

Supporting Information

**Substituent Effects on Photoresponsive Nitric Oxide Release by
N-Nitrosoaniline Derivatives**

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1. Supporting Figures and Tables

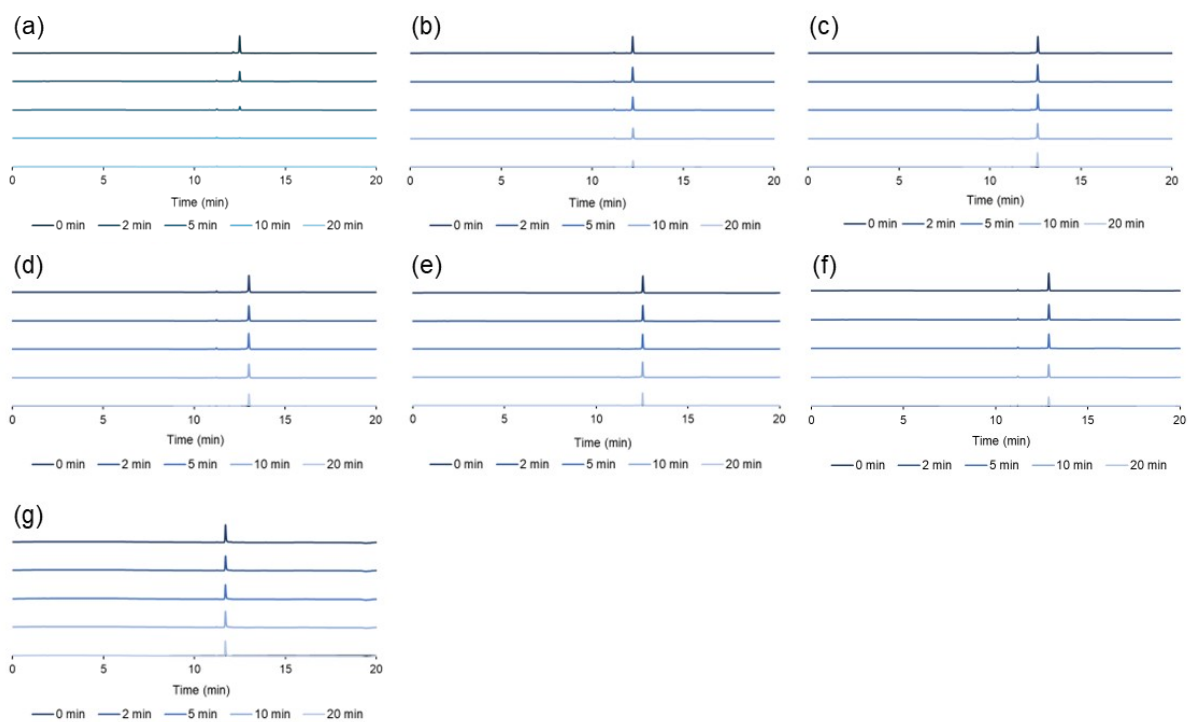


Figure S1 (a)–(g) Monitoring photodecomposition: chromatograms at 650 nm of solutions of **1** (a), **2** (b), **3**(c), **4** (d), **5** (e), **6** (f) and **7** (g) at various irradiation times.

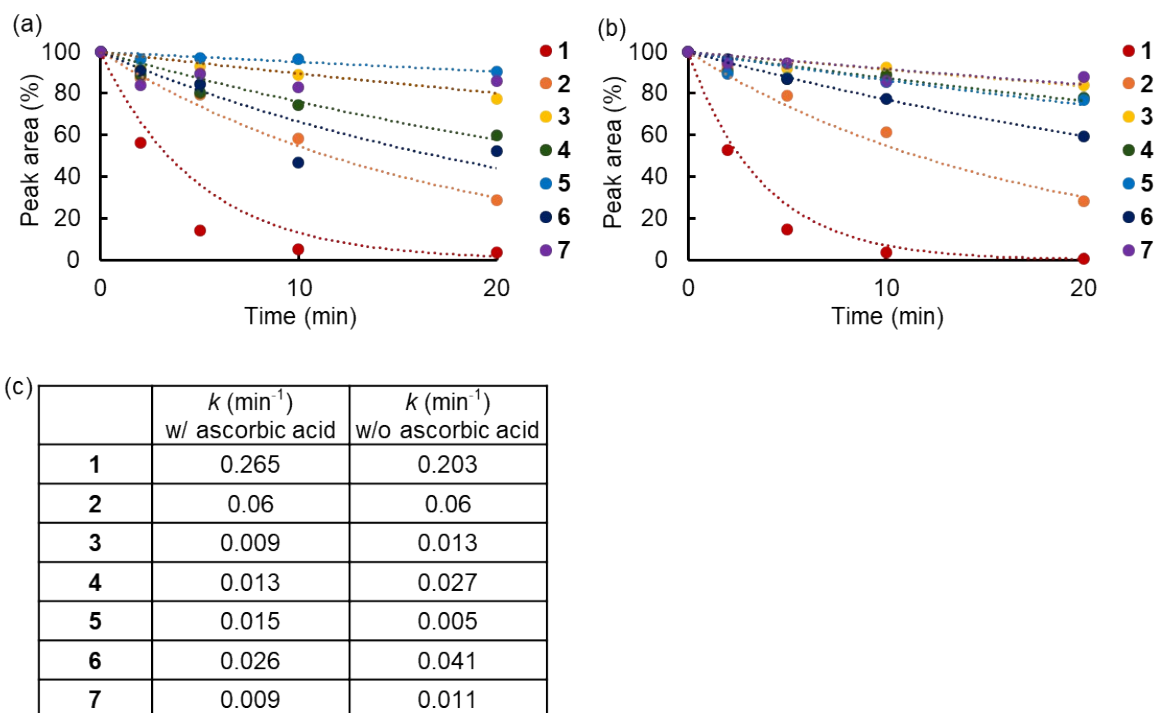


Figure S2 (a) Change of HPLC peak area of solutions of 1–8 with irradiation time in the presence of ascorbic acid. (b) Change of HPLC peak area of solutions of 1–8 with irradiation time in the absence of ascorbic acid. Each compound (10 μM) was dissolved in HEPES buffer (100 mM, pH 7.4, DMSO 0.1%). (c) Photodecomposition rate constants in the presence or absence of ascorbic acid.

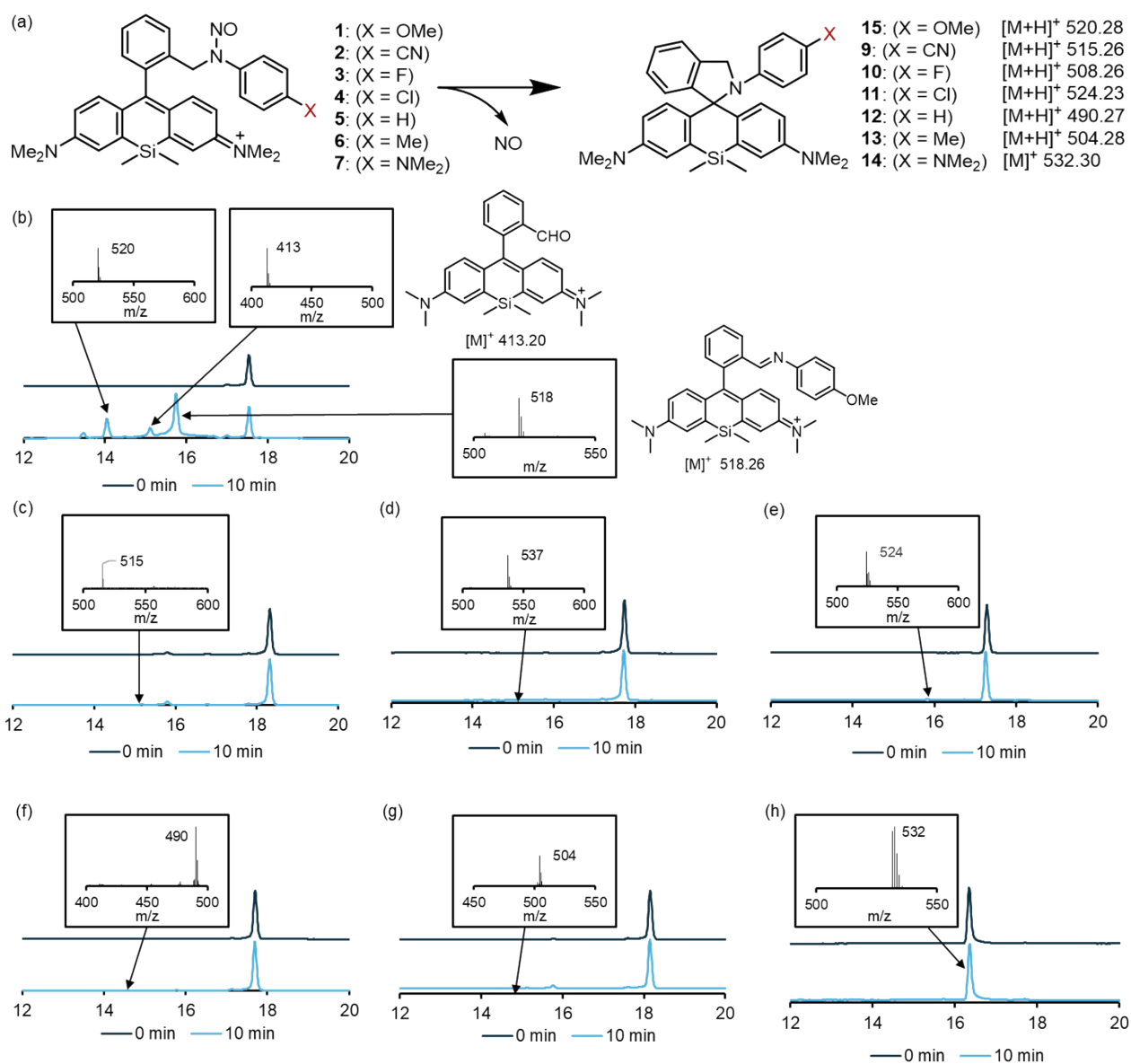


Figure S3 (a) Putative photodecomposition products of NORD-2 derivatives. (b)–(h) LC-MS charts of solutions of **1** (b), **2** (c), **3** (d), **4** (e), **5** (f), **6** (g), and **7** (h). Each compound (10 μM) was dissolved in HEPES buffer (100 mM, pH 7.4, DMSO 0.1%).

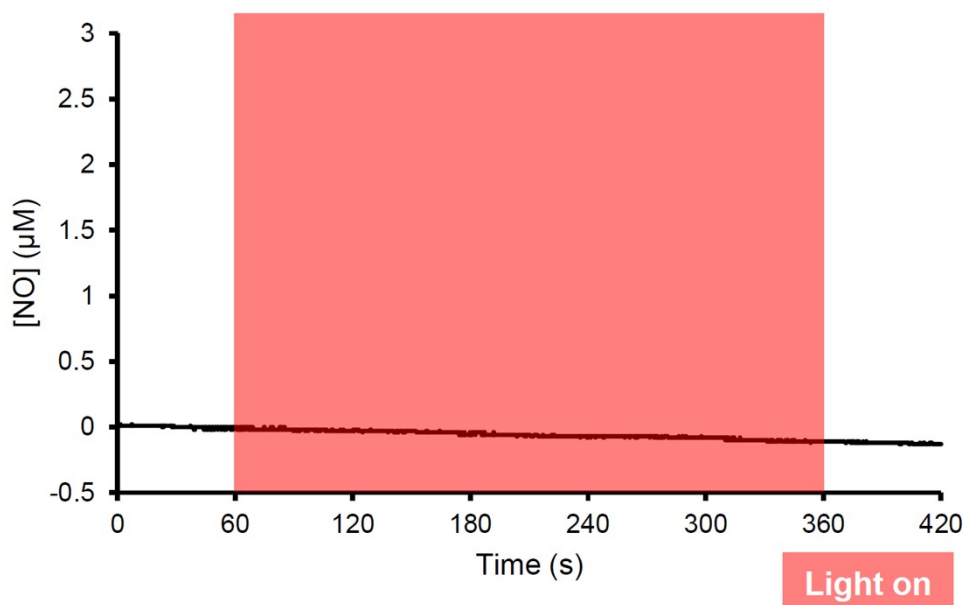


Figure S4. Effect of light irradiation on the NO electrode signal. NO electrode response of 100 mM HEPES buffer (pH 7.3) containing 0.1% DMSO in the absence of NO releasers. The sample was irradiated with 660 nm light at 133 mW cm^{-2} during the red shaded period. No increase in the NO signal was observed.

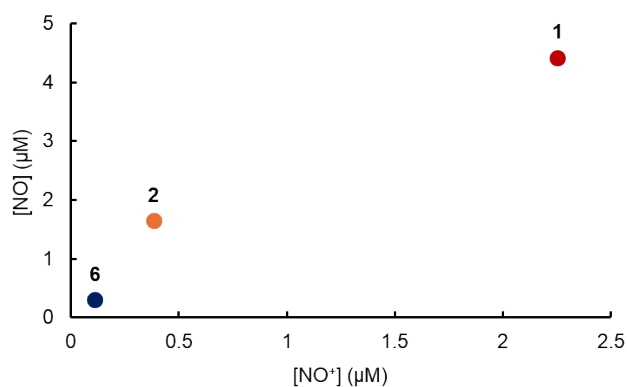


Figure S5 Comparison of amounts of NO and NO⁺ released from **1**, **2** and **6**.

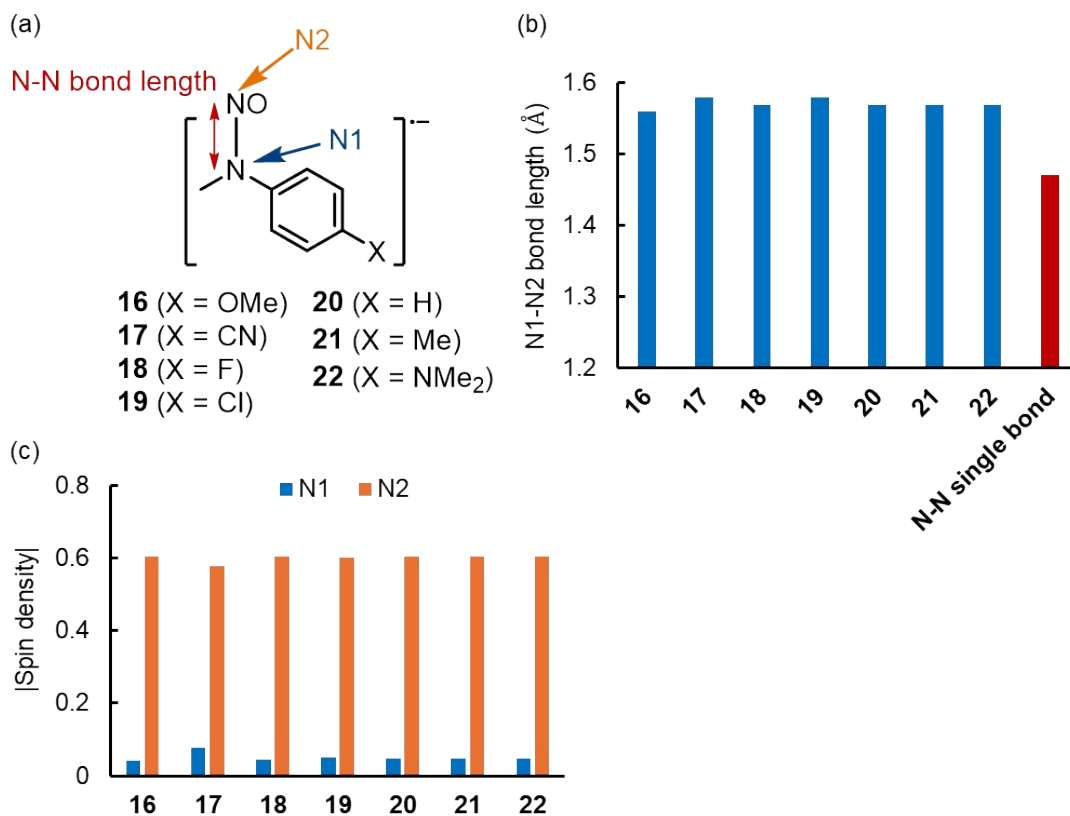


Figure S6 (a) Structures of model radical anion intermediates **16–22**. (b) N1-N2 bond lengths of **16–22**. The N–N single-bond length is based on the reported value for hydrazine.¹ (c) Spin densities of N1 and N2 in **16–22**. Calculations were conducted using U ω B97X-D/6-31G (d,p).

