FCD	ωB97x-D/6-31+G(d,p)

3. Resonance Structures

Figure S2 shows the electron-rich centers of 1N and 2N using resonance structures. Figure S3 shows the energetically feasible configurations of the naphthol-$CHCl_3$ system. As expected from the resonance structures, during electron transfer, the electron-accepting $CHCl_3$ molecule moves from its initial position with the C-H bond pointing towards the center of the aromatic rings to one of the electron-rich centers.

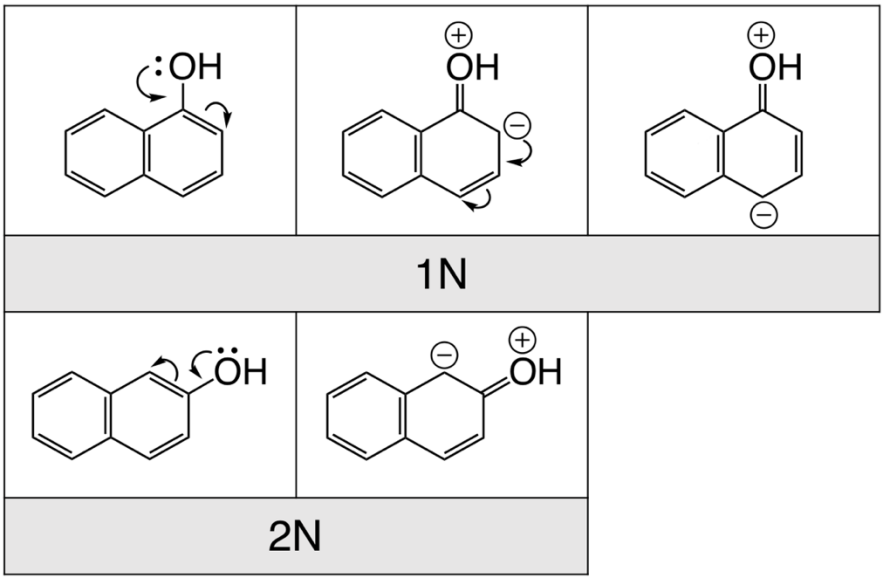


Figure S2. Resonance structures of 1N and 2N showing negatively charged atoms.

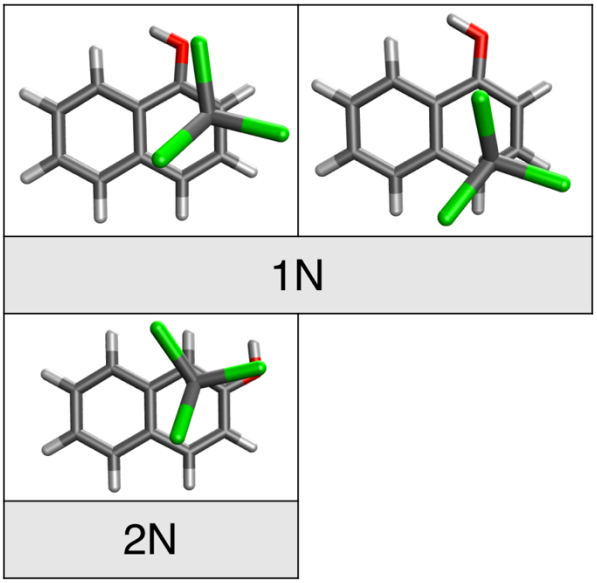


Figure S3. Top view of the energetically favorable structures of 1N and 2N in the charge separated state.

4. Chloroform Structures

$CHCl_3^-$ molecule was optimized at different levels of theory to obtain an undissociated structure. C-Cl and C-H bond lengths from the undissociated structure were used to constrain the bond lengths of the $CHCl_3^-$ molecule in the charge separated state CDFT calculations.

