

## Supporting Online Material



Figure S1: Isosurface plots of the density changes for the excitations to the  $S_1$  and  $S_2$  states from the SCS-CC2/cc-pVTZ calculations, isosurface value 0.001.

Table S1: B3-LYP/cc-pVTZ calculated optimized  $S_0$  cartesian coordinates of 5CI (in bohr).

c	2.33945506	-3.45666728	-0.06658526
c	1.27758598	-0.96529945	-0.00746652
c	-1.39128359	-1.25172758	-0.06878124
n	-1.88418188	-3.79426572	-0.15945308
c	0.36744358	-5.11258413	-0.15768127
c	2.30066152	1.46262037	0.09063558
c	0.67194214	3.52928432	0.12554779
c	-1.97971352	3.19668763	0.06173556
c	-3.02957847	0.81302010	-0.03550986
c	1.68232260	6.03072950	0.23184740
n	2.49030247	8.05337799	0.32241414
h	4.31287105	-3.94921688	-0.04395390
h	0.37172822	-7.14615943	-0.22234068
h	-3.61004990	-4.57988505	-0.21756163
h	4.32226751	1.75508990	0.13982414
h	-5.05904804	0.56889883	-0.08351262
h	-3.18272473	4.84609688	0.09084145

Table S2: CC2/cc-pVTZ calculated optimized  $S_0$  cartesian coordinates of 5CI (in bohr).

c	2.34866071	-3.45461961	-0.06573146
c	1.28588288	-0.97298158	-0.00621903
c	-1.39162059	-1.25666760	-0.06905693
n	-1.88641656	-3.80029826	-0.16206036
c	0.35993795	-5.12372640	-0.15974757
c	2.31426076	1.46331070	0.09373932
c	0.67074549	3.52440059	0.12816663
c	-1.98471158	3.19916416	0.06435097
c	-3.04143246	0.80551644	-0.03491131
c	1.67858227	6.02946434	0.23040246
n	2.50391614	8.10273261	0.31498826
h	4.32141862	-3.95276763	-0.04256228
h	0.35749085	-7.15832311	-0.22588515
h	-3.61777002	-4.58336081	-0.22039897
h	4.33653914	1.76470859	0.14398175
h	-5.07141596	0.56034515	-0.08349399
h	-3.18406763	4.85310243	0.09443765

Table S3: SCS-CC2/cc-pVTZ calculated optimized  $S_0$  cartesian coordinates of 5CI (in bohr).

c	2.35019781	-3.46398276	-0.06583061
c	1.28135652	-0.97281537	-0.00578832
c	-1.38961411	-1.25884087	-0.06860637
n	-1.89043978	-3.80593228	-0.16184733
c	0.36301331	-5.13025296	-0.16013315
c	2.31302511	1.46736094	0.09439528
c	0.67241128	3.52912870	0.12867474
c	-1.98699674	3.20244899	0.06483292
c	-3.04346320	0.80888173	-0.03428126
c	1.68504998	6.04595455	0.23055902
n	2.50559442	8.11020028	0.31366763
h	4.32368942	-3.96057592	-0.04256695
h	0.36148410	-7.16517968	-0.22675658
h	-3.61968003	-4.58790024	-0.22239344
h	4.33593391	1.76399170	0.14448228
h	-5.07329575	0.56211543	-0.08298895
h	-3.18826627	4.85539776	0.09458110

Table S4: SOS-CC2/cc-pVTZ calculated optimized  $S_0$  cartesian coordinates of 5CI (in bohr).

c	2.35102810	-3.46904980	-0.06604163
c	1.27902081	-0.97274404	-0.00620427
c	-1.38846243	-1.25996994	-0.06890684
n	-1.89247812	-3.80885041	-0.16198615
c	0.36476636	-5.13390410	-0.16001384
c	2.31233792	1.46958771	0.09405537
c	0.67338194	3.53168923	0.12857275
c	-1.98841842	3.20406912	0.06472837
c	-3.04456502	0.81075712	-0.03447609
c	1.68841242	6.05430446	0.23111756
n	2.50671476	8.11433835	0.31466840
h	4.32497993	-3.96481052	-0.04264033
h	0.36354001	-7.16907279	-0.22632140
h	-3.62084748	-4.59020965	-0.22211651
h	4.33562386	1.76406254	0.14405859
h	-5.07440541	0.56318085	-0.08312208
h	-3.19062924	4.85662187	0.09462809

Table S5: TD B3-LYP/cc-pVTZ calculated optimized  $S_1$  cartesian coordinates of 5CI (in bohr).

c	2.31357707	-3.43231040	-0.06596908
c	1.27578852	-0.94146559	-0.00652449
c	-1.33482974	-1.23814460	-0.06797896
n	-1.86432685	-3.88163417	-0.16245019
c	0.26806961	-5.19358398	-0.16258137
c	2.40425058	1.47170395	0.09411758
c	0.69997771	3.61381750	0.13136188
c	-1.93478521	3.20232448	0.06469666
c	-3.03984999	0.81054241	-0.03575725
c	1.61725269	6.10762535	0.23372599
n	2.41076371	8.15620458	0.31925587
h	4.28088074	-3.95684469	-0.04404838
h	0.31035691	-7.22566512	-0.22691714
h	-3.60981466	-4.63725253	-0.22124075
h	4.42378165	1.72702484	0.14086329
h	-5.06540963	0.57513465	-0.08413035
h	-3.15568311	4.84252333	0.09357669