(a)

	1	2	3	4	5	6	7
Excitation Energy [eV]	2.74	2.57	2.57	2.58	2.58	2.58	2.72
π - π^* [eV]	2.69	2.49	2.50	2.46	2.45	2.45	2.54
CT-MECI [eV]	2.70	2.93	3.01	2.66	3.06	2.55	2.54
CT [eV]	2.10	2.93	2.48	2.56	2.56	2.47	1.69

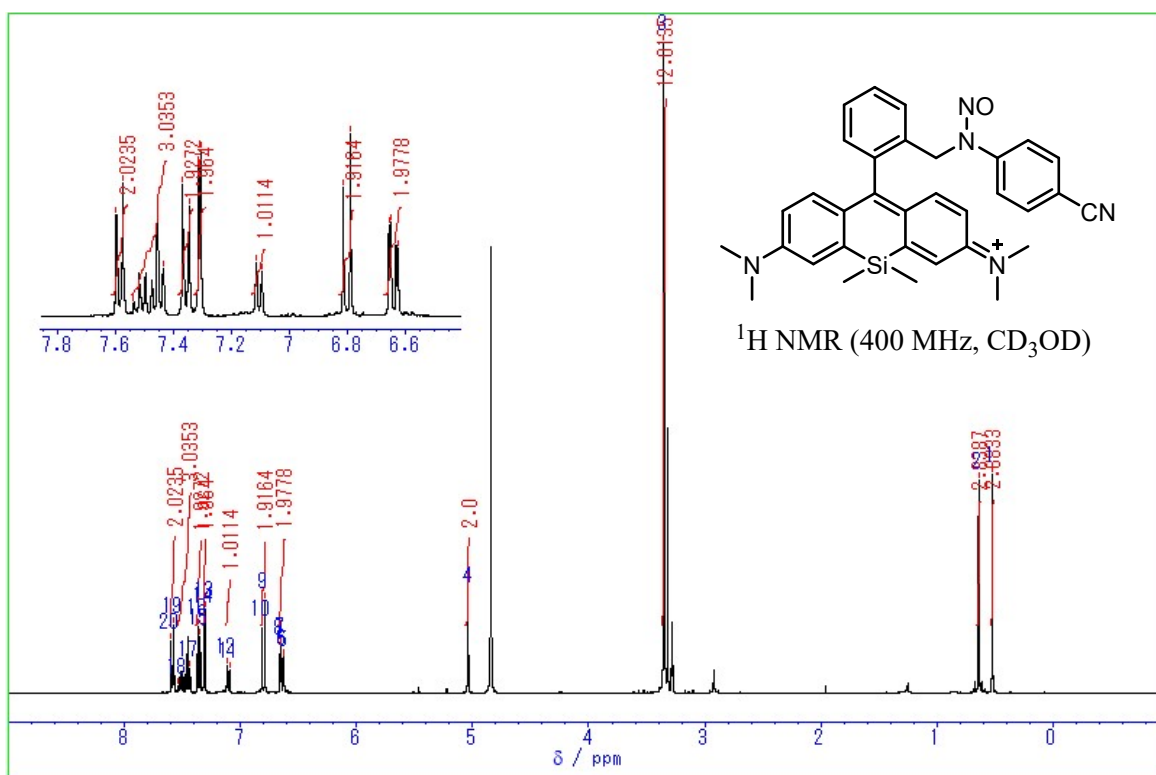
(b)

	1	7
GS-MECI [eV]	3.20	2.28

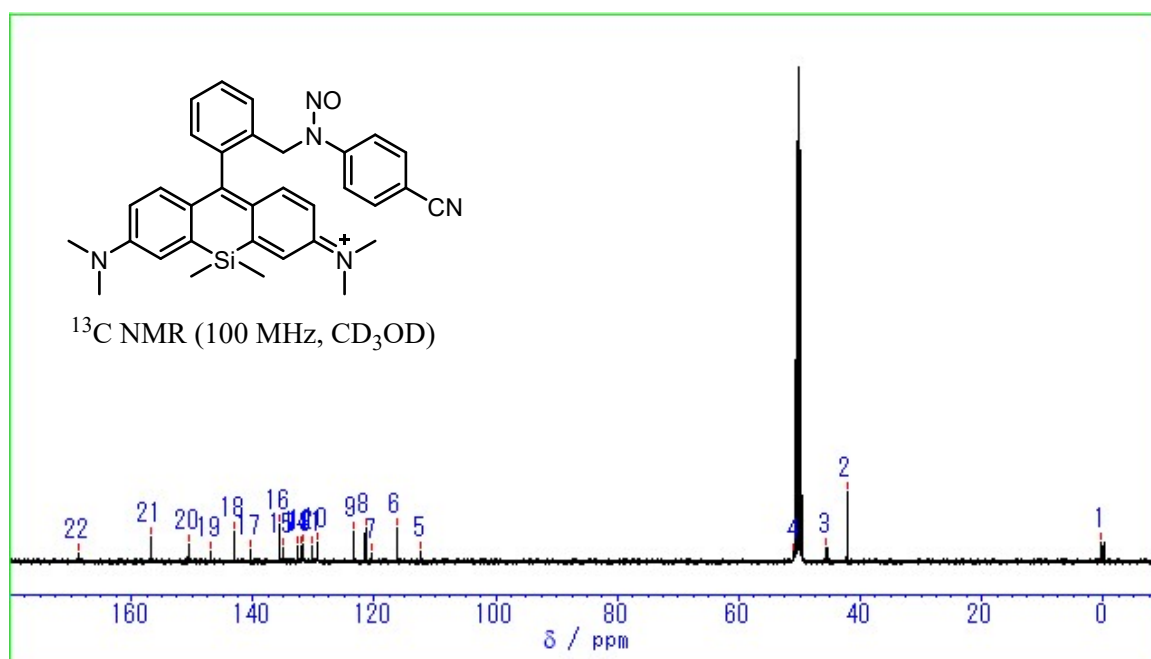
Figure S7 (a) Energy of each excited state and CT-MECI of **1–7**. Calculations were conducted using ω B97XD/6-31G (d,p). (b) GS-MECI of **1** and **7**.

2. NMR charts of 2–13

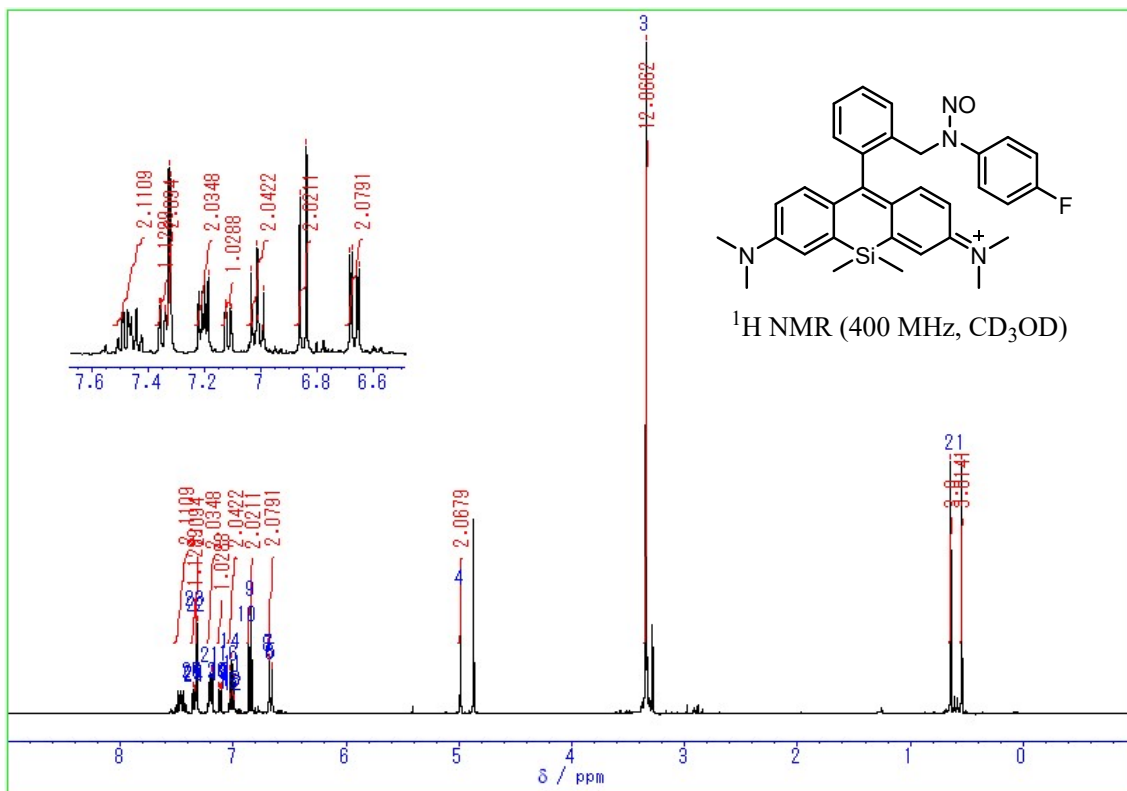
^1H NMR of 2



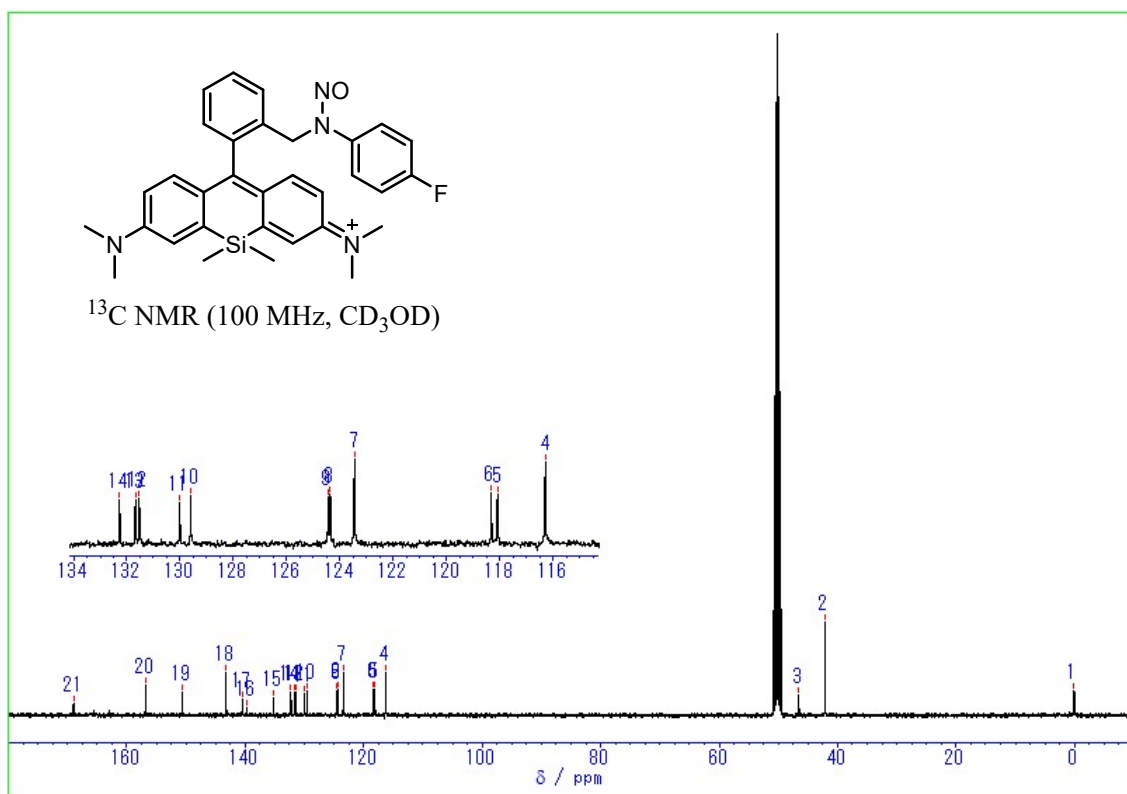
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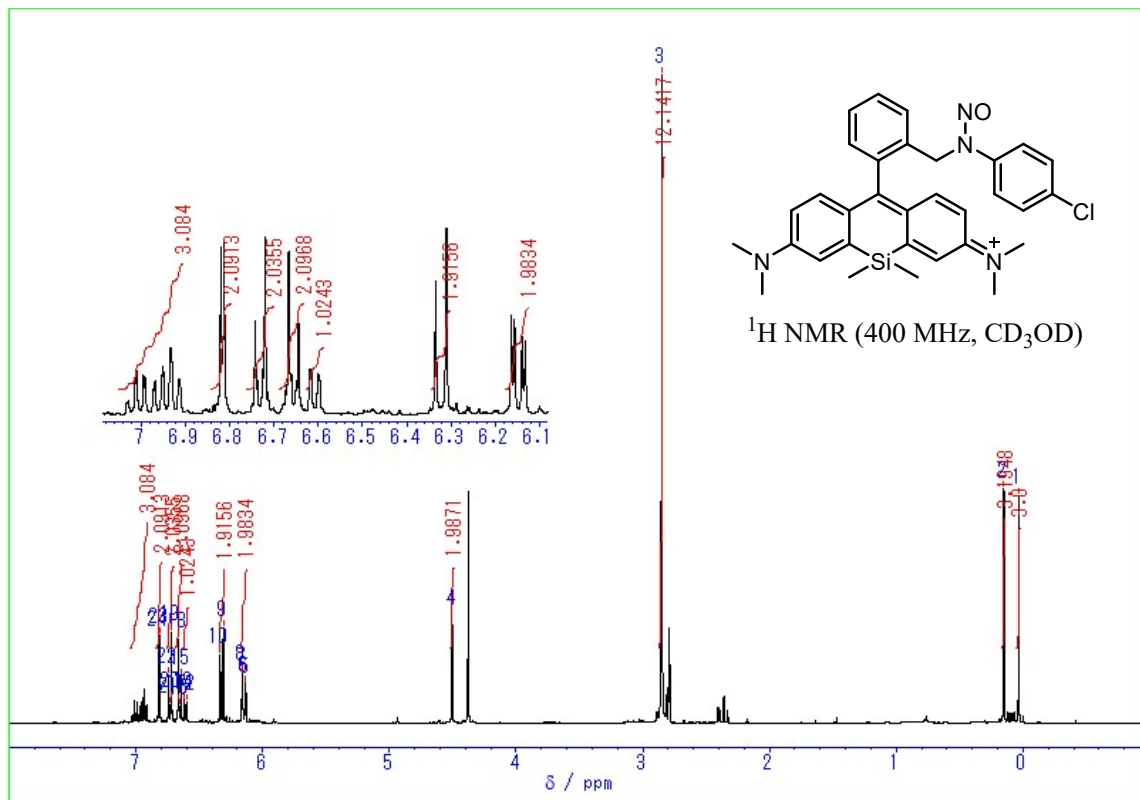
¹H NMR of **3**