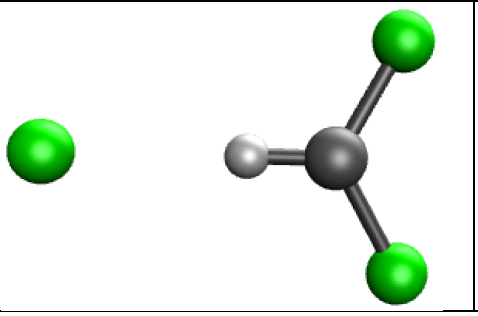
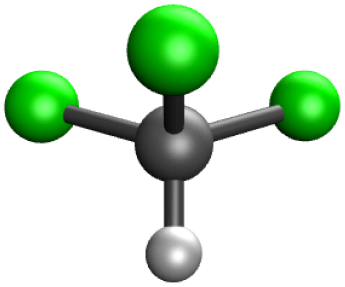
B3LYP/6-31+G(d,p)	MP2/6-311++G(d,p)
	

Figure S4. (Left) Dissociated $CHCl_3^-$ optimized at B3LYP/6-31+G(d,p) level **(Right)** Undissociated $CHCl_3^-$ optimized at MP2/6-311++G(d,p) level

5. Comparison of Free and Reorganization Energies with and without an Explicit Solvent Molecule

For comparison, calculations were performed without assuming any solvent shell order (i.e. infinitely separated solute and explicit solvent) as well as without any explicit solvent (i.e. oxidation of photoexcited naphthol). As expected, the free energy (ΔG^0) for the oxidation of naphthol was greater than the free energy for electron transfer without assuming specific solvent shell, which in turn was greater than the free energy for the model with the explicit solvent molecule in the first solvation shell. The reorganization energies (λ) for both the models including explicit solvent were found to be comparable while for just the oxidation of naphthol, the reorganization energy was noticeably lower due to the complete absence of solvent reorganization.

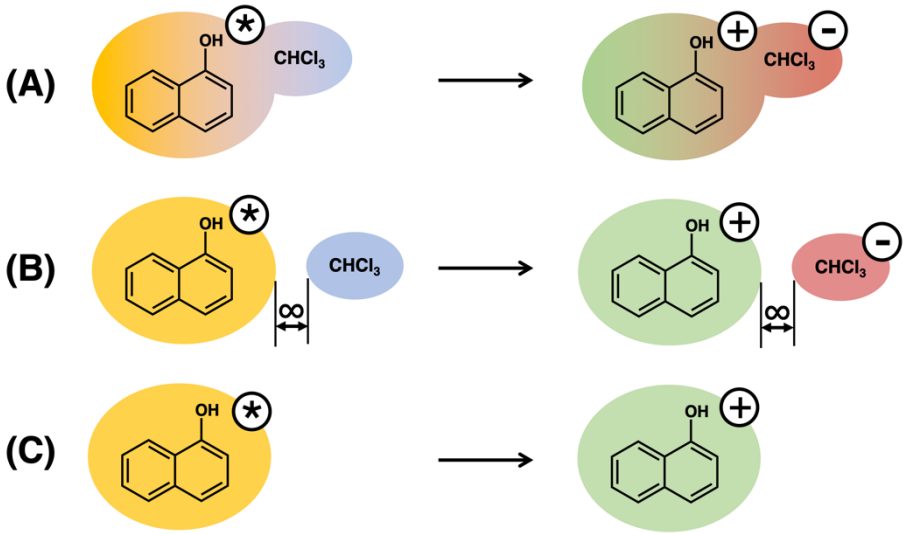


Figure S5. Electron transfer processes for (A) model used in the article i.e. keeping an explicit electron accepting solvent in the first solvation shell, (B) model assuming not solvent order i.e.

infinitely separated solute and solvent, and (C) oxidation of photoexcited naphthol in dielectric continuum of $CHCl_3$

Table S2. Free energies (ΔG^0) and reorganization energies (λ) for electron transfer processes with and without explicit solvent

Isomer	ET with explicit solvent inside first solvation sphere		ET with explicit solvent at infinite separation		Oxidation of naphthol	
	ΔG^0	λ	ΔG^0	λ	ΔG^0	λ
	eV		eV		eV	
cis1N	-0.41 — -0.48	1.25 — 1.37	0.52	1.21	1.74	0.15
trans1N	-0.45 — -0.52	1.27 — 1.37	0.48	1.20	1.70	0.15
cis2N	-0.31 — -0.47	1.42	0.61	1.25	1.82	0.13
trans2N	-0.29 — -0.46	1.39 — 1.40	0.60	1.25	1.81	0.13

6. EOM-CCSD for Excited States

Due to the absence of correlation from doubly excited configurations and inconsistent description of electronic excited states of naphthol photoacids (revealed by excitation analysis based on the one- electron transition density matrix), TDDFT fails dramatically at predicting the energy and ordering of the ^1L_a and ^1L_b excited states as observed experimentally, while EOM-CCSD accurately predicts the excited states.[1]

