

ELECTRONIC SUPPLEMENTARY INFORMATION

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**State-Interaction Pair Density Functional Theory for Locally Avoided  
Crossings of Potential Energy Surfaces in Methylamine**

Chen Zhou, Laura Gagliardi,\* and Donald G. Truhlar\*

*Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of  
Minnesota, Minneapolis MN 55455-0431*

\*email: [gagliardi@umn.edu](mailto:gagliardi@umn.edu), [truhlar@umn.edu](mailto:truhlar@umn.edu)

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## Equilibrium geometries of methylamine in Angstrom

### (1) eclipsed conformation

N	0.00204548	0.00000628	0.70120476
H	0.86019472	-0.00004443	1.22059368
H	-0.85421062	-0.00004310	1.22119778
C	0.00189000	-0.00000336	-0.73696735
H	0.48596395	-0.88475017	-1.15933997
H	-1.02936905	0.00030991	-1.08536656
H	0.48647422	0.88448059	-1.15929482

### (2) staggered conformation

N	-0.12310328	0.00071775	0.72548952
H	-0.14497838	-0.94901180	1.08504480
H	-0.14273413	0.94922612	1.08510310
C	-0.00066684	0.00002564	-0.72911010
H	-0.50666214	0.87808667	-1.12875744
H	1.02787763	0.00059336	-1.10940810
H	-0.50604478	-0.87873943	-1.12824836

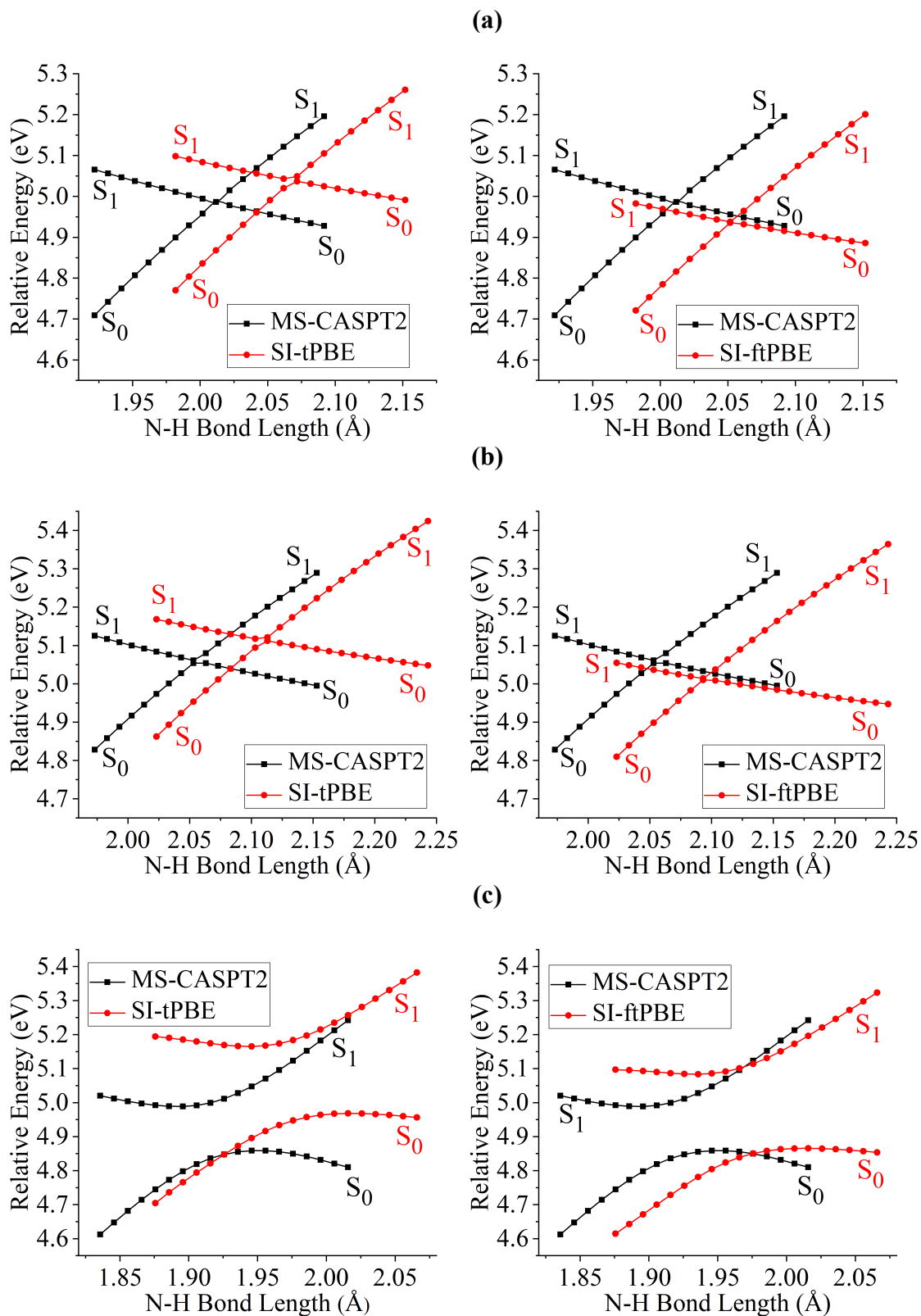
### (3) H6-C4-N1-H3 dihedral angle equaling 95°