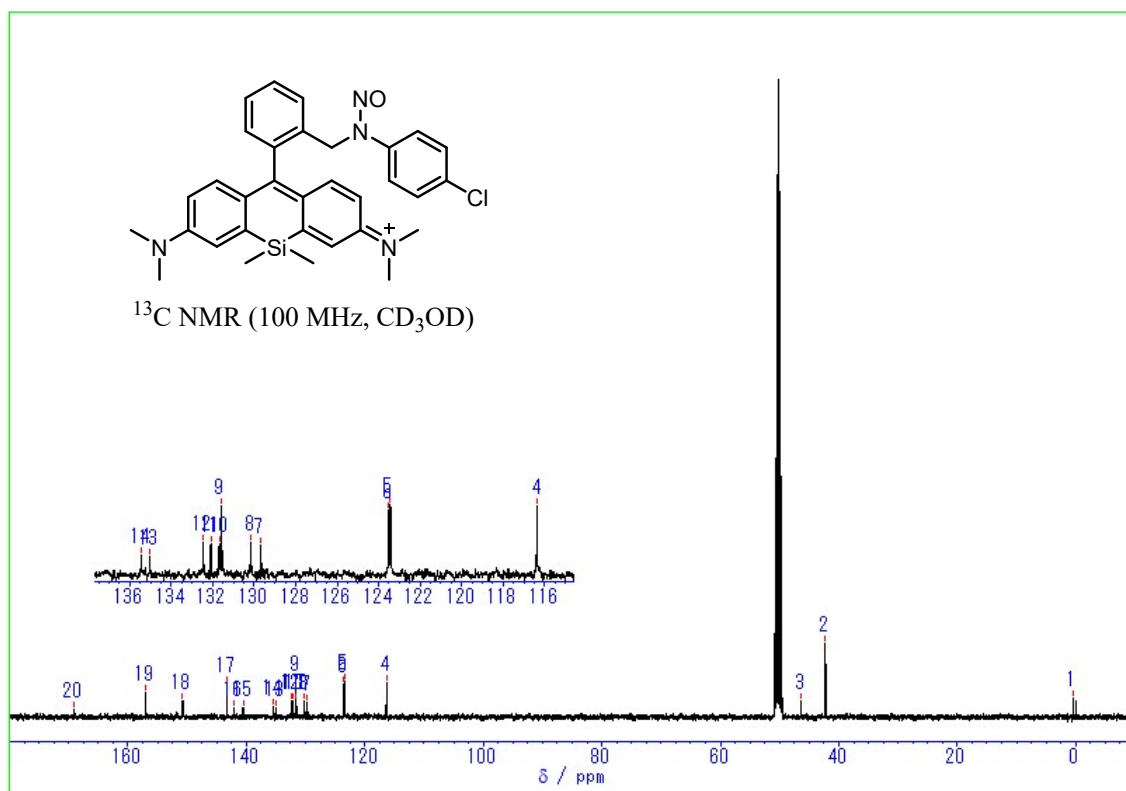
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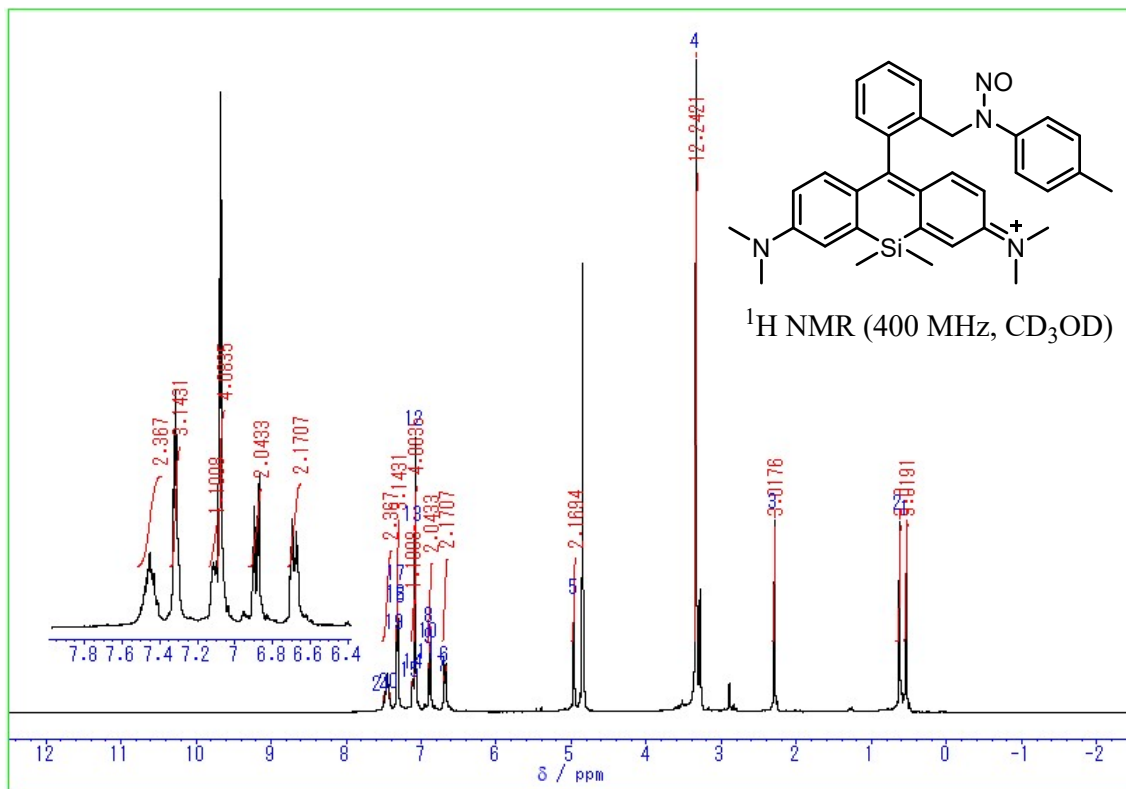
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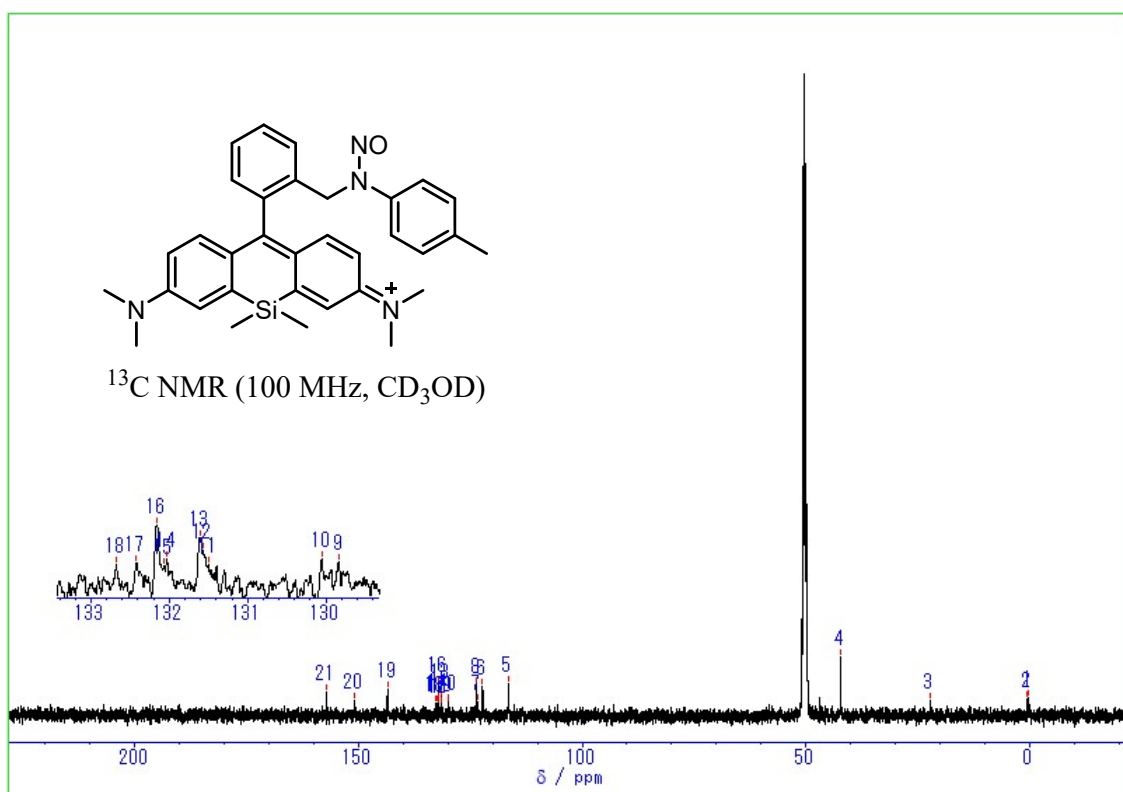
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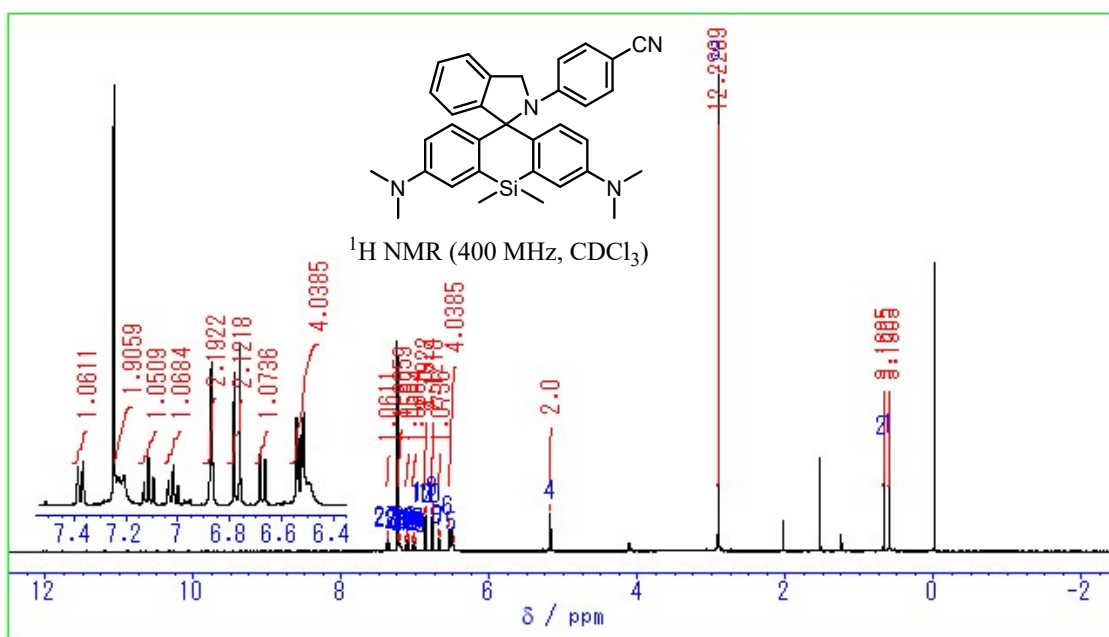
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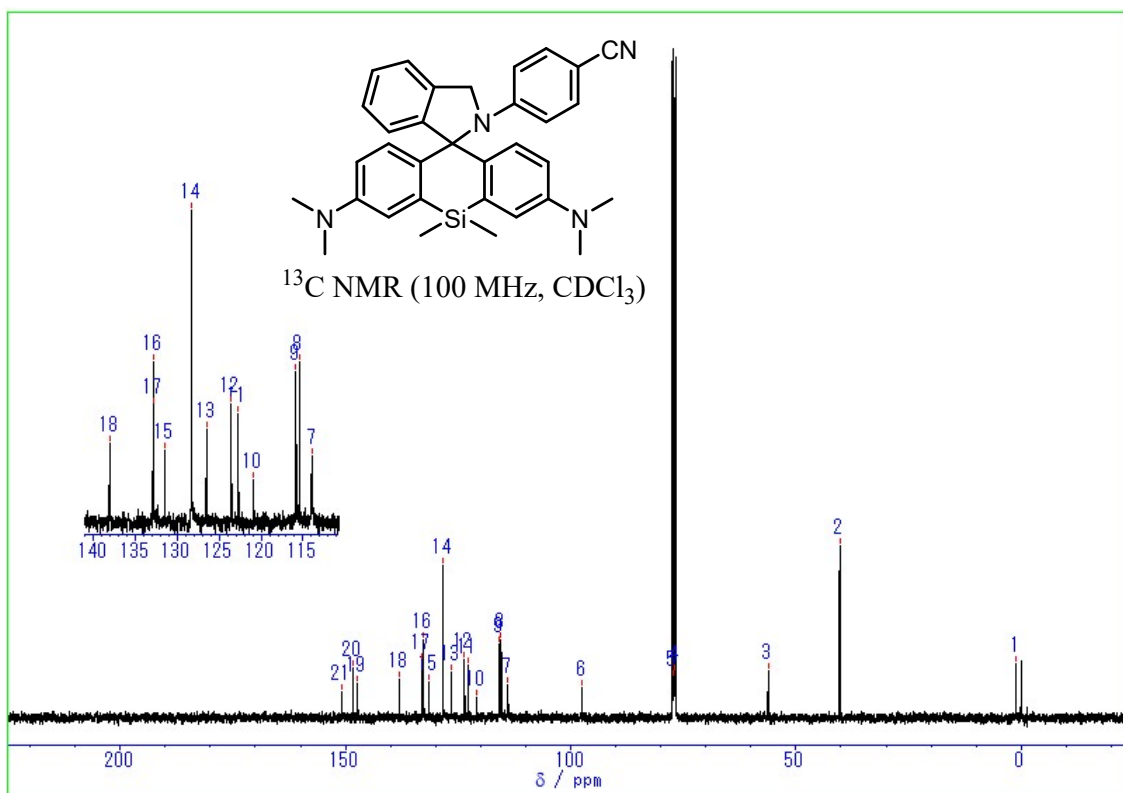
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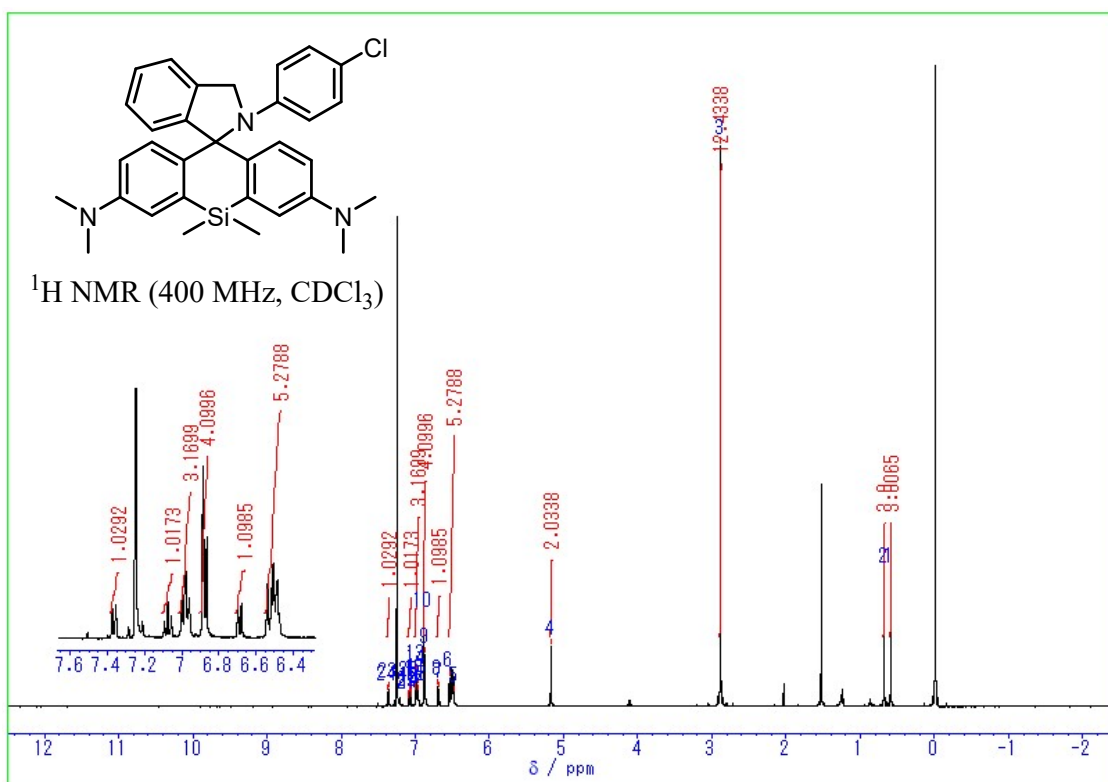
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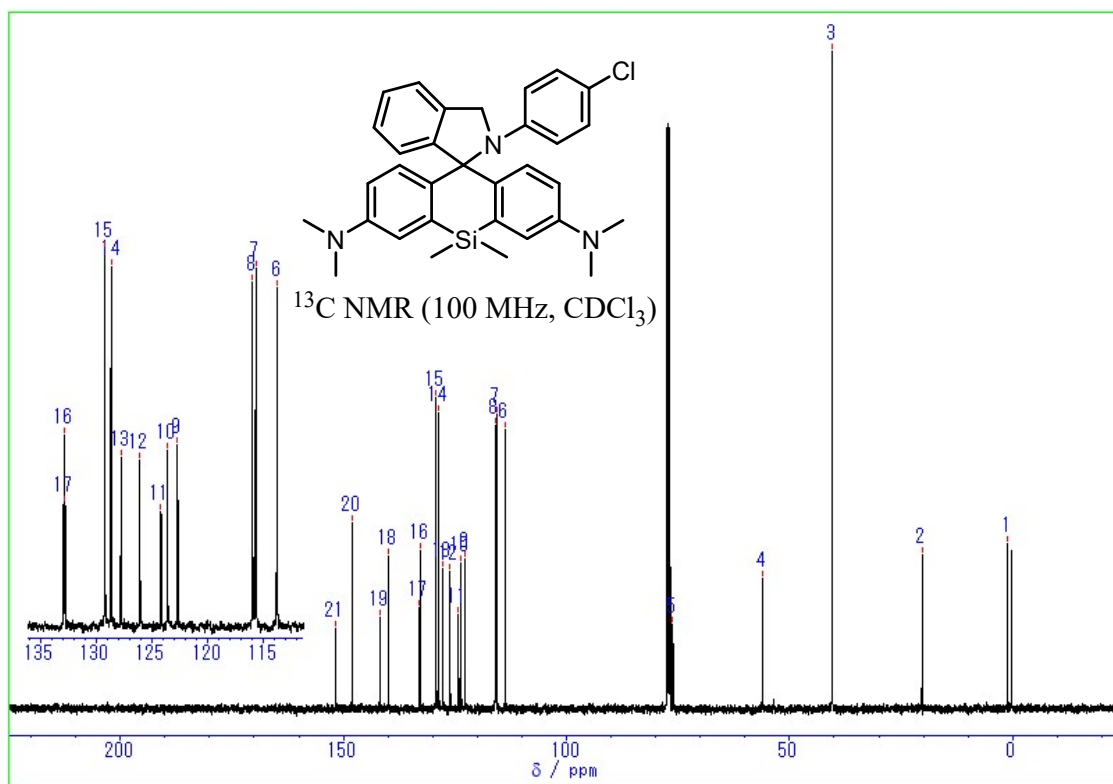
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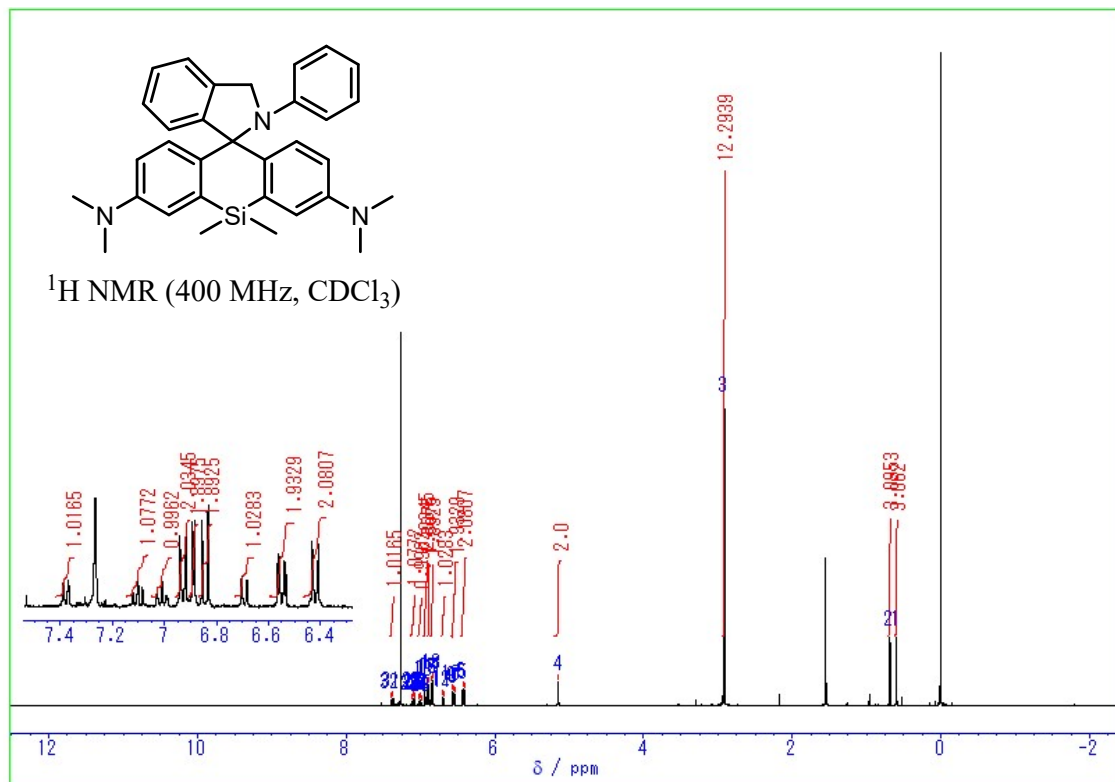
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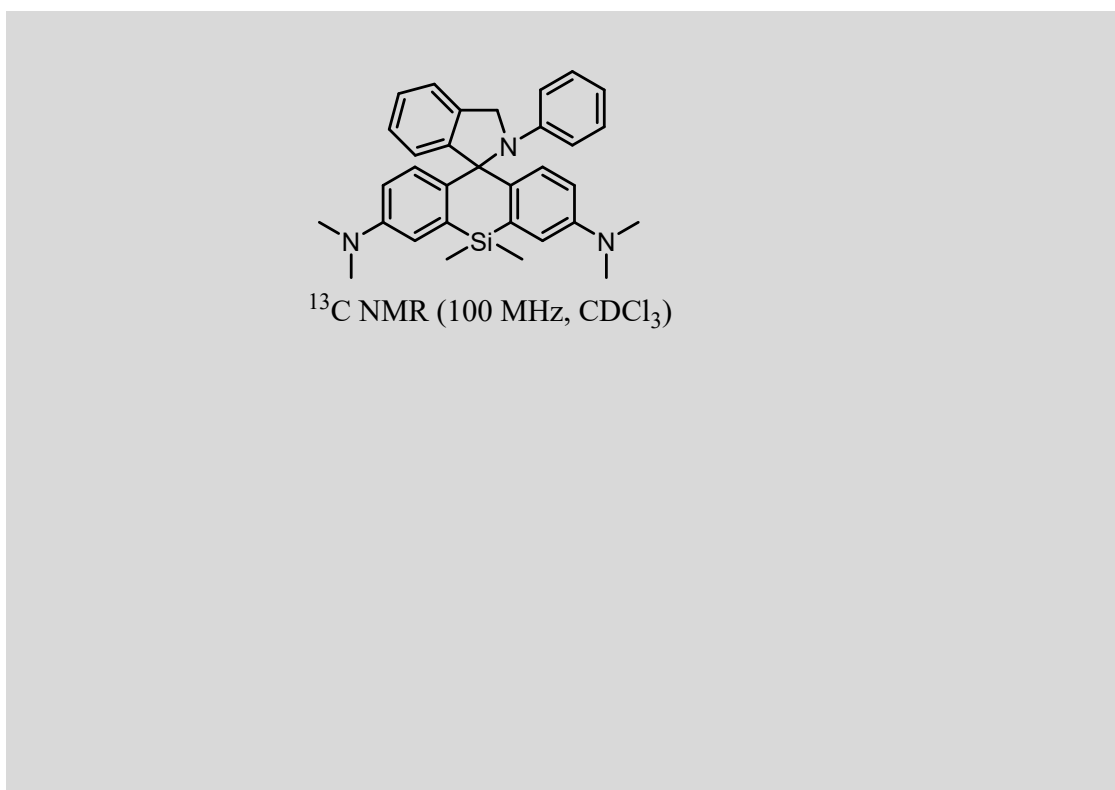
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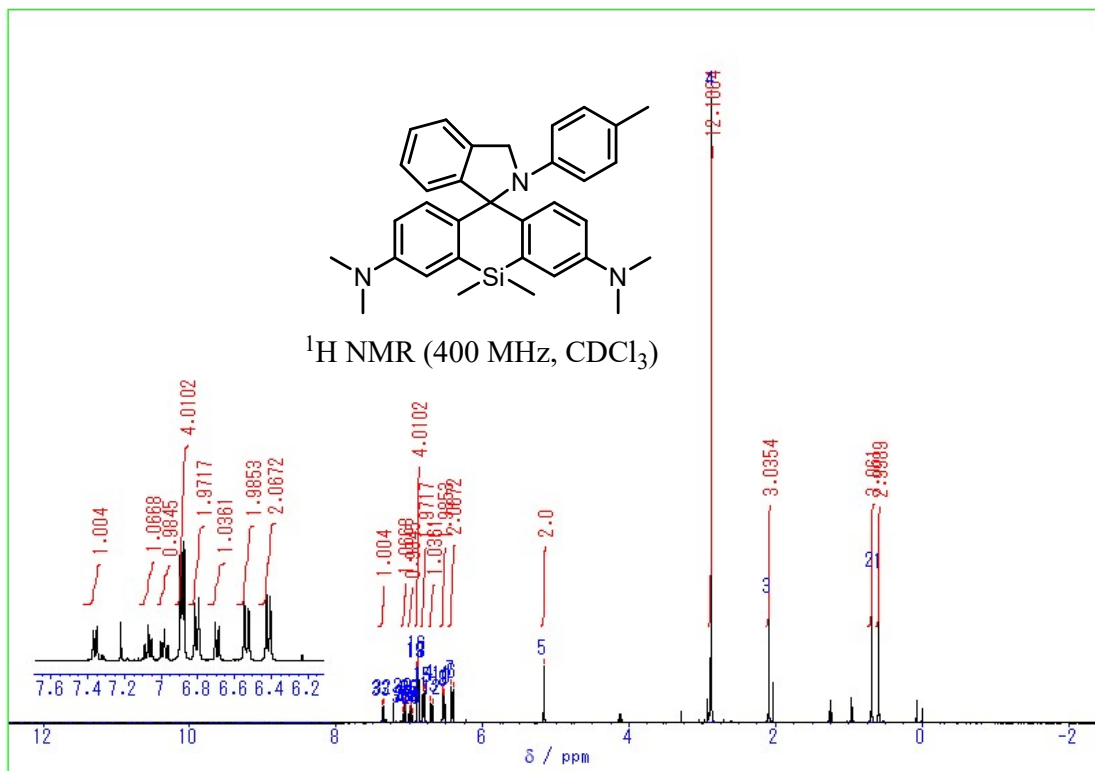
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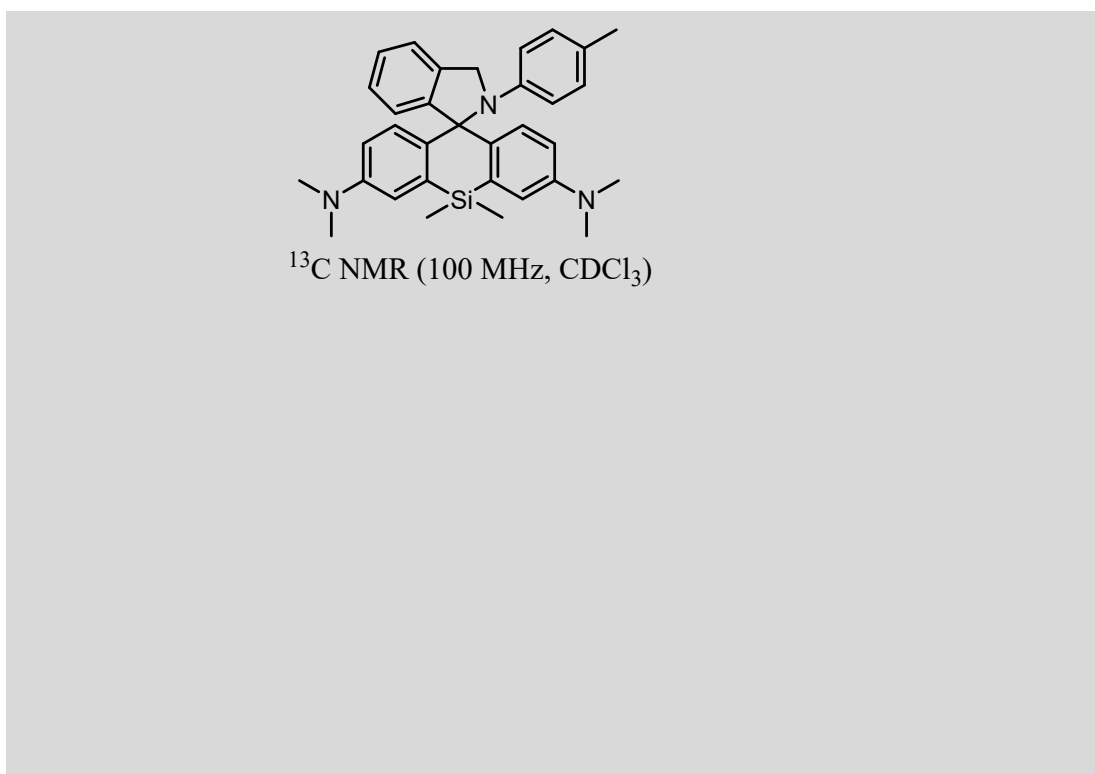
¹³C NMR of **12**