7. Optimized Structures

7.1. Ground State

7.1.1. cis1N with $CHCl_3$ on $R^{(1)}$

C	-1.5960581148	4.8996910729	-0.2568846119
C	-2.5837890967	4.3405089675	0.5240113095
C	-2.7379811098	2.9285403386	0.6190792213
C	-1.8388421305	2.0852588628	-0.1210962542
C	-0.8288265608	2.6948379437	-0.9172866773
C	-0.7100563546	4.0671428797	-0.9851735127
H	-4.4137882955	2.9983857867	1.9919039349
H	-1.4922377712	5.9789704095	-0.3162472221

H	-3.2646071551	4.9733654317	1.0869534046
C	-3.7478349439	2.3472071380	1.4338001902
C	-2.0038037901	0.6666690838	-0.0079982294
H	-0.1268210988	2.0900533000	-1.4849538970
H	0.0684135373	4.5120629835	-1.5973319991
C	-2.9916671370	0.1297875402	0.7962750472
C	-3.8646470680	0.9755692509	1.5181611416
H	-3.0847174967	-0.9492751615	0.8646257341
H	-4.6297930066	0.5294924370	2.1461910657
O	-1.1996294325	-0.2207375743	-0.6714903177
H	-0.5615270162	0.2297777683	-1.2408983429
C	-0.6384090691	1.6848836670	3.4628836609
Cl	0.9515151918	2.0826965048	2.7407873289
Cl	-1.2645502287	3.0532326176	4.4333442195
Cl	-0.5470281865	0.1886832245	4.4437790997
H	-1.3387095761	1.5031132372	2.6535335462

7.1.2. trans1N with $CHCl_3$ on $R^{(1)}$

C	-1.7590335285	4.9582833867	-0.2789157307
C	-2.7188935324	4.3539571411	0.5053094223
C	-2.7924602990	2.9367575209	0.6118716492
C	-1.8424642114	2.1467257813	-0.1170265003
C	-0.8631231261	2.7947042352	-0.9176750665
C	-0.8233303124	4.1716251754	-0.9972486395
H	-4.4837127406	2.9008330414	1.9722014244
H	-1.7169401903	6.0413211320	-0.3487446565
H	-3.4367309536	4.9543907514	1.0578445791
C	-3.7713026087	2.2932600021	1.4219996149
C	-1.9134397917	0.7236902514	0.0000349652
H	-0.1453625353	2.1927608983	-1.4635651216
H	-0.0711537976	4.6573796722	-1.6116626729
C	-2.8719313965	0.1230883336	0.7938413793
C	-3.8044572088	0.9174295181	1.5052500739
H	-2.9039438546	-0.9600483538	0.8778048652
H	-4.5447858067	0.4254171075	2.1286976613
O	-0.9828396741	0.0095936374	-0.7042569248
H	-1.1043188672	-0.9386222679	-0.5497844609
C	-0.7130349476	1.7024368116	3.5311057890
Cl	0.8865044201	1.4457348102	2.7691912321
Cl	-0.7283982904	3.2013138414	4.5119425997
Cl	-1.1973707187	0.2848434518	4.5133928625
H	-1.4472278780	1.8213194909	2.7406075157

7.1.3. cis2N with $CHCl_3$ on $R^{(1)}$

C	-1.5774894912	4.9108803073	-0.2634386697
C	-2.5942192660	4.3645282344	0.4923132763
C	-2.7595858204	2.9549544399	0.5779781748
C	-1.8536472470	2.0990908708	-0.1322132708
C	-0.8159084144	2.6935599825	-0.9038169539
C	-0.6823731262	4.0650319713	-0.9679153748
H	-4.4809441744	2.9981316753	1.8967605166
H	-1.4586912511	5.9886611872	-0.3218933934
H	-3.2839457234	5.0053497630	1.0358179079
C	-3.7934070942	2.3558051497	1.3532933926
C	-2.0081741900	0.6882440492	-0.0372027921
H	-0.1275878926	2.0475102856	-1.4423163913
H	0.1156945208	4.5037468922	-1.5599363673
C	-3.0238988929	0.1479845365	0.7261437099
C	-3.9274557549	0.9882252681	1.4299508377
H	-4.7113076145	0.5318879775	2.0260127504
H	-1.3147763389	0.0397278979	-0.5678038300
O	-3.2244171635	-1.1995925745	0.8646184624
H	-2.5586344048	-1.6918745788	0.3617685115
C	-0.6109517969	1.7016696795	3.3823907187
Cl	0.9480435382	2.2916297018	2.7285079906
Cl	-1.1513953230	2.7057634511	4.7639296948
Cl	-0.5072216981	-0.0260225827	3.8416800725
H	-1.3560733908	1.7922843451	2.5984091365