Table S6: CC2/cc-pVTZ calculated optimized  $S_1$  cartesian coordinates of 5CI (in bohr).

c	2.31585845	-3.41484509	-0.06490768
c	1.30577360	-0.96042241	-0.00504083
c	-1.36970026	-1.25659061	-0.06827680
n	-1.88727595	-3.88212253	-0.16431213
c	0.27520815	-5.18176957	-0.16341134
c	2.43378690	1.47064612	0.09679913
c	0.72457486	3.60116087	0.13189270
c	-1.95198092	3.20005606	0.06511778
c	-3.07385379	0.78845848	-0.03586216
c	1.63673208	6.09790242	0.23147970
n	2.42216473	8.20364841	0.31582232
h	4.28583748	-3.94260095	-0.04272687
h	0.31785691	-7.21668471	-0.22891149
h	-3.63112979	-4.65002493	-0.22423454
h	4.45801202	1.72834672	0.14583851
h	-5.10262265	0.56261114	-0.08389526
h	-3.15924181	4.85223060	0.09462895

Table S7: SCS-CC2/cc-pVTZ calculated optimized  $S_1$  cartesian coordinates of 5CI (in bohr).

c	2.34807092	-3.45121350	-0.06567041
c	1.31745932	-0.98607006	-0.00698208
c	-1.42925839	-1.27098536	-0.07067684
n	-1.90275426	-3.83626947	-0.16247871
c	0.34811237	-5.16343948	-0.16031102
c	2.41402094	1.45822464	0.09393837
c	0.70538740	3.58187038	0.12996315
c	-2.00778801	3.23347115	0.06409216
c	-3.10968351	0.78973714	-0.03755976
c	1.67494416	6.07294292	0.23293712
n	2.48621201	8.15247905	0.31986988
h	4.32112387	-3.95620480	-0.04261124
h	0.36191796	-7.19766887	-0.22525079
h	-3.62911603	-4.62778158	-0.22186540
h	4.43380807	1.74901566	0.14363946
h	-5.13799148	0.55595816	-0.08572679
h	-3.19446532	4.89593403	0.09469290

Table S8: SOS-CC2/cc-pVTZ calculated optimized  $S_1$  cartesian coordinates of 5CI (in bohr).

c	2.35226942	-3.46239233	-0.06573919
c	1.31812857	-0.98841405	-0.00598642
c	-1.43226280	-1.27175836	-0.07042719
n	-1.90339558	-3.83208549	-0.16319968
c	0.35766589	-5.16696185	-0.16115348
c	2.41190269	1.45852425	0.09603533
c	0.69850358	3.58134896	0.13080435
c	-2.01266968	3.24104174	0.06549913
c	-3.11513747	0.79065788	-0.03678312
c	1.67815665	6.07879570	0.23147273
n	2.49391618	8.14979937	0.31502987
h	4.32582519	-3.96532381	-0.04262314
h	0.36645777	-7.20107419	-0.22706635
h	-3.62872758	-4.62351533	-0.22352907
h	4.43096484	1.75341044	0.14662323
h	-5.14307438	0.55417524	-0.08532347
h	-3.19852329	4.90377184	0.09636648

Table S9: SCS-CC2/cc-pVTZ calculated optimized  $S_2$  cartesian coordinates of 5CI (in bohr).

c	1.2410487	-1.8388334	-0.0350051
c	0.6970113	-0.5115760	-0.0023882
c	-0.7171235	-0.6468323	-0.0352273
n	-0.9721944	-2.0166550	-0.0852949
c	0.1686789	-2.7682496	-0.0870437
c	1.2647933	0.7835091	0.0514377
c	0.3300143	1.8937713	0.0685636
c	-1.0466920	1.7243175	0.0353670
c	-1.6284286	0.4077290	-0.0190492
c	0.8633120	3.2192908	0.1218805
n	1.3282576	4.3020695	0.1658065
h	2.2857520	-2.1086299	-0.0229029
h	0.1470518	-3.8424047	-0.1227854
h	-1.9058414	-2.4069084	-0.1168937
h	2.3303580	0.9571404	0.0784388
h	-2.6984262	0.2575186	-0.0454691
h	-1.6875719	2.5947432	0.0505655

Table S10: SOS-CC2/cc-pVTZ calculated optimized  $S_2$  cartesian coordinates of 5CI (in bohr).

c	1.2416001	-1.8357107	-0.0349116
c	0.6989162	-0.5122907	-0.0024090
c	-0.7187272	-0.6488737	-0.0353441
n	-0.9749239	-2.0216711	-0.0854678
c	0.1641626	-2.7678644	-0.0871156
c	1.2651374	0.7847714	0.0512860
c	0.3317399	1.8954735	0.0685831
c	-1.0442140	1.7257604	0.0354217
c	-1.6271748	0.4052765	-0.0192046
c	0.8658013	3.2250174	0.1221988
n	1.3275542	4.3061124	0.1661573
h	2.2853360	-2.1089267	-0.0229618
h	0.1460917	-3.8423888	-0.1226017
h	-1.9070397	-2.4134770	-0.1170485
h	2.3309092	0.9572736	0.0783753
h	-2.6975700	0.2571653	-0.0455793
h	-1.6875992	2.5943525	0.0506219