¹H NMR of **13**



¹³C NMR of **13**



3. Cartesian Coordinates

1 (Ground state)

Total Energy = -1938.0169181 A.U

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1 (π - π^* state)

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H	6.98833068	-1.97775547	0.95753056
H	6.66750219	-0.68554838	-0.20631068
H	6.11668079	-0.52832227	1.48035108
C	-5.94285365	0.21923573	-0.77876434
H	-5.98723214	0.93802174	-1.60291973
H	-6.88266603	-0.32708861	-0.75082971
H	-5.83369849	0.76682227	0.16338769
C	-5.15074393	-2.14695788	-1.03220077
H	-4.61362320	-2.69658205	-0.25237877
H	-6.21782621	-2.29308185	-0.88166397
H	-4.87839424	-2.56367924	-2.00790017
O	-0.89026269	-3.45452669	2.40388018
C	-2.15527095	-4.06424245	2.21043880

H	-2.56036765	-3.82463954	1.22034167
H	-1.98634616	-5.13792943	2.28005653
H	-2.87038280	-3.75904267	2.98189839

1 (CT-MECI)

Total Energy = -1937.8992854 A.U

C	2.13422259	-1.21453554	-2.15410330
C	1.94819686	0.18817935	-1.96552771
C	0.68504844	0.71611248	-1.91992314
C	-0.38951877	-0.16301370	-2.08523521
C	-0.18658774	-1.49558901	-2.25514780
C	1.09702352	-2.05364684	-2.27947575
H	3.15489810	-1.58212761	-2.22672134
H	2.78132204	0.87270797	-1.88657491
H	-1.39592297	0.20501998	-1.97591179
H	-1.00679216	-2.18509843	-2.33969700
N	0.48310146	2.05282874	-1.57104827
N	1.70421701	2.93512910	-1.64512142
O	1.44351493	4.05041687	-1.60830632
C	-0.78472897	2.76012193	-1.29987499
H	-1.57553036	2.03337266	-1.49185301
H	-0.86232208	3.56695090	-2.06564723
C	-0.89665104	3.39501858	0.07019222
C	-1.07114576	4.75900927	0.18130372
C	-0.91976915	2.60105374	1.21716016
C	-1.23769382	5.34079362	1.42421485
H	-1.04014722	5.39025774	-0.70221789
C	-1.04038854	3.19825391	2.45050126
C	-1.20530995	4.56696529	2.55870802
H	-1.38744698	6.40450407	1.49642214
H	-1.03287769	2.57021236	3.33684190
H	-1.35185395	5.01454313	3.53316925
C	-0.85596992	1.12036819	1.16153666
C	-1.73102523	0.33536559	0.90468606

C	-1.14946037	4.77367161	0.20447701	H	0.36870812	-2.45837559	4.07308486
C	-0.79680563	2.55416022	1.18293025	H	-0.70404940	-1.05531931	3.96266584
C	-1.21280903	5.35245092	1.46613143	N	-4.83321714	-2.19355413	-0.99998984
H	-1.27545754	5.39868270	-0.67607339	N	4.86034159	-0.78919994	0.63344236
C	-0.85931386	3.17412454	2.43388351	C	-4.82531472	-3.60984786	-0.68863245
C	-1.06173759	4.54345302	2.58452895	H	-5.62838156	-4.10121110	-1.24087443
H	-1.38361580	6.41857080	1.56704247	H	-3.88687296	-4.07056677	-1.01076759
H	-0.75581746	2.54350605	3.31077220	H	-4.95834391	-3.82498524	0.38395979
H	-1.11453468	4.97708900	3.57769974	C	-6.16592521	-1.61835017	-1.06644573
C	-0.58440735	1.07444619	1.08875962	H	-6.83942428	-2.33364771	-1.54187472
C	-1.72813285	0.22449698	0.76233844	H	-6.57725324	-1.35795733	-0.07852010
C	0.78292506	0.57583363	1.17575321	H	-6.17147804	-0.71849264	-1.68722546
C	-1.68804751	-1.19151267	0.82031209	C	5.91339431	0.16298148	0.95352963
C	-2.94715278	0.76601623	0.29680469	H	5.92052820	0.46881839	2.01175639
C	1.12650924	-0.80046364	1.26424606	H	6.88151381	-0.28216308	0.71553131
C	1.89222689	1.44976130	1.12692343	H	5.81911643	1.06370602	0.34148354
C	-2.71710019	-1.96480312	0.25427584	C	5.17673569	-2.12912886	1.09381490
C	-3.95957590	-0.01154137	-0.25018940	H	4.55758626	-2.87299234	0.58159706
H	-3.12382839	1.83582228	0.37349388	H	6.21602074	-2.35592907	0.84784868
C	2.46766575	-1.22118288	1.13600572	H	5.03258435	-2.26964046	2.17650144
C	3.20638669	1.01743978	1.01393248	O	1.15646229	-3.04388669	-2.37865980
H	1.72171446	2.52036269	1.20172073	C	2.44018689	-3.72912685	-2.27457731
C	-3.85022610	-1.40990783	-0.34527537	H	2.90043475	-3.46760857	-1.32687129
H	-2.62835581	-3.04462034	0.32541596	H	2.18200479	-4.78212349	-2.30640592
H	-4.85845635	0.49350619	-0.58449623	H	3.05522349	-3.45763019	-3.13107695
H	2.66192764	-2.28696650	1.22338295	-----			
C	3.53224159	-0.34688736	0.94666202	2 (Ground state)			
H	3.98306276	1.77438402	0.99672247	Total Energy = -1915.7304924 A.U			
Si	-0.25194167	-1.96712704	1.70583776	-----			
C	0.07661604	-3.72555697	1.08172029	C	-4.06893271	1.27043865	1.36493982
H	0.06730797	-3.79398208	-0.00918882	C	-3.06195973	2.21778859	1.26406728
H	1.03689720	-4.10549281	1.44725484	C	-1.74415110	1.86475984	1.55852049
H	-0.69268615	-4.41174182	1.45041209	C	-1.42706243	0.55645942	1.92709804
C	-0.51267358	-2.05562477	3.56336907	C	-2.42855945	-0.39683302	2.01131237
H	-1.37093124	-2.68742337	3.81431682	C	-3.75344120	-0.03979496	1.73825797