7.1.4. trans2N with $CHCl_3$ on $R^{(1)}$

C	-1.7657744939	4.9918057768	-0.2453870310
C	-2.7847130782	4.3754891540	0.4500301312
C	-2.8437223237	2.9577056628	0.5487347037
C	-1.8286471129	2.1674238878	-0.0884338964
C	-0.7898792342	2.8351961700	-0.7985888003
C	-0.7599148897	4.2117420743	-0.8741031225
H	-4.6445569689	2.8775914764	1.7537780906
H	-1.7283557718	6.0748914792	-0.3139657016
H	-3.5579373594	4.9654333782	0.9356877991
C	-3.8737977840	2.2876900481	1.2653360973
C	-1.8770164349	0.7517767027	0.0165923097
H	-0.0179977244	2.2400008560	-1.2792520815
H	0.0395616565	4.7067343700	-1.4179160958
C	-2.8930622766	0.1390467347	0.7229409094
C	-3.9042151153	0.9130802887	1.3533828929
H	-4.6926756975	0.4127474981	1.9098464615
H	-1.1062847608	0.1475111528	-0.4526340710
O	-2.8912419209	-1.2287432598	0.8015097761
H	-3.6306113686	-1.5369830758	1.3452994922

C	-0.6690356270	1.7268253531	3.4172571144
Cl	0.9938772511	1.4052473448	2.8391423259
Cl	-0.7449055510	3.2501042857	4.3565536249
Cl	-1.2975202352	0.3481215285	4.3738854263
H	-1.3048421486	1.8436745529	2.5456038948

7.1.5. cis1N with $CHCl_3$ on $R^{(2)}$

C	-2.0450486984	5.0700492226	-0.8238241254
C	-2.7955132708	4.5211090777	0.1935932081
C	-2.6618144283	3.1507660689	0.5555017610
C	-1.7205075056	2.3365368652	-0.1661809198
C	-0.9603955963	2.9340280956	-1.2115683958
C	-1.1175764810	4.2671301340	-1.5336555456
H	-4.1333052185	3.2145527302	2.1444723389
H	-2.1573912660	6.1188422885	-1.0810999991
H	-3.5035010070	5.1337167935	0.7451357472
C	-3.4282422117	2.5850733816	1.6096563171
C	-1.5924923935	0.9622613793	0.2151484873
H	-0.2337630984	2.3533812383	-1.7732828601
H	-0.5222084614	4.7037063634	-2.3294002942
C	-2.3493690308	0.4409202707	1.2465670394
C	-3.2686410096	1.2569865024	1.9433655043
H	-2.2265912902	-0.6043975376	1.5114926347
H	-3.8518419425	0.8222418678	2.7496399055
O	-0.7259552638	0.1045012726	-0.4088035690
H	-0.2407145745	0.5389912315	-1.1228948735
C	0.7984245784	4.2616521191	1.7932107518
Cl	2.4359857247	3.8382552969	1.1997714923
Cl	0.6916119763	6.0014378860	2.2049602106
Cl	0.3321063744	3.2376735212	3.1847423361
H	0.1000690549	4.0682399204	0.9849904085

7.1.6. trans1N with $CHCl_3$ on $R^{(2)}$

C	-2.0537987209	5.0686245062	-0.8305136650
C	-2.8066513506	4.5328825910	0.1936180241
C	-2.6803085191	3.1636247439	0.5605825654
C	-1.7464171898	2.3479748268	-0.1615679313
C	-0.9845144871	2.9233764208	-1.2153717778
C	-1.1348333792	4.2566059843	-1.5424055894
H	-4.1461217050	3.2223568189	2.1586375659
H	-2.1593729770	6.1173340062	-1.0919468599
H	-3.5078566491	5.1550726081	0.7432096247
C	-3.4428429767	2.5950455673	1.6187833586
C	-1.6118629271	0.9762568859	0.2162378228