C	-1.12181774	0.67469222	2.03625194	H	-1.58216419	1.49907808	-1.65175660
C	-2.13632756	-0.26575507	2.10602893	C	4.61333416	-1.15733892	0.17840823
C	-3.45406959	0.11375385	1.83295241	H	3.53824283	-2.98737827	0.60190816
H	-4.77580511	1.72471173	1.27306295	H	5.30629260	0.82943642	-0.41823513
H	-2.95133069	3.39440877	1.12461392	H	-2.01347125	-3.28243088	-0.48008015
H	-0.10493448	0.38011751	2.26750334	C	-3.06083135	-1.52594136	-1.18669881
H	-1.90959276	-1.29155066	2.37112781	H	-3.73143724	0.46401296	-1.79649262
N	-0.38729092	2.96339215	1.61931324	Si	0.74881249	-2.68460925	-0.00082928
N	-0.68396497	4.14619161	2.16018653	C	0.43369601	-3.17027203	1.78695684
O	0.17600681	5.00771004	2.05490914	H	0.37805086	-2.29043238	2.43468530
C	0.89729293	2.70818685	0.95513147	H	-0.50584555	-3.72549633	1.87670413
H	1.20625696	1.69217010	1.19517822	H	1.23868293	-3.81149547	2.16027039
H	1.61236126	3.39697344	1.40540960	C	1.02500827	-4.22209066	-1.04081081
C	0.82830428	2.92136558	-0.54312556	H	1.88808670	-4.78738240	-0.67472003
C	0.81833557	4.22848867	-1.03982800	H	0.15188505	-4.88100537	-0.99487344
C	0.78620516	1.84317020	-1.44200433	H	1.20373776	-3.96160880	-2.08767115
C	0.77147760	4.47546054	-2.40591731	N	5.82007498	-1.61973081	0.56278526
H	0.84937844	5.05430516	-0.33677857	N	-4.27158879	-2.11445344	-1.26860817
C	0.75054471	2.10579692	-2.81670497	C	5.96662872	-2.98273554	1.05498113
C	0.74119731	3.40826131	-3.29967087	H	7.00853987	-3.15881440	1.31160249
H	0.76560303	5.49688920	-2.77138326	H	5.35750117	-3.14419655	1.95053657
H	0.72479551	1.26915792	-3.50814586	H	5.67101786	-3.70963055	0.29122111
H	0.71284002	3.58859329	-4.36911537	C	7.00026784	-0.76807515	0.48815183
C	0.77901923	0.41791353	-0.98694869	H	7.85885160	-1.31698562	0.86770930
C	2.03266535	-0.16185290	-0.60721679	H	7.20869371	-0.47281308	-0.54546557
C	-0.47906811	-0.27108743	-1.02103477	H	6.87220235	0.13374121	1.09514479
C	2.19689279	-1.51193813	-0.12733919	C	-5.44718816	-1.34242253	-1.64594648
C	3.22448704	0.63442524	-0.69620482	H	-5.32354593	-0.89965400	-2.63896298
C	-0.65990032	-1.65625652	-0.66553010	H	-6.31168998	-2.00159117	-1.67001053
C	-1.65748525	0.44504784	-1.41710934	H	-5.64391101	-0.54459182	-0.92163083
C	3.44404762	-1.96792437	0.24416419	C	-4.43944492	-3.51135829	-0.89550125
C	4.45153742	0.17265454	-0.32242523	H	-4.20387445	-3.66351177	0.16344647
H	3.15641813	1.64466465	-1.08053487	H	-5.47403172	-3.80200895	-1.06197764
C	-1.90585963	-2.24039136	-0.76062807	H	-3.79768764	-4.15752797	-1.50260014
C	-2.88483166	-0.14188883	-1.50094984	C	-4.49912607	-0.86858992	1.88030475

N -5.34099047 -1.66626270 1.90386087

2 (CT state)

Total Energy = -1915.6228175 A.U

C -2.40878757 -0.59519450 2.14484339
C -2.01799732 0.71449455 2.10392320
C -0.62850703 1.03628115 2.03268337
C 0.34208746 -0.00376687 2.07521550
C -0.06393690 -1.31411312 2.12027201
C -1.43735256 -1.62027839 2.12059320
H -3.46091297 -0.84896241 2.16673791
H -2.75481238 1.50280294 2.09395791
H 1.39893823 0.21815026 2.08952626
H 0.67455129 -2.10475103 2.14803560
N -0.24736972 2.34477835 1.92594026
N -1.22940764 3.27735290 2.28620456
O -0.86883627 4.41141476 2.17998583
C 1.03883002 2.82892843 1.41273053
H 1.76918110 2.02847060 1.49186066
H 1.36171098 3.64359811 2.06075169
C 0.86812922 3.31115193 -0.01439013
C 0.98829051 4.67793149 -0.27394716
C 0.56248280 2.42191850 -1.06590006
C 0.81801125 5.17942665 -1.55727094
H 1.21792264 5.35371087 0.54325382
C 0.36797686 2.95269661 -2.34953446
C 0.49787633 4.31089271 -2.59953918
H 0.92828665 6.24235930 -1.74226114
H 0.12169987 2.27168008 -3.15819218
H 0.35461059 4.69213896 -3.60496044
C 0.45123973 0.94441150 -0.90391434
C 1.68546892 0.19812229 -0.70932845
C -0.86018810 0.36691507 -1.01558017
C 1.75321702 -1.22390777 -0.72676322

C 2.90258140 0.87344447 -0.44903312
C -1.11094589 -1.03655493 -1.07631802
C -2.01429227 1.20189799 -0.98006784
C 2.91828525 -1.88336801 -0.35495177
C 4.05705854 0.21439184 -0.08157701
H 2.94976810 1.95367255 -0.53338401
C -2.41436572 -1.52623302 -0.99857773
C -3.30031054 0.70839422 -0.93673344
H -1.88897841 2.27946728 -0.97896359
C 4.09004368 -1.19531832 0.03046197
H 2.92639110 -2.96766884 -0.38150704
H 4.94386152 0.80310723 0.11716063
H -2.55971777 -2.60092004 -1.02527085
C -3.54773542 -0.68324754 -0.89995329
H -4.11956397 1.41480709 -0.89210050
Si 0.31874501 -2.18910338 -1.42208189
C 0.14022492 -3.88708931 -0.64315179
H 0.22675973 -3.86552787 0.44577938
H -0.82288682 -4.34166266 -0.89589842
H 0.92265012 -4.55043919 -1.02609637
C 0.51248836 -2.36723580 -3.28420258
H 1.40311135 -2.95623614 -3.52564879
H -0.35833893 -2.86922031 -3.71807922
H 0.61201796 -1.38492646 -3.75600928
N 5.20856549 -1.85679264 0.46019697
N -4.80802191 -1.19103820 -0.76918513
C 5.23303401 -3.30699203 0.46728808
H 6.17260063 -3.64718013 0.90055446
H 4.41793872 -3.71089928 1.07752309
H 5.14811170 -3.72922331 -0.54281491
C 6.43765147 -1.12312198 0.69731862
H 7.20254485 -1.81200631 1.05295897
H 6.81143483 -0.63728181 -0.21328476
H 6.29787748 -0.35406981 1.46485326
C -5.93425794 -0.29171613 -0.59958360

H	-6.05551268	0.36692152	-1.46702299	C	0.05683634	4.46500320	-2.51990975
H	-6.84653619	-0.87596465	-0.49225991	H	0.26526547	6.36720066	-1.53849400
H	-5.82038161	0.33324728	0.29504287	H	-0.08962105	2.43708761	-3.20850438
C	-5.00996921	-2.62550741	-0.67389557	H	-0.21404810	4.88844792	-3.48116843
H	-4.47512508	-3.05481706	0.18265490	C	0.45496960	1.01041385	-1.06646298
H	-6.07173685	-2.82862665	-0.54514567	C	1.64102225	0.24938112	-1.11220915
H	-4.67629746	-3.14010061	-1.58212618	C	-0.82997470	0.34597289	-1.21341103
C	-1.86910169	-2.98381515	2.13315681	C	1.64679254	-1.22055820	-1.14517283
N	-2.23103196	-4.08546543	2.12714141	C	2.92332509	0.90643466	-0.92396673

2 (CT-MECI)

Total Energy = -1915.6228099 A.U

C	-2.08433496	-0.48742096	2.39874744	C	3.86217468	0.24933764	-0.21882575
C	-1.61482315	0.81692840	2.44425476	H	3.03521598	1.95770212	-1.16360975
C	-0.25228800	1.07198798	2.29497028	C	-2.19217666	-1.70291729	-1.20507280
C	0.64230350	0.01163256	2.18103837	C	-3.17928830	0.48279268	-0.69887721
C	0.17396721	-1.28816625	2.09875591	H	-1.94880850	2.18985718	-0.87734712
C	-1.19581306	-1.54052876	2.17458995	C	3.66800767	-1.14871947	0.19105586
H	-3.14611868	-0.69258711	2.48398675	H	2.63158993	-2.94504166	-0.36685516
H	-2.29480788	1.64988212	2.57174160	H	4.77879720	0.75853567	0.05482356
H	1.70850622	0.19467810	2.10944418	H	-2.33128499	-2.74371108	-1.46973222
H	0.86128846	-2.11100164	1.93660711	C	-3.30921393	-0.97009133	-0.75515921
N	0.20290248	2.41594704	2.20747557	H	-4.02171842	1.07511716	-0.36132481
N	-0.34313500	3.28427633	3.08868254	Si	0.40504532	-2.06431701	-2.21741608
O	0.08547379	4.38138659	2.98779102	C	0.22935596	-3.88266241	-1.81861823
C	1.26233983	2.82210891	1.29203476	H	-0.11431174	-4.04921222	-0.79289571
H	1.94435185	1.98501529	1.15576622	H	-0.49073792	-4.36829888	-2.48566620
H	1.79492620	3.62376774	1.80836221	H	1.17524532	-4.41661935	-1.96062572
C	0.78653151	3.34606650	-0.05204125	C	0.67628267	-1.74993334	-4.04327150
C	0.69782805	4.72949824	-0.22025628	H	1.56248327	-2.27796673	-4.40968564
C	0.48124490	2.50761663	-1.13834282	H	-0.17894068	-2.09065746	-4.63601269
C	0.33031610	5.28935435	-1.43838151	H	0.81822797	-0.68485137	-4.24845126
H	0.89995079	5.36717024	0.63392723	N	4.61032420	-1.74318617	0.95916031
C	0.13206639	3.08533723	-2.36466417	N	-4.50222599	-1.52897419	-0.51104801
				C	4.37107060	-3.07834261	1.47834921

H	4.99922115	-3.24866169	2.35370291
H	3.32471251	-3.17122013	1.78236023
H	4.58903833	-3.85873642	0.73586810
C	5.93056050	-1.15668923	1.17347103
H	6.56802651	-1.89283653	1.66200756
H	6.40820908	-0.88408668	0.22806469
H	5.88067417	-0.27444590	1.82230914
C	-5.73714166	-0.74219992	-0.50675659
H	-5.79588153	-0.08152447	-1.37472533
H	-6.58591674	-1.42314322	-0.55177361
H	-5.83315239	-0.14973365	0.41009253
C	-4.64189424	-2.98342612	-0.46204885
H	-3.78810670	-3.43809720	0.04389174
H	-5.53796596	-3.23331901	0.10653961
H	-4.74109719	-3.40113752	-1.47230684
C	-1.68301811	-2.85416581	1.87063649
N	-2.06506907	-3.88359120	1.49874251

3 (Ground state)

Total Energy = -1922.7295345 A.U

C	-4.22182324	1.09325889	1.33188086
C	-3.22117178	2.05785539	1.29916601
C	-1.91760100	1.72183192	1.65921988
C	-1.60492450	0.41579826	2.03688761
C	-2.59369541	-0.55780771	2.05236339
C	-3.88631276	-0.19849580	1.70249093
H	-5.24230726	1.33306088	1.05774828
H	-3.44942812	3.07179907	0.99287741
H	-0.59535738	0.15290237	2.33217800
H	-2.37032218	-1.58031540	2.33193973
N	-0.91136094	2.73312422	1.67104159
N	-1.24533478	3.85941913	2.29270037
O	-0.40255866	4.74858963	2.27474882
C	0.41298995	2.54042212	1.07102446

H	0.72007615	1.51321403	1.26272389
H	1.09001310	3.20226060	1.61313723
C	0.45481745	2.85835169	-0.41030945
C	0.31165912	4.18324981	-0.83227254
C	0.65796290	1.86062956	-1.37356701
C	0.37510316	4.51654796	-2.17920602
H	0.15406715	4.95352645	-0.08478121
C	0.73277077	2.20148883	-2.72699035
C	0.59300866	3.52315811	-3.13042809
H	0.26201788	5.55100769	-2.48545255
H	0.89285936	1.41922144	-3.46207830
H	0.65151721	3.77467175	-4.18389797
C	0.77365218	0.41622296	-0.98715585
C	2.06977428	-0.04068998	-0.60333859
C	-0.42754671	-0.33798559	-1.04262286
C	2.34434252	-1.37339398	-0.15659850
C	3.17228837	0.85979414	-0.66036581
C	-0.52117173	-1.71736707	-0.66153894
C	-1.63394602	0.29412537	-1.47260185
C	3.62355244	-1.73737551	0.19323613
C	4.44362835	0.49422141	-0.31202020
H	3.01332112	1.87645314	-0.99904289
C	-1.73026469	-2.36627951	-0.70121165
C	-2.83102938	-0.35803817	-1.52368112
H	-1.61733042	1.33670534	-1.76296855
C	4.72145323	-0.82870136	0.13162372
H	3.80511577	-2.75116035	0.53174541
H	5.23572767	1.22751996	-0.38351851
H	-1.77951932	-3.40417568	-0.39219787
C	-2.93374009	-1.71594525	-1.11026171
H	-3.70956275	0.18812237	-1.83857128
Si	0.97225020	-2.64138558	-0.00934581
C	0.69443511	-3.09364871	1.78896583
H	0.51879596	-2.20076198	2.39564246
H	-0.17343679	-3.75324868	1.88890101

H	1.56661700	-3.61494873	2.19537578	H	-3.34954947	3.08396322	1.04488720
C	1.33980218	-4.15144346	-1.05442341	H	-0.42110930	0.20602873	2.31191090
H	2.24056710	-4.65889041	-0.69520817	H	-2.15743239	-1.56825491	2.28663739
H	0.51011270	-4.86358177	-1.00491669	N	-0.79922622	2.78709093	1.69805019
H	1.49449827	-3.87523736	-2.10094965	N	-1.15984650	3.90726759	2.31532556
N	5.96566008	-1.20832881	0.47841977	O	-0.34282543	4.82004178	2.28611906
N	-4.11684832	-2.35148638	-1.08134041	C	0.51391682	2.63329590	1.06225736
C	6.22858502	-2.57215340	0.92151425	H	0.86539838	1.62168138	1.26087149
H	7.28877604	-2.67533535	1.14166386	H	1.17874617	3.33332873	1.56937886
H	5.66586971	-2.80908612	1.82995441	C	0.48513479	2.91883717	-0.42474060
H	5.96904329	-3.29762249	0.14424742	C	0.34636111	4.24106631	-0.85829190
C	7.07027692	-0.25930984	0.41256618	C	0.61114313	1.89301959	-1.37491686
H	7.98239361	-0.75157075	0.74286899	C	0.33851442	4.55330066	-2.21164108
H	7.22442710	0.09761191	-0.61065138	H	0.24658149	5.02585585	-0.11548893
H	6.89058476	0.60102487	1.06462158	C	0.61577528	2.22189412	-2.73553210
C	-5.33541064	-1.66300192	-1.48991876	C	0.47942495	3.53907008	-3.15564307
H	-5.23929453	-1.27028412	-2.50521387	H	0.23018066	5.58525739	-2.52849247
H	-6.16179047	-2.37033632	-1.47941712	H	0.71937859	1.42533113	-3.46599630
H	-5.57380067	-0.84170148	-0.80685065	H	0.48326939	3.77236285	-4.21521334
C	-4.22545713	-3.68648834	-0.50468726	C	0.72571894	0.45572485	-0.97649204
H	-3.87732422	-3.69150313	0.53270508	C	2.01794942	-0.02498390	-0.59173507
H	-5.26919478	-3.99239905	-0.51526799	C	-0.47195798	-0.33188397	-1.03542509
H	-3.64995983	-4.41646003	-1.08109368	C	2.28738681	-1.36481912	-0.13096879
F	-4.84286735	-1.14512674	1.70408818	C	3.14026481	0.86870052	-0.65410652

3 (π - π^* state)

Total Energy = -1922.6378012 A.U

C	-4.07280470	1.08122116	1.34263052
C	-3.09663153	2.06971869	1.32983594
C	-1.78328237	1.75660289	1.67747076
C	-1.43878884	0.45055936	2.02813089
C	-2.40478527	-0.54558934	2.02902622
C	-3.70472816	-0.21105975	1.68381113
H	-5.09905275	1.30110431	1.07350347

C	-0.54988485	-1.72440686	-0.67324326
C	-1.69353135	0.28741742	-1.46173504
C	3.56776679	-1.72820363	0.22967348
C	4.40096414	0.49765622	-0.29087618
H	2.98873436	1.88037719	-1.01001586
C	-1.75411038	-2.39302806	-0.74374672
C	-2.87783290	-0.38370934	-1.52438462
H	-1.68921097	1.33536852	-1.73208810
C	4.67004620	-0.82828418	0.17313978
H	3.74209437	-2.74151863	0.57465615
H	5.20039753	1.22343543	-0.36601451

H	-1.78743265	-3.43546464	-0.44630255	C	-2.14932826	-1.27034591	2.24734021
C	-2.96244028	-1.76077230	-1.15025312	C	-2.03534862	0.08848162	2.23379995
H	-3.76365987	0.15338724	-1.83674863	C	-0.74276330	0.69550187	2.10260060
Si	0.92803435	-2.63851850	0.00562088	C	0.42389914	-0.12562336	2.07830144
C	0.63222669	-3.11515483	1.79926586	C	0.30041219	-1.48934387	2.09778569
H	0.44477061	-2.23221388	2.41752801	C	-0.98234243	-2.04695378	2.14659041
H	-0.23177736	-3.78271077	1.88291985	H	-3.11333199	-1.75708808	2.30856804
H	1.50171986	-3.63774664	2.21068899	H	-2.91707376	0.70747721	2.28020318
C	1.32346337	-4.16813795	-1.00728262	H	1.41218107	0.30748685	2.04776497
H	2.22006945	-4.66590584	-0.62397584	H	1.17061607	-2.13102894	2.06517773
H	0.49857949	-4.88647321	-0.96007765	N	-0.64930427	2.05202077	1.98848667
H	1.49530662	-3.91125212	-2.05619445	N	-1.82293573	2.75269017	2.29955408
N	5.91294679	-1.20509903	0.53645928	O	-1.70437976	3.93772038	2.20557744
N	-4.14241628	-2.41480190	-1.15233680	C	0.52166925	2.81271841	1.53828251
C	6.16874442	-2.56457696	0.99187390	H	1.39408269	2.16799076	1.59786434
H	7.22578243	-2.66969443	1.22429864	H	0.66397399	3.63033846	2.24543585
H	5.59152864	-2.79187407	1.89435559	C	0.31957784	3.35287832	0.13453417
H	5.91157676	-3.29314605	0.21595041	C	0.27518490	4.73648329	-0.04538545
C	7.02180526	-0.26157310	0.47748754	C	0.18626741	2.49730321	-0.97431329
H	7.92514042	-0.75199900	0.83272890	C	0.10105456	5.28812973	-1.30844439
H	7.19477567	0.07954551	-0.54854223	H	0.37316151	5.38674917	0.81812602
H	6.83055803	0.60907744	1.11269629	C	-0.00738815	3.07121012	-2.23644036
C	-5.37323557	-1.72087051	-1.50428469	C	-0.04804986	4.44922776	-2.40904097
H	-5.31036284	-1.29641738	-2.51026931	H	0.07513330	6.36561376	-1.43003969
H	-6.19800368	-2.42968052	-1.48564331	H	-0.11885416	2.41214835	-3.09195469
H	-5.58909583	-0.91894941	-0.79010248	H	-0.19182474	4.86633557	-3.40026994
C	-4.22674020	-3.77939172	-0.65378303	C	0.25543718	1.00682316	-0.88835900
H	-3.93087841	-3.82707780	0.40017651	C	1.57328135	0.40968445	-0.73986985
H	-5.25293478	-4.12852999	-0.74163298	C	-0.97609405	0.28311111	-0.98437886
H	-3.58602026	-4.45061283	-1.23370475	C	1.81795718	-0.99008833	-0.83456559
F	-4.63786805	-1.18008409	1.66285982	C	2.69268749	1.21539558	-0.41825452
-----				C	-1.05689537	-1.14083293	-1.11397698
3 (CT state)				C	-2.21723949	0.96575745	-0.84727989
Total Energy = -1922.6383623 A.U				C	3.05625833	-1.51756241	-0.48769186
-----				C	3.91918146	0.68564893	-0.07362862
				H	2.60022690	2.29608010	-0.43043344
				C	-2.27803456	-1.79167215	-1.00695224
				C	-3.42511407	0.30932912	-0.75402050

H	-2.22457033	2.04936127	-0.79074373
C	4.12951633	-0.71212789	-0.04727195
H	3.20046106	-2.58940531	-0.57104013
H	4.72335289	1.36730526	0.17431501
H	-2.29362368	-2.87240969	-1.09911711
C	-3.49376787	-1.10374054	-0.78193921
H	-4.32329002	0.90074172	-0.62638291
Si	0.49186284	-2.07850483	-1.56497987
C	0.51707879	-3.83321740	-0.89933302
H	0.38276384	-3.87934740	0.18315628
H	-0.27887885	-4.42566098	-1.36250764
H	1.46673752	-4.31915171	-1.14577403
C	0.67625060	-2.11833265	-3.43728601
H	1.62123590	-2.59042647	-3.72509674
H	-0.14195751	-2.68206284	-3.89706089
H	0.66347210	-1.10273387	-3.84488719
N	5.32092447	-1.25349558	0.35980720
N	-4.67254481	-1.77135757	-0.59871052
C	5.53463041	-2.68440829	0.26444437
H	6.51304929	-2.92835630	0.67631156
H	4.78290737	-3.23500724	0.84093794
H	5.50069197	-3.04232844	-0.77323023
C	6.44031485	-0.38545959	0.67069269
H	7.28318772	-0.99213187	0.99915068
H	6.76158480	0.20489728	-0.19756557
H	6.19112846	0.30681812	1.48257176
C	-5.89225719	-1.03125814	-0.33626049
H	-6.15139368	-0.36942957	-1.17089578
H	-6.71408965	-1.73177962	-0.19679062
H	-5.80631208	-0.42199030	0.57210019
C	-4.69267272	-3.22194362	-0.59689118
H	-4.02716529	-3.63379777	0.17205610
H	-5.70408893	-3.56621673	-0.38697792
H	-4.38984220	-3.63319278	-1.56720063
F	-1.10548467	-3.35626859	2.12319040

Total Energy = -1922.6188927 A.U

C	-3.57829097	1.93311683	0.89726757
C	-2.40170493	2.65659784	1.05306804
C	-1.20757525	1.99738126	1.33226643
C	-1.18126932	0.60391506	1.42395464
C	-2.34877427	-0.12748735	1.27577207
C	-3.53072734	0.55228715	1.01933251
H	-4.52716718	2.42760796	0.72383170
H	-2.40651630	3.73817243	0.99627352
H	-0.25210222	0.09091506	1.64888740
H	-2.35846070	-1.20595592	1.37377882
N	-0.03983074	2.75759883	1.63037586
N	-0.16948847	3.57571484	2.69638561
O	0.83351596	4.09206494	3.02890217
C	1.23578526	2.49502964	0.99010322
H	1.46867221	1.43143561	1.06511588
H	1.95278318	3.04845586	1.60356290
C	1.26936058	2.98720353	-0.43871203
C	1.37229183	4.36152017	-0.66195256
C	1.21074985	2.11884899	-1.53501062
C	1.42068248	4.87881013	-1.95123155
H	1.41741251	5.02779541	0.19509971
C	1.28206364	2.64701041	-2.82870397
C	1.38479872	4.01798225	-3.04018233
H	1.49961547	5.94995647	-2.10224123
H	1.25312690	1.96958975	-3.67829820
H	1.44287287	4.40706147	-4.05117769
C	1.05023249	0.64278237	-1.35800627
C	2.15502105	-0.14811868	-0.93480105
C	-0.20867702	0.03203454	-1.73128916
C	2.09873828	-1.60294074	-0.75281712
C	3.38483590	0.51445844	-0.53787700
C	-0.47047922	-1.41326246	-1.71937214
C	-1.30829062	0.87965795	-2.08414826

3 (CT-MECI)

C	2.96537220	-2.18548099	0.15818200
C	4.23862223	-0.09498978	0.30587628
H	3.53667846	1.55267263	-0.80421614
C	-1.76366720	-1.87179650	-1.64071020
C	-2.57802750	0.40093137	-2.03867042
H	-1.15113726	1.94168998	-2.21222736
C	4.00655650	-1.45872127	0.76285639
H	2.94916596	-3.26405681	0.27746818
H	5.10046131	0.45054974	0.67068047
H	-1.95422610	-2.93946199	-1.68534508
C	-2.86091899	-0.99515190	-1.73901107
H	-3.40079879	1.09583843	-2.14966570
Si	0.96284396	-2.58801647	-1.82424063
C	0.54944056	-4.25713496	-1.06728094
H	0.17998793	-4.16354769	-0.04219924
H	-0.20992296	-4.78448012	-1.65424481
H	1.42512076	-4.91520717	-1.05523475
C	1.60968676	-2.81199609	-3.56967756
H	2.50814446	-3.43790067	-3.58109851
H	0.86224742	-3.29310066	-4.20938006
H	1.86924364	-1.85259216	-4.02641548
N	4.88534613	-2.03135278	1.61966729
N	-4.13587484	-1.41387080	-1.67343627
C	4.57330725	-3.30931980	2.23470204
H	5.14830121	-3.41819277	3.15511437
H	3.51077292	-3.35597332	2.48841544
H	4.81618550	-4.15210362	1.57249855
C	6.17509616	-1.42676309	1.93173212
H	6.80034246	-2.16617750	2.43137115
H	6.69720800	-1.11311811	1.02410661
H	6.06474959	-0.56508792	2.60224827
C	-5.26269404	-0.62747537	-2.16083068
H	-5.00005982	-0.08068064	-3.06693164
H	-6.07818739	-1.30549810	-2.41769840
H	-5.61514433	0.06397089	-1.38707406

C	-4.45496653	-2.68467595	-1.04788173
H	-3.73747392	-2.89817659	-0.25242940
H	-5.44794489	-2.62018567	-0.60016598
H	-4.44477969	-3.51080679	-1.77101852
F	-4.66556873	-0.15462473	0.88229427

4 (Ground state)

Total Energy = -2283.1022479 A.U

C	4.02702782	1.21078272	-1.26274846
C	3.02202804	2.16939231	-1.21116189
C	1.71491152	1.82877899	-1.55376147
C	1.40345126	0.51874264	-1.91495610
C	2.39886037	-0.44824161	-1.94597305
C	3.70466779	-0.08900435	-1.63237073
H	5.04654334	1.47346393	-1.00639904
H	3.25304747	3.18369290	-0.90898722
H	0.39205950	0.24412136	-2.19251448
H	2.16067145	-1.46803440	-2.22391480
N	0.71006815	2.83889318	-1.56486372
N	1.07054975	3.98636865	-2.13550772
O	0.22645103	4.87250773	-2.12795102
C	-0.64234043	2.63051873	-1.03560889
H	-0.93631711	1.60629167	-1.25896007
H	-1.29425999	3.29812941	-1.60054238
C	-0.75919435	2.92395464	0.44664902
C	-0.70723442	4.24859081	0.89014292
C	-0.93850365	1.90220320	1.38930556
C	-0.83600442	4.55836058	2.23804026
H	-0.56740331	5.03692687	0.15838482
C	-1.07600250	2.21893835	2.74378116
C	-1.02670725	3.54031900	3.16859387
H	-0.79410070	5.59314015	2.56071112
H	-1.21606548	1.41839358	3.46309541
H	-1.13493680	3.77241755	4.22258434

C	-3.24336822	2.00483322	1.28944620	C	4.73271643	-0.68823848	0.27773217
C	-1.92833543	1.71884918	1.64263841	H	3.85824390	-2.63145843	0.67086422
C	-1.57458994	0.42490670	2.02552432	H	5.20763638	1.37271054	-0.25516710
C	-2.54253470	-0.56746544	2.06478897	H	-1.65099531	-3.47815980	-0.50525358
C	-3.87700211	-0.29426935	1.74562746	C	-2.84318451	-1.81539090	-1.22012188
H	-5.23308158	1.23832782	1.08572164	H	-3.67863998	0.08946963	-1.87582367
H	-3.50764142	3.00649375	0.97005252	Si	1.04247527	-2.60824956	0.03812537
H	-0.55356037	0.19164256	2.30870552	C	0.70891128	-3.05040959	1.82959026
H	-2.25684590	-1.57321805	2.35890750	H	0.46759985	-2.15807729	2.41445734
N	-0.95589144	2.76435032	1.64321696	H	-0.13325947	-3.74596227	1.90136485
N	-1.33266173	3.89252503	2.23305434	H	1.58457644	-3.52757781	2.28031638
O	-0.51867504	4.80955027	2.20308983	C	1.49666771	-4.11510109	-0.97711828
C	0.38131591	2.60341873	1.06395037	H	2.39752640	-4.59155024	-0.57794259
H	0.71890206	1.59094910	1.28025352	H	0.68845564	-4.85282782	-0.95476354
H	1.03045853	3.29830805	1.59845226	H	1.68479305	-3.84229045	-2.01905916
C	0.42642303	2.89087003	-0.42298320	N	5.97594400	-1.02893745	0.66638538
C	0.26637019	4.20436219	-0.87383833	N	-3.99125349	-2.51056910	-1.30204176
C	0.64071052	1.87482443	-1.36397448	C	6.26312711	-2.38002918	1.13259727
C	0.32479462	4.50882630	-2.22777388	H	7.31866295	-2.45105934	1.38548135
H	0.09809586	4.98789976	-0.14268099	H	5.67992744	-2.62319322	2.02636224
C	0.70756793	2.18649795	-2.72496898	H	6.04749447	-3.12072259	0.35622519
C	0.55225033	3.49716860	-3.15729072	C	7.05564635	-0.05059855	0.62072342
H	0.19923423	5.53490523	-2.55658351	H	7.96885061	-0.51116223	0.99130517
H	0.87553640	1.39017970	-3.44299434	H	7.23552216	0.29306440	-0.40290153
H	0.60596869	3.72594021	-4.21619562	H	6.82979235	0.81535703	1.25055433
C	0.78194561	0.44018375	-0.95103997	C	-5.22467027	-1.84874499	-1.71062189
C	2.08214471	0.01949148	-0.53911494	H	-5.16645033	-1.50476756	-2.74819738
C	-0.39806584	-0.34523026	-1.02352414	H	-6.05036337	-2.55164329	-1.62515370
C	2.38045044	-1.30074850	-0.07146365	H	-5.43845007	-0.99257972	-1.06414534
C	3.16260182	0.94703981	-0.58184497	C	-4.01891247	-3.93884050	-1.00868817
C	-0.45349890	-1.73453882	-0.67341600	H	-3.73986158	-4.13741212	0.03142656
C	-1.61857972	0.25982920	-1.45149752	H	-5.02771236	-4.31346654	-1.16677049
C	3.65871732	-1.62598250	0.31810512	H	-3.34077566	-4.48948889	-1.66728886
C	4.43292947	0.62017866	-0.19346412	C	-4.92112378	-1.37497110	1.84813514
H	2.98732247	1.95410844	-0.94038822	H	-4.58631018	-2.29352547	1.35853424
C	-1.63205217	-2.43040724	-0.78295846	H	-5.12250067	-1.62038027	2.89591222
C	-2.78932287	-0.43316278	-1.55192113	H	-5.86439446	-1.06671921	1.39118339
H	-1.63371495	1.31191228	-1.70509711		-----		

6 (π - π^* state)

Total Energy = -1862.7433638 A.U

C	-2.32466400	-1.32432200	2.26381700
C	-2.13509500	0.04145000	2.12812900
C	-0.84137700	0.57058800	2.12129700
C	0.24705200	-0.28816300	2.24454100
C	0.03778300	-1.66013800	2.35987900
C	-1.24465600	-2.20524300	2.37310600
H	-3.33846500	-1.71540600	2.26531500
H	-2.98563900	0.70052000	2.01349500
H	1.26485100	0.08322600	2.25518800
H	0.90253800	-2.31168500	2.44785400
N	-0.66727800	1.98286500	1.99600000
N	-1.66337400	2.72816000	2.46381600
O	-1.48887900	3.93784700	2.37839300
C	0.55480300	2.63522900	1.51579000
H	1.34407700	1.88724400	1.50418900
H	0.82305900	3.39335200	2.25438100
C	0.43092000	3.28591800	0.14995500
C	0.41419900	4.67837600	0.05881100
C	0.39582800	2.52302200	-1.03016000
C	0.36127300	5.31906500	-1.17398800
H	0.43238500	5.26267200	0.97279200
C	0.33959200	3.17652200	-2.26501600
C	0.32231400	4.56476900	-2.34228500
H	0.34856600	6.40292500	-1.22026400
H	0.31118900	2.57983800	-3.17171000
H	0.28081200	5.05275500	-3.31045000
C	0.40691100	1.02807800	-1.01852800
C	1.66252400	0.36876800	-0.83222000
C	-0.85981100	0.36417400	-1.12962500
C	1.83603100	-1.06344700	-0.86416100
C	2.83005900	1.14593100	-0.52988600
C	-1.01832100	-1.06584400	-1.22895500
C	-2.06305600	1.14240300	-1.08105000
C	3.02173300	-1.62678900	-0.44810700