H	-0.2783777039	2.3025574012	-1.7551334341
H	-0.5434564534	4.6880371477	-2.3442615812
C	-2.3622928601	0.4486514192	1.2486586349
C	-3.2815787487	1.2672628780	1.9494897196
H	-2.2458438210	-0.5967196321	1.5230786329
H	-3.8614332574	0.8310967708	2.7574921557
O	-0.7075877564	0.2362275519	-0.4976156857
H	-0.6864631464	-0.6732513881	-0.1659851614
C	0.7921041474	4.2007169290	1.7896220383
Cl	2.4408170584	3.7996244705	1.2126661731
Cl	0.6599693828	5.9373050018	2.2075680649
Cl	0.3236885436	3.1659305150	3.1733446640
H	0.1036572570	4.0016993456	0.9739855909

7.1.7. cis2N with $CHCl_3$ on $R^{(2)}$

C	-1.9740008605	5.0760970660	-0.8557076412
C	-2.8599211071	4.5610167440	0.0700411843
C	-2.8041752844	3.1914299986	0.4479856010
C	-1.8140943859	2.3410896898	-0.1471321576
C	-0.9166785742	2.9013377923	-1.0995535094
C	-0.9945401923	4.2356472164	-1.4449392133
H	-4.4428304605	3.2727877971	1.8653787659
H	-2.0207339544	6.1252118386	-1.1314801758
H	-3.6090561718	5.1996930222	0.5308170469
C	-3.6933195874	2.6318338848	1.4092290213
C	-1.7493837331	0.9731240307	0.2347645838
H	-0.1621803199	2.2604100711	-1.5479364165
H	-0.2990964320	4.6491755768	-2.1694186698
C	-2.6304980277	0.4709669320	1.1704468766
C	-3.6144367394	1.3060472760	1.7645891285
H	-4.2894931604	0.8776680943	2.4987326591
H	-0.9958263333	0.3297178240	-0.2137391098
O	-2.6213503577	-0.8341969789	1.5870346764
H	-1.9206373117	-1.3265820945	1.1343144874
C	0.0369033611	4.5374960051	2.3683446462
Cl	1.6984182300	4.9169156328	1.8139247315
Cl	-0.6481870791	5.8907436476	3.3229171388
Cl	-0.0005450714	3.0104787488	3.3002432411
H	-0.5854710968	4.4109123044	1.4874666047

7.1.8. trans2N with $CHCl_3$ on $R^{(2)}$

C	-1.9682452125	5.0668785982	-0.8597981123
C	-2.8569652668	4.5635305657	0.0685880195

C	-2.8101509681	3.1947189861	0.4539333897
C	-1.8260533538	2.3331043127	-0.1375417861
C	-0.9250218093	2.8836268541	-1.0939621218
C	-0.9942296743	4.2159630847	-1.4454157479
H	-4.4455646728	3.2938038755	1.8730002106
H	-2.0073314630	6.1148349798	-1.1411857421
H	-3.6013146709	5.2098279457	0.5265141357
C	-3.7002088941	2.6472505292	1.4179390088
C	-1.7688626462	0.9689470363	0.2498290161
H	-0.1752629331	2.2351999667	-1.5392991013
H	-0.2964949272	4.6216837812	-2.1721237601
C	-2.6508745193	0.4755454358	1.1895194156
C	-3.6281883939	1.3208051630	1.7801179869
H	-4.3123536274	0.9129440264	2.5200887641
H	-1.0247268383	0.3114678699	-0.1901096854
O	-2.5542698502	-0.8475548573	1.5355013947
H	-3.2187956457	-1.0712636258	2.2030370472
C	0.0318597746	4.5360712864	2.3731087443
Cl	1.6922979493	4.9256847324	1.8235299600
Cl	-0.6622427248	5.8829417790	3.3309943589
Cl	-0.0000555789	3.0059567742	3.2999821506
H	-0.5883654533	4.4097590402	1.4906640243

7.2. Charge Separated State

7.2.1. cis1N with C-H bond of $CHCl_3$ pointing towards $C^{(2)}$

C	-1.6857707680	4.9343442952	-0.2203610601
C	-2.6236114937	4.3204888562	0.5902274534
C	-2.6399578584	2.9132816253	0.7406971955
C	-1.6713426333	2.1315871289	0.0226666792
C	-0.7240133227	2.7877965292	-0.8058968762
C	-0.7277275295	4.1653766911	-0.9169847446
H	-4.3740909531	2.8905569531	2.0498675224
H	-1.6826406925	6.0150228838	-0.3218756259
H	-3.3582903266	4.9131021349	1.1266606152
C	-3.6156748519	2.2759033245	1.5736625134
C	-1.7550535628	0.7014009961	0.1380648341
H	0.0274565590	2.2270034676	-1.3538388781
H	0.0089694530	4.6578152079	-1.5429728347
C	-2.5996966602	0.1113559194	1.1128428782
C	-3.6157387790	0.9110364084	1.7381229471
H	-2.6911710638	-0.9773727280	1.0984568247
H	-4.4013576496	0.4236167929	2.3093381165
O	-1.0776520990	-0.1433611857	-0.6385865353
H	-0.4760434136	0.2990637132	-1.2593662646

C	-0.9990473907	1.0024444247	2.9629745287
Cl	0.5754706146	0.3251706766	2.4864916328
Cl	-0.6145107324	2.5909112843	3.6503127926
Cl	-1.5481279619	-0.0180930664	4.3100984203
H	-1.6918425537	0.8027086269	2.1229810854

7.2.2. trans1N with C-H bond of $CHCl_3$ pointing towards $C^{(2)}$

C	-1.6739549593	4.9140102285	-0.2283808710
C	-2.6098269292	4.3177368246	0.5996274612
C	-2.6381141188	2.9121979192	0.7583703190
C	-1.6823189939	2.1229133817	0.0367980806
C	-0.7425300474	2.7535089225	-0.8175570325
C	-0.7360698576	4.1310495700	-0.9378420600
H	-4.3705994788	2.8923648445	2.0729074515
H	-1.6611852263	5.9940743570	-0.3370538917
H	-3.3318817946	4.9231996845	1.1389472702
C	-3.6137057547	2.2770905545	1.5948282919
C	-1.7599382355	0.6964702372	0.1574913721
H	-0.0323420800	2.1507954386	-1.3720528653
H	-0.0098819048	4.6141645443	-1.5834012002
C	-2.6029656012	0.1059191469	1.1339377609
C	-3.6187209735	0.9119072076	1.7576881931
H	-2.7060786524	-0.9831475479	1.1324112452
H	-4.4059041694	0.4266529659	2.3286908085
O	-1.0070558726	-0.0237004452	-0.6732800034
H	-1.1491222946	-0.9794564894	-0.5657123300
C	-1.0149781768	1.0114101725	2.9880063551
Cl	0.5768990708	0.3714271095	2.5176967305
Cl	-0.6652587351	2.5992505852	3.6951049627
Cl	-1.5498326043	-0.0324455144	4.3229314769
H	-1.7008014801	0.8044046423	2.1440610847

7.2.3. cis1N with C-H bond of $CHCl_3$ pointing towards $C^{(4)}$

C	-1.8586596894	5.0428239289	-0.5009076276
C	-2.7957514469	4.4896040423	0.3549466775
C	-2.7322007941	3.1171105136	0.6995868538
C	-1.7123639635	2.3002998096	0.1113671457
C	-0.7553748464	2.8990304193	-0.7470666860
C	-0.8238480920	4.2488802148	-1.0388743660
H	-4.5381116193	3.1247093892	1.9352128530
H	-1.9241759213	6.0928774379	-0.7679372917
H	-3.6082335165	5.0981009474	0.7412530028
C	-3.6836443585	2.5237495041	1.6146254478

C	-1.7516891491	0.8845263216	0.3753386131
H	0.0412804700	2.3157123512	-1.1991929211
H	-0.0869088102	4.6951935173	-1.6983947820
C	-2.7789299874	0.3090297900	1.1439133234
C	-3.7716958999	1.1127848656	1.6942034133
H	-2.8017717897	-0.7707610981	1.2484017703
H	-4.6218975644	0.6504649649	2.1906536075
O	-0.8596294953	0.0267757263	-0.1215697782
H	-0.1587541512	0.4531207498	-0.6391472490
C	-1.7582264802	2.4264199389	3.3480789983
Cl	-0.0256974747	2.0237351097	3.3159725376
Cl	-1.8097467956	4.1290524017	3.8399302461
Cl	-2.4373574848	1.5172523933	4.7155308179
H	-2.4932300597	2.3587259708	2.5230724635