C	4.00266700	0.57799200	-0.12489700
H	2.77602300	2.22676500	-0.58850000
C	-2.27043000	-1.62995700	-1.13565700
C	-3.30007600	0.57279000	-1.00846600
H	-1.99337500	2.22294400	-1.05619600
C	4.13155300	-0.84359400	-0.01844400
H	3.12235300	-2.70592100	-0.47390300
H	4.83658500	1.22255200	0.12077400
H	-2.36212700	-2.70827600	-1.19790300
C	-3.45043100	-0.84929900	-0.97719900
H	-4.16755500	1.21617100	-0.93857800
Si	0.47500000	-2.13380500	-1.55969700
C	0.39540600	-3.80838200	-0.72541000
H	0.39271300	-3.70815300	0.36220200
H	-0.50550800	-4.35397000	-1.02371800
H	1.25622700	-4.42008700	-1.01387000
C	0.70911300	-2.33822800	-3.41366700
H	1.63564300	-2.88063400	-3.62758300
H	-0.12435700	-2.90138500	-3.84585600
H	0.75858300	-1.36450900	-3.91018300
N	5.26786900	-1.41162100	0.43390100
N	-4.66063600	-1.42142200	-0.81268300
C	5.37347600	-2.85941600	0.54699300
H	6.32339800	-3.11250800	1.01220800
H	4.56665200	-3.26051900	1.16829600
H	5.33120900	-3.33796900	-0.43781300
C	6.41450200	-0.59125100	0.80137000
H	7.22062700	-1.23831400	1.13919600
H	6.77452400	-0.01017700	-0.05390700
H	6.16055200	0.09619200	1.61476800
C	-5.86005800	-0.60290300	-0.69727300
H	-5.99876100	0.01945700	-1.58678600
H	-6.72597200	-1.25317300	-0.59696300
H	-5.80979500	0.04553100	0.18398500
C	-4.78529900	-2.86894000	-0.72269800
H	-4.14919300	-3.26482400	0.07560400
H	-5.81802600	-3.12513600	-0.49766700
H	-4.50636200	-3.35084000	-1.66629000

C	-1.47400500	-3.69032600	2.47059600
H	-1.80481900	-4.09479600	1.50756300
H	-0.56105900	-4.21872300	2.75625600
H	-2.24933300	-3.92353200	3.20590400

6 (CT state)

Total Energy = -1862.7424502 A.U

C	3.79454371	1.04483642	-1.84459244
C	2.81621694	2.02968581	-1.80555122
C	1.47990335	1.68352476	-1.99944200
C	1.13013132	0.35123928	-2.21178591
C	2.11902202	-0.62311515	-2.23423068
C	3.46462718	-0.29746356	-2.05683727
H	4.83295272	1.32288430	-1.68901647
H	3.08062151	3.06409598	-1.61862854
H	0.09487790	0.06893347	-2.37117392
H	1.83564647	-1.65903226	-2.39231742
N	0.48056297	2.70105814	-2.00070604
N	0.77950943	3.79442568	-2.69151346
O	-0.05197342	4.69536679	-2.65412700
C	-0.79187642	2.55967104	-1.28412311
H	-1.12378623	1.52834026	-1.39367080
H	-1.50338906	3.20636307	-1.79851001
C	-0.69309953	2.94631682	0.17681492
C	-0.63430544	4.30125869	0.51800334
C	-0.67602441	1.97976447	1.19496021
C	-0.56549180	4.70321104	1.84587256
H	-0.64413675	5.03917053	-0.27738696
C	-0.61879628	2.39791178	2.52969280
C	-0.56258753	3.74668107	2.85789422
H	-0.52124506	5.75936922	2.09020064
H	-0.61135411	1.64641721	3.31331327
H	-0.51739586	4.04910002	3.89889016
C	-0.70527789	0.51231054	0.90456124
C	-1.97825903	-0.08742393	0.64433201
C	0.54755804	-0.18489273	0.96024473

C	-2.17541233	-1.48136737	0.33133079
C	-3.15689100	0.73172617	0.68882885
C	0.70365514	-1.60176986	0.74683813
C	1.74376212	0.55579673	1.23637022
C	-3.44415915	-1.96227367	0.08472248
C	-4.40540390	0.24428509	0.43869454
H	-3.05904797	1.78145138	0.93723727
C	1.94894126	-2.18535732	0.85135023
C	2.96955431	-0.03136631	1.33022870
H	1.68327079	1.62822839	1.36814368
C	-4.60324135	-1.13586182	0.12013434
H	-3.56442644	-3.01467528	-0.14804945
H	-5.24934530	0.91980710	0.49205666
H	2.03897079	-3.25287443	0.68168935
C	3.12396948	-1.44021440	1.14888172
H	3.83005652	0.59206296	1.53390197
Si	-0.73958477	-2.67359147	0.24800365
C	-0.51561222	-3.32673620	-1.49981646
H	-0.46385327	-2.50924903	-2.22482161
H	0.40496113	-3.91471005	-1.57713332
H	-1.35273732	-3.97437276	-1.77972279
C	-0.97678621	-4.10710741	1.43649235
H	-1.85729094	-4.69661831	1.16111786
H	-0.10967493	-4.77521618	1.41452389
H	-1.10908803	-3.75040603	2.46168591
N	-5.83370713	-1.62812680	-0.13056348
N	4.33554586	-2.02802501	1.24500908
C	-6.01536285	-3.03990777	-0.43826231
H	-7.07256497	-3.23625077	-0.60021946
H	-5.46867049	-3.31789944	-1.34550608
H	-5.66976642	-3.66946633	0.38838086
C	-7.00264189	-0.75896678	-0.09384869
H	-7.88660724	-1.34141981	-0.34300829
H	-7.14256466	-0.32853102	0.90325245
H	-6.91021744	0.05434513	-0.82066412
C	5.51687656	-1.24134036	1.57149042
H	5.42788936	-0.78919948	2.56516427
H	6.38959560	-1.89018780	1.56376913

H	5.67665430	-0.44427690	0.83791325
C	4.47421719	-3.46581669	1.06792126
H	4.14286866	-3.77283509	0.07020267
H	5.52062470	-3.74015046	1.17956195
H	3.88976786	-4.01308883	1.81534174
C	4.52981354	-1.36001644	-2.12033104
H	5.32268847	-1.17870697	-1.39013370
H	4.11040188	-2.35176350	-1.93406835
H	4.99823295	-1.38013758	-3.11008036

6 (CT-MECI)

Total Energy = -1862.7396735 A.U

C	2.42318042	-0.56879765	-2.87059377
C	2.29984078	0.65396502	-2.21622025
C	1.10412876	0.99431420	-1.58667683
C	0.04044171	0.11230761	-1.66937838
C	0.18035011	-1.10648718	-2.32968197
C	1.37371754	-1.48205641	-2.93044065
H	3.36086680	-0.79539514	-3.37422636
H	3.12875268	1.35369119	-2.21126218
H	-0.91499604	0.34084004	-1.21290512
H	-0.68075105	-1.77495135	-2.36466601
N	0.99965373	2.24151574	-0.86524854
N	2.13184939	2.87450423	-0.63837658
O	1.98575475	3.95724636	-0.12604872
C	-0.26016500	2.89452761	-0.50443822
H	-1.07223123	2.30279377	-0.92770692
H	-0.25852764	3.86830902	-1.00526658
C	-0.49321466	3.14390614	0.98213375
C	-0.60558790	4.46847029	1.40971151
C	-0.65007659	2.12290418	1.93370876
C	-0.88388282	4.78800970	2.73068778
H	-0.43588391	5.26434290	0.69100120
C	-0.91687208	2.45202926	3.26920631

C	-1.04140403	3.77425559	3.66959523
H	-0.96295820	5.82869958	3.02751788
H	-1.03198151	1.65113173	3.99380973
H	-1.24745630	4.01274272	4.70788190
C	-0.55230989	0.68050639	1.58012974
C	-1.71523788	-0.04978567	1.24724697
C	0.72509687	0.02105459	1.61290607
C	-1.70641971	-1.45450450	0.85811117
C	-2.96547547	0.65059028	1.09558554
C	0.91853347	-1.37882003	1.28175159
C	1.90005533	0.80477974	1.82745885
C	-2.61367099	-1.88599139	-0.09912057
C	-3.87729024	0.19014609	0.20356848
H	-3.09194048	1.62244697	1.55996704
C	2.10285986	-1.77902979	0.69742864
C	3.06632964	0.39780538	1.26805840
H	1.81219301	1.81118504	2.22363065
C	-3.69077124	-1.07139701	-0.49796260
H	-2.59860406	-2.92369392	-0.41335847
H	-4.74885577	0.79492656	-0.01304421
H	2.24878022	-2.82245354	0.43852225
C	3.19568938	-0.89300044	0.61344154
H	3.89568136	1.09167807	1.24751693
Si	-0.45502256	-2.58261094	1.64217447
C	-0.24890082	-4.15986935	0.65674300
H	-0.04574729	-3.93686871	-0.39531162
H	0.57908247	-4.76370671	1.04376275
H	-1.14308342	-4.78989300	0.71292306
C	-0.73771069	-2.88525611	3.46230130
H	-1.63418647	-3.49089902	3.62874805
H	0.11212440	-3.41558512	3.90365031
H	-0.86124348	-1.94440065	4.00451842
N	-4.60813162	-1.47139212	-1.40470030
N	4.37686637	-1.25033556	0.07440118
C	-4.35700375	-2.65489592	-2.20802976

H	-5.01432057	-2.64744161	-3.07801146	C	1.06871958	2.64639243	0.98185194
H	-3.32243772	-2.65198549	-2.56282377	H	1.30937107	1.61274521	1.22754026
H	-4.53392877	-3.58186552	-1.64433530	H	1.83411117	3.28906512	1.41739627
C	-5.91365698	-0.82686828	-1.51242963	C	0.99001483	2.86209283	-0.51501807
H	-6.54983736	-1.42630542	-2.16258912	C	0.92683571	4.17097764	-1.00136427
H	-6.40669434	-0.75934848	-0.53871448	C	0.96870981	1.79783132	-1.42796157
H	-5.83381401	0.17559762	-1.94885476	C	0.86406991	4.42784291	-2.36468726
C	5.59013035	-0.46967368	0.29336391	H	0.93229273	4.99005118	-0.28913565
H	5.74353704	-0.26308254	1.35509280	C	0.91143658	2.06285920	-2.80052089
H	6.44575143	-1.04381612	-0.05570899	C	0.86430945	3.36896215	-3.26926125
H	5.56076278	0.47663335	-0.25866470	H	0.82082004	5.45147273	-2.72101279
C	4.47318858	-2.47749001	-0.69431890	H	0.90041835	1.23200119	-3.49867357
H	3.61067641	-2.56252676	-1.36124644	H	0.82360158	3.55792612	-4.33651682
H	5.37858693	-2.45346280	-1.30201596	C	1.00622875	0.36833034	-0.97925008
H	4.51699073	-3.36280435	-0.04467718	C	2.27644762	-0.13078724	-0.55026095
C	1.53064040	-2.81829428	-3.61485933	C	-0.21685022	-0.34855332	-1.05664751
H	1.91559929	-3.58212079	-2.92938542	C	2.47665588	-1.43939669	-0.00544030
H	0.57666368	-3.18352565	-4.00357798	C	3.42798899	0.69967167	-0.66265983
H	2.22327987	-2.75773996	-4.45706512	C	-0.34981188	-1.73025618	-0.69565065

7 (Ground state)

Total Energy = -1957.4647165 A.U

C	-3.63434154	1.72721717	1.05293319
C	-2.54072530	2.57563587	1.12400437
C	-1.31259070	2.10744658	1.58060855
C	-1.19223030	0.77434887	1.96230341
C	-2.27358811	-0.08567561	1.87217787
C	-3.52198036	0.36386840	1.39357000
H	-4.57306984	2.12965715	0.69522528
H	-2.63974466	3.61279335	0.82206504
H	-0.24742518	0.39965683	2.34391497
H	-2.13465763	-1.11413253	2.17815588
N	-0.18917608	2.98334014	1.65286286
N	-0.38099376	4.14059616	2.26571948
O	0.55590391	4.93519999	2.22221559

C	1.06871958	2.64639243	0.98185194
H	1.30937107	1.61274521	1.22754026
H	1.83411117	3.28906512	1.41739627
C	0.99001483	2.86209283	-0.51501807
C	0.92683571	4.17097764	-1.00136427
C	0.96870981	1.79783132	-1.42796157
C	0.86406991	4.42784291	-2.36468726
H	0.93229273	4.99005118	-0.28913565
C	0.91143658	2.06285920	-2.80052089
C	0.86430945	3.36896215	-3.26926125
H	0.82082004	5.45147273	-2.72101279
H	0.90041835	1.23200119	-3.49867357
H	0.82360158	3.55792612	-4.33651682
C	1.00622875	0.36833034	-0.97925008
C	2.27644762	-0.13078724	-0.55026095
C	-0.21685022	-0.34855332	-1.05664751
C	2.47665588	-1.43939669	-0.00544030
C	3.42798899	0.69967167	-0.66265983
C	-0.34981188	-1.73025618	-0.69565065
C	-1.39968425	0.30968065	-1.51321235
C	3.72758448	-1.83648245	0.40762782
C	4.67152355	0.30096490	-0.25351808
H	3.33444796	1.68681263	-1.09857803
C	-1.54379492	-2.38341675	-0.87542053
C	-2.58761107	-0.34076528	-1.68177207
H	-1.37154787	1.36993582	-1.72836456
C	4.86965567	-0.98829201	0.31288372
H	3.85087573	-2.83253166	0.81735040
H	5.50317274	0.98185505	-0.37591868
H	-1.61991745	-3.42641326	-0.58879316
C	-2.70058023	-1.73073143	-1.39761944
H	-3.44686557	0.22103350	-2.02169326
Si	1.04703153	-2.63851152	0.15736855
C	0.59520960	-2.89518137	1.95962724
H	0.41351692	-1.93966642	2.45965438
H	-0.31241609	-3.50217861	2.03939254
H	1.40003411	-3.41120977	2.49207608
C	1.43241333	-4.26098425	-0.69411930

H	2.27444154	-4.76222861	-0.20675534	C	-0.90320519	0.87242905	1.62923776
H	0.57084726	-4.93443595	-0.64802736	C	-1.88816439	-0.05579219	1.88055496
H	1.68837246	-4.10094550	-1.74493895	C	-3.25625386	0.25068277	1.67617495
N	6.08332982	-1.39512348	0.73244776	H	-4.60091953	1.84576821	1.04131892
N	-3.85023287	-2.39920378	-1.59026252	H	-2.84379024	3.46201505	0.59224799
C	6.26574540	-2.72847535	1.29224486	H	0.12721328	0.59782433	1.82095949
H	7.30900985	-2.85548135	1.57291518	H	-1.59189783	-1.02496164	2.25501998
H	5.65168801	-2.86934456	2.18723753	N	-0.23739434	3.13762490	0.96708489
H	6.01119312	-3.50359362	0.56237982	N	-0.59320474	4.38092476	1.30788853
C	7.23617713	-0.51068703	0.61864890	O	0.24759340	5.24452681	1.10746145
H	8.11006195	-1.01092096	1.03038918	C	1.10132219	2.84349008	0.44103478
H	7.44399486	-0.26222962	-0.42710751	H	1.40496981	1.86716123	0.81454974
H	7.07820343	0.41665998	1.17783752	H	1.76678023	3.59409209	0.86789305
C	-5.05036351	-1.68957440	-2.01433505	C	1.15856087	2.88513896	-1.07200196
H	-4.94070498	-1.29207742	-3.02838182	C	1.24979262	4.12189557	-1.71766127
H	-5.89330960	-2.37710709	-2.00165252	C	1.13597821	1.70680388	-1.83599069
H	-5.26692892	-0.86929837	-1.32585489	C	1.31732684	4.20261258	-3.10312196
C	-3.92491880	-3.83765265	-1.36569180	H	1.26640196	5.02510402	-1.11726122
H	-3.81667904	-4.08627034	-0.30454679	C	1.21231489	1.80282852	-3.22993303
H	-4.89447268	-4.19793241	-1.70294730	C	1.30006534	3.03659011	-3.86350206
H	-3.15122895	-4.36195423	-1.93307096	H	1.38841596	5.17151387	-3.58617403
C	-5.92942720	0.05521715	1.14664437	H	1.19757496	0.88950676	-3.81693204
H	-6.04521995	0.67577249	0.25249491	H	1.35795159	3.08649249	-4.94592592
H	-6.64735392	-0.76135917	1.06868627	C	1.02952012	0.34829976	-1.21923287
H	-6.18902296	0.66476390	2.02328265	C	2.23291174	-0.23148588	-0.68336488
C	-4.47322637	-1.85859669	1.73055722	C	-0.26183318	-0.26404865	-1.22642358
H	-4.41295451	-1.91247808	2.82736121	C	2.30643958	-1.53651673	-0.09559143
H	-5.34057597	-2.43235013	1.40158547	C	3.44465492	0.52206629	-0.69959951
H	-3.58454843	-2.34203826	1.31509412	C	-0.52824602	-1.60181136	-0.77374334
N	-4.58943376	-0.50109323	1.23372908	C	-1.39556379	0.49169076	-1.66859548
-----				C	3.49042069	-1.98635518	0.46433466
7 (π-π^* state)				C	4.61174784	0.06684487	-0.14346360
Total Energy = -1957.3714268 A.U				H	3.45505776	1.49999047	-1.16659599
-----				C	-1.82268035	-2.08547000	-0.75583644
C	-3.57199044	1.55735512	1.21151529	C	-2.67263064	0.00781404	-1.62382246
C	-2.58146668	2.47851447	0.96122754	H	-1.24873148	1.49886681	-2.03825029
C	-1.23173740	2.15333586	1.16661738	C	4.67569472	-1.20874466	0.48149179
				H	3.51109725	-2.97955085	0.90071996