7.2.4. trans1N with C-H bond of $CHCl_3$ pointing towards $C^{(4)}$

C	-1.8375598216	5.0257592490	-0.5000479028
C	-2.7858576467	4.4894307708	0.3560782341
C	-2.7372011988	3.1180787781	0.7068013062
C	-1.7224747982	2.2951577495	0.1248438909
C	-0.7521581407	2.8695662765	-0.7327835598
C	-0.8081853987	4.2191096720	-1.0316838955
H	-4.5515732277	3.1241288592	1.9347306367
H	-1.8914391243	6.0751724997	-0.7727675844
H	-3.5925181951	5.1102415084	0.7350274185
C	-3.6943968024	2.5254597489	1.6172215681
C	-1.7590443489	0.8833317876	0.3886028314
H	0.0231338512	2.2438705100	-1.1595815835
H	-0.0658824089	4.6579254151	-1.6905718767
C	-2.7813792378	0.3065826046	1.1616387781
C	-3.7781180021	1.1152576923	1.7042337398
H	-2.8168630798	-0.7731265154	1.2792322141
H	-4.6305078949	0.6536401662	2.1978792837
O	-0.8001766089	0.1475828146	-0.1749356658
H	-0.8834861639	-0.7929317677	0.0548253220
C	-1.7778061243	2.4213531084	3.3659451636
Cl	-0.0441953226	2.0231215335	3.3368273599
Cl	-1.8377693391	4.1229358902	3.8604648755
Cl	-2.4572767652	1.5076447034	4.7301979351
H	-2.5085863206	2.3505635351	2.5374539708

7.2.5. cis2N with C-H bond of $CHCl_3$ pointing towards $C^{(1)}$

C	-1.6509071544	4.9436422859	-0.2578541071

C	-2.6103399223	4.3772836015	0.5657781187
C	-2.6442381685	2.9758360805	0.7587116025
C	-1.6639263321	2.1510889081	0.1235965203
C	-0.7125900842	2.7485812920	-0.7360006711
C	-0.7131692880	4.1246712443	-0.9205293234
H	-4.4052929109	2.9824638766	2.0252127369
H	-1.6286677956	6.0183081030	-0.4074337433
H	-3.3503887959	4.9980599183	1.0624033568
C	-3.6695265638	2.3495499796	1.5353030893
C	-1.6914460321	0.7206970376	0.3755122592
H	-0.0125016929	2.1258925272	-1.2854086289
H	0.0096873383	4.5747830508	-1.5939246312
C	-2.8572210134	0.1522401161	0.9612078026
C	-3.7869016514	0.9799720573	1.6418730435
H	-4.6130957859	0.5228245768	2.1765271627
H	-1.0658120311	0.0730899972	-0.2484727038
O	-3.1206336578	-1.1550217038	0.9346618729
H	-2.4708498205	-1.6520100355	0.4086001753
C	-0.6829994767	1.2356434952	2.6896658994
Cl	1.0278111330	1.2939127682	2.2053388849
Cl	-0.8942243227	2.5469942004	3.8640896582
Cl	-0.8611401380	-0.2741643147	3.6097065713
H	-1.2353061131	1.1042946576	1.7393224343

7.2.6. trans2N with C-H bond of $CHCl_3$ pointing towards $C^{(1)}$

C	-1.6371255897	4.9460478592	-0.2635953351
C	-2.5973231480	4.3927934538	0.5672833562
C	-2.6466799633	2.9913266664	0.7616196820
C	-1.6800833128	2.1530707580	0.1214956974
C	-0.7290767661	2.7387091296	-0.7471025374
C	-0.7150027892	4.1142498755	-0.9332440665
H	-4.4057923444	3.0198246361	2.0289587966
H	-1.6024617676	6.0201632882	-0.4146796704
H	-3.3265274633	5.0230586403	1.0679844658
C	-3.6767469758	2.3786610164	1.5396142563
C	-1.7201828424	0.7260731893	0.3774666036
H	-0.0409041537	2.1064528941	-1.3004984231
H	0.0073488882	4.5549187426	-1.6134193350
C	-2.8868932575	0.1703901256	0.9716009889
C	-3.8074975298	1.0092702344	1.6514138951
H	-4.6410803668	0.5729910291	2.1949114548
H	-1.1089901322	0.0605155036	-0.2395773773
O	-3.0567666139	-1.1486542584	0.8679429403
H	-3.8321464700	-1.4569234996	1.3678296674
C	-0.6987321759	1.2209684329	2.6951211597

Cl	1.0074933357	1.3291098959	2.2032463429
Cl	-0.9382644711	2.4951740761	3.9044813334
Cl	-0.8431150417	-0.3182548224	3.5712911841
H	-1.2577178587	1.1003000635	1.7472699106

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