H	5.48954558	0.69885122	-0.19122404
H	-1.99165871	-3.10225457	-0.41498711
C	-2.94424935	-1.30325527	-1.14488555
H	-3.47576525	0.64418623	-1.97112883
Si	0.84065523	-2.69198325	-0.13090831
C	0.44114720	-3.32641974	1.59348287
H	0.33969742	-2.50012299	2.30333507
H	-0.49241449	-3.89884115	1.59487420
H	1.23477476	-3.98707407	1.95769944
C	1.15922779	-4.14681896	-1.27776850
H	1.99848257	-4.74877244	-0.91426348
H	0.27827551	-4.79482433	-1.33262350
H	1.39568960	-3.80434391	-2.28929022
N	5.82155602	-1.66247559	1.05379422
N	-4.21480900	-1.78349085	-1.05980009
C	5.85956097	-2.97480539	1.67626470
H	6.85058136	-3.14501090	2.09257320
H	5.12986028	-3.04998797	2.49036533
H	5.65240876	-3.76942094	0.95001899
C	7.02504588	-0.84786362	1.03260520
H	7.82447810	-1.37798772	1.54661382
H	7.35408974	-0.64530286	0.00694749
H	6.86755912	0.10897647	1.54277041
C	-5.33130299	-0.97071874	-1.50743416
H	-5.35542219	-0.86971337	-2.60008938
H	-6.26234371	-1.42980611	-1.17784513
H	-5.27629622	0.03054597	-1.07199047
C	-4.45287466	-3.20141535	-0.83923012
H	-4.04814684	-3.53237789	0.12104071
H	-5.52595215	-3.38283718	-0.82682077
H	-4.00374413	-3.81064277	-1.63241694
C	-5.63001005	-0.27462607	1.94616958
H	-5.94248218	0.14970438	0.98928566
H	-6.24164566	-1.15506973	2.13193934
H	-5.82335276	0.46064455	2.73446030
C	-3.87052784	-1.97734848	2.43417713
H	-3.48198828	-1.92170755	3.45782024
H	-4.75030146	-2.61817971	2.42916428

H	-3.10717791	-2.43885190	1.80055096
N	-4.22897674	-0.66792975	1.92052741

7 (CT state)

Total Energy = -1957.4026148 A.U

C	-3.19512236	0.60025674	1.89482199
C	-2.38378206	1.69087908	1.86327128
C	-0.96837004	1.54514251	1.84153206
C	-0.41406548	0.24873615	1.90788824
C	-1.22330536	-0.85245026	1.92529967
C	-2.64732872	-0.72299177	1.89615818
H	-4.26522266	0.74929873	1.88088872
H	-2.81824748	2.67841694	1.81764971
H	0.65575374	0.09773776	1.93314482
H	-0.76433008	-1.82899971	1.97919897
N	-0.16778247	2.67631934	1.78428550
N	-0.78467408	3.83578243	2.15105397
O	-0.07914505	4.81586481	2.10329223
C	1.24374878	2.70335413	1.37569707
H	1.66312925	1.71395853	1.53575171
H	1.74943235	3.39338971	2.05162935
C	1.41707784	3.15103317	-0.06375765
C	1.75592128	4.48123900	-0.32325450
C	1.26500683	2.25063422	-1.13349457
C	1.92700616	4.93762309	-1.62489312
H	1.88106151	5.16483756	0.50933703
C	1.43461973	2.72863629	-2.43752890
C	1.75763635	4.05720540	-2.68849295
H	2.19063719	5.97445443	-1.80502413
H	1.31545275	2.03322091	-3.26285661
H	1.88608179	4.39946583	-3.71023395
C	0.96917637	0.79465549	-0.95851181
C	2.08447856	-0.05816813	-0.54472516
C	-0.34729618	0.35334620	-1.23760626
C	2.01957202	-1.47626958	-0.51136872
C	3.30081093	0.51581650	-0.11291077

C	-2.64102945	-0.76273173	2.06751891	H	2.93175155	-3.29326603	0.07567094
H	-4.29702121	0.68849673	2.10916422	H	5.22656711	0.25419482	0.79132813
H	-2.91452547	2.63332296	1.90721764	H	-2.33598306	-2.39564457	-1.27211940
H	0.64577440	0.07712742	1.73660090	C	-3.14981652	-0.40027266	-1.27640990
H	-0.72415104	-1.84080806	2.04215040	H	-3.50231971	1.71247712	-1.55779670
N	-0.26850560	2.61269067	1.61175444	Si	0.58516864	-2.27634571	-1.32586674
N	-1.04827348	3.88940943	1.77634761	C	0.07740191	-3.86369632	-0.41425819
O	-0.35393576	4.82275614	1.80114400	H	0.03281898	-3.72951122	0.67239213
C	1.17731625	2.73271763	1.32591470	H	-0.88526512	-4.25328905	-0.76576128
H	1.64768901	1.76911493	1.49869138	H	0.81154535	-4.65503730	-0.59675456
H	1.58504291	3.44155302	2.05026843	C	0.98123523	-2.74067361	-3.10053599
C	1.41160547	3.20497501	-0.09704534	H	1.81732704	-3.44603211	-3.14749780
C	1.80327898	4.52248512	-0.32294517	H	0.12012110	-3.19847351	-3.59886423
C	1.30090984	2.28596101	-1.15903081	H	1.26278250	-1.84710973	-3.66484418
C	2.05663428	4.97251194	-1.61446208	N	5.22783971	-2.42736940	1.18906511
H	1.91870285	5.20852879	0.51071938	N	-4.53374358	-0.81360315	-1.22185753
C	1.56596377	2.76669952	-2.44147302	C	5.20889826	-3.84907012	0.91062355
C	1.92522935	4.09120640	-2.67924099	H	6.06077422	-4.32124489	1.40274105
H	2.35940697	6.00051469	-1.78122736	H	4.30636668	-4.31258824	1.32045704
H	1.49109997	2.06649020	-3.26847562	H	5.25650355	-4.08445526	-0.16483106
H	2.11785827	4.42940668	-3.69178897	C	6.54851291	-1.83161963	1.26723517
C	0.97794117	0.84057066	-0.95505100	H	7.24039893	-2.55419696	1.70318982
C	2.08185374	-0.03279697	-0.50774727	H	6.94440586	-1.52191618	0.28707725
C	-0.35630398	0.39619775	-1.19604578	H	6.54394731	-0.95814094	1.92548530
C	2.00574481	-1.44626638	-0.47062262	C	-5.46728988	0.17488150	-1.74912138
C	3.29768300	0.51358899	-0.04916445	H	-5.25083289	0.46588451	-2.78911068
C	-0.75076755	-0.98412058	-1.23581461	H	-6.48064997	-0.23153217	-1.71049643
C	-1.42883998	1.31947734	-1.35086236	H	-5.45966679	1.08065660	-1.13635472
C	3.04461857	-2.21334147	0.08082422	C	-4.78527394	-2.12881554	-1.80470790
C	4.32362034	-0.25684422	0.47846696	H	-4.31558159	-2.91874581	-1.21141051
H	3.47536768	1.58174468	-0.13116055	H	-5.86046940	-2.32245926	-1.80104370
C	-2.09584912	-1.33510655	-1.23263436	H	-4.41866381	-2.22183671	-2.83839702
C	-2.76388917	0.93260388	-1.41373208	C	-4.87333870	-1.71683452	2.00353315
H	-1.19993448	2.37473425	-1.47501860	H	-5.11860908	-1.25557656	1.04930310
C	4.21604063	-1.65144616	0.59686596	H	-5.29118384	-2.71757310	2.04367041

H	-5.25598914	-1.15268394	2.85405961
C	-2.81484413	-3.17852430	2.03912333
H	-2.09535833	-3.31636276	2.84494761
H	-3.61249919	-3.90384908	2.16394318
H	-2.34020229	-3.32262935	1.07016268
N	-3.39570240	-1.82399305	2.08546629

16

Total Energy = -570.4446927 A.U

C	-1.06920138	-0.08316022	-0.50324221
C	0.31901463	-0.09698721	-0.58348579
C	1.08579735	1.08809957	-0.40361802
C	0.35231799	2.27863572	-0.13858736
C	-1.03631286	2.27523064	-0.06143424
C	-1.76706941	1.09556160	-0.24244984
H	-1.64018813	-1.00472951	-0.64461653
H	0.82606327	-1.04120265	-0.78935465
H	0.91868630	3.19661110	0.00231487
H	-1.54137757	3.22156202	0.14485814
N	2.43236358	1.10916972	-0.47517433
N	3.15493847	2.47513606	-0.25718906
O	4.40063103	2.32213985	-0.35733242
C	3.22301307	-0.04225751	-0.73626065
H	3.11253226	-0.83399111	0.03421562
H	3.01306903	-0.50333166	-1.72413246
H	4.26053356	0.34247525	-0.72255899
C	-3.85367279	2.17117720	0.07499129
H	-4.92142265	1.90745570	0.08450271
H	-3.58966790	2.61459439	1.05542963
H	-3.68639380	2.94326995	-0.70183016
O	-3.15089379	0.99509138	-0.18371427

17

Total Energy = -548.2284253 A.U

C	-1.08002989	-0.19769715	-0.36591108
C	0.28823060	-0.15224044	-0.53879458
C	1.02228387	1.05990451	-0.33314100
C	0.26770859	2.21772071	0.05926492
C	-1.09408682	2.14918064	0.22549931
C	-1.81027593	0.94458505	0.01942466
H	-1.61205041	-1.13807221	-0.53050521
H	0.81793748	-1.05739616	-0.83766684
H	0.81591185	3.14332855	0.21789973
H	-1.64416830	3.04506362	0.52460836
N	2.34373178	1.14106774	-0.49068967
N	3.04663065	2.52901107	-0.23613411
O	4.27640722	2.42264028	-0.42853468
C	3.16564786	0.04069014	-0.87758249
H	3.13284481	-0.79257797	-0.15027966
H	2.90136034	-0.35906977	-1.87499119
H	4.18579028	0.46584447	-0.90783410
C	-3.22313814	0.88651947	0.19519058
N	-4.37989671	0.83697987	0.33859020

18

Total Energy = -555.211406 A.U

C	-1.08105082	-0.20754689	-0.29400759
C	0.29746295	-0.15350429	-0.50104763
C	1.02824053	1.05341659	-0.31583180
C	0.28086450	2.20189151	0.09092173
C	-1.08845074	2.13101136	0.29229182
C	-1.76565007	0.92947241	0.10005721
H	-1.62970349	-1.14122176	-0.43989038
H	0.82080683	-1.05893882	-0.81143116
H	0.82884138	3.13032309	0.23548783
H	-1.65081657	3.01504676	0.60343235
N	2.35738991	1.14198790	-0.50677181
N	3.04877688	2.53425256	-0.26973112
O	4.28161199	2.43900574	-0.48997367
C	3.16793669	0.04717857	-0.91073982

H	3.16109548	-0.79286569	-0.18523624
H	2.88602125	-0.36277299	-1.90297289
H	4.18605628	0.47749990	-0.96589880
F	-3.11890545	0.87429871	0.30264998

19

Total Energy = -915.6080909 A.U

C	-1.08066211	-0.20761124	-0.30751991
C	0.29489836	-0.15452039	-0.50716323
C	1.02809011	1.05328473	-0.31839900
C	0.27819289	2.20335790	0.08546600
C	-1.08903631	2.13506933	0.28002249
C	-1.77481892	0.93162718	0.08502179
H	-1.61736505	-1.14661115	-0.45942600
H	0.81768218	-1.06114083	-0.81494940
H	0.82437573	3.13238674	0.23333234
H	-1.63998633	3.02645512	0.58836218
N	2.35311534	1.14024457	-0.50166906
N	3.05227604	2.53979322	-0.26118724
O	4.28162331	2.43912965	-0.47843164
C	3.16793513	0.04577289	-0.90306340
H	3.15754030	-0.79262561	-0.17732725
H	2.88992362	-0.36152660	-1.89638145
H	4.18613130	0.47602206	-0.95403391
Cl	-3.52938805	0.85949532	0.33858760

20

Total Energy = -455.9843927 A.U

C	-1.07480237	-0.20261121	-0.28799402
C	0.29993783	-0.15249874	-0.49801645
C	1.02955078	1.05794904	-0.31326619
C	0.27865566	2.20457199	0.09526049
C	-1.08804178	2.12161530	0.29573808
C	-1.79640523	0.92386741	0.11068294

H	-1.59493281	-1.15425878	-0.44191010
H	0.82790545	-1.05564277	-0.80940790
H	0.82379207	3.13492578	0.23987280
H	-1.62707262	3.02250371	0.60848351
N	2.35695926	1.14555857	-0.50637571
N	3.05566793	2.53302578	-0.27175146
O	4.28813119	2.43233864	-0.49523391
C	3.16563396	0.04799032	-0.91152752
H	3.15712728	-0.79051466	-0.18511422
H	2.87956349	-0.36114946	-1.90222401
H	4.18433664	0.47571908	-0.96899624
H	-2.87547919	0.87509807	0.27313377

21

Total Energy = -495.2660511 A.U

C	-1.06313948	-0.18696828	-0.34149920
C	0.32016421	-0.15177698	-0.50422037
C	1.04702594	1.06184756	-0.35656947
C	0.28085538	2.22568729	-0.03515613
C	-1.09075659	2.15182746	0.11861096
C	-1.80985770	0.95050160	-0.02792925
H	-1.57965600	-1.14632730	-0.46535767
H	0.85199743	-1.07291738	-0.74891633
H	0.82076763	3.16313044	0.08197055
H	-1.63825777	3.06964733	0.36513624
N	2.38121451	1.14299679	-0.50451512
N	3.06692721	2.54040526	-0.31431021
O	4.30770467	2.43339946	-0.48674937
C	3.20400678	0.02786536	-0.82274845
H	3.16794135	-0.77279584	-0.05534468
H	2.95424120	-0.43204246	-1.80110835
H	4.22418314	0.45432002	-0.86404400
C	-3.30736266	0.90596323	0.14619414
H	-3.62116585	1.23133128	1.15462298
H	-3.83221661	1.55867170	-0.57484569
H	-3.69335406	-0.11584160	-0.00015174

22

Total Energy = -589.8475709 A.U

C	-0.96581962	-0.25397236	-0.09686664
C	0.42391211	-0.19846890	-0.13219923
C	1.10446520	0.99948368	-0.49512762
C	0.28631788	2.12832834	-0.81712609
C	-1.09272582	2.04096238	-0.77249652
C	-1.75396117	0.85245473	-0.41268426
H	-1.47119183	-1.18273948	0.18418260
H	1.00068574	-1.08907643	0.12286507
H	0.79130666	3.05060631	-1.09625650
H	-1.68303761	2.92847793	-1.02640071
N	-3.19295753	0.74023880	-0.35983723
N	2.44348388	1.09477648	-0.54152496
N	3.08142991	2.47335840	-0.95683990
O	4.33342072	2.38160792	-0.94753236
C	3.31836576	0.01619965	-0.23538166
H	3.21269731	-0.34708517	0.80743113
H	3.18861635	-0.85421447	-0.91074274
H	4.32868325	0.44451775	-0.37594991
C	-3.79864970	1.58633627	0.64838206
H	-4.87097270	1.34091913	0.75213601
H	-3.30746345	1.41165649	1.61645234
H	-3.72647549	2.67563762	0.42328919
C	-3.83025984	0.90832100	-1.65011789
H	-3.36218426	0.23288655	-2.38061255
H	-4.90293066	0.65355150	-1.57701568
H	-3.76087597	1.94495059	-2.05391822

Reference

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