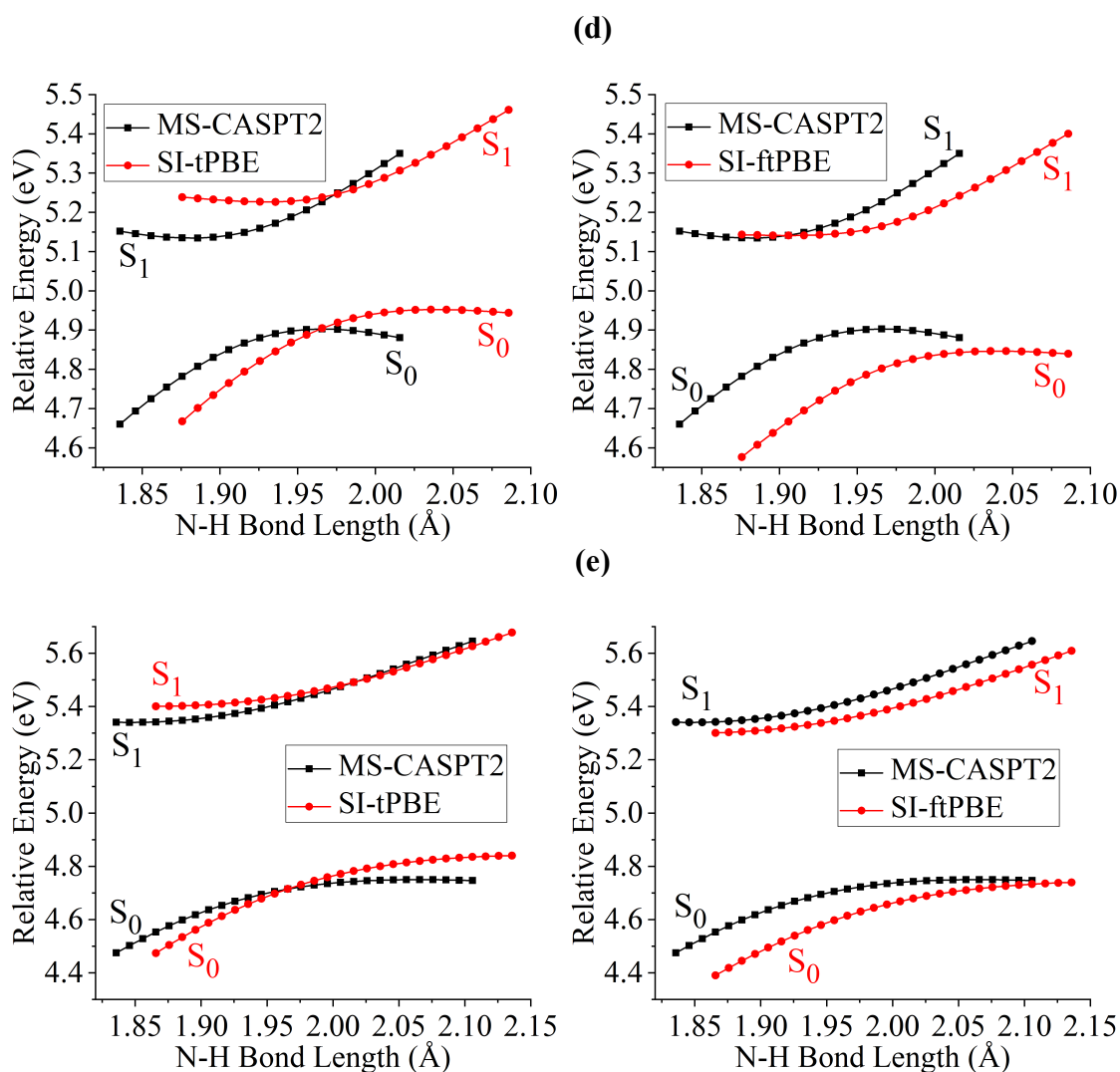
N	-0.12310328	0.00071775	0.72548952
H	-0.23506087	-0.94550075	1.07746126
H	-0.23641226	0.94561052	1.07721977
C	-0.00066684	0.00002564	-0.72911010
H	-0.50666214	0.87808667	-1.12875744
H	1.02787763	0.00059336	-1.10940810
H	-0.50604478	-0.87873943	-1.12824836

### (4) H6-C4-N1-H3 dihedral angle equaling 100°

N	-0.12310328	0.00071775	0.72548952
H	-0.30947164	-0.93603241	1.07119290
H	-0.30699192	0.93665960	1.07128320
C	-0.00066684	0.00002564	-0.72911010
H	-0.50666214	0.87808667	-1.12875744
H	1.02787763	0.00059336	-1.10940810
H	-0.50604478	-0.87873943	-1.12824836

### SI-PDFT PESs for N-H bond fission of methylamine near the LAC region compared with MS-CASPT2





**Figure S1.** SI-PDFT PESs for N-H bond fission of methylamine with (a) eclipsed-H3 conformation, (b) eclipsed-H2 conformation, (c) staggered conformation, (d) H6-C4-N1-H3 dihedral angle equaling  $95^\circ$  and (e)  $100^\circ$  near the LAC region compared with MS-CASPT2 method. The relative energies are compared with those of ground state geometry for each method.

## Absolute energies (in a.u.) for the PESs of N-H Bond fission

### (1) N-H3 bond fission of eclipsed conformation

$R_{N-H}$ (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
0.602	-95.14323782	-94.94263956	-95.14952539	-94.95053699	-95.30344282	-95.09055447	-95.34388245	-95.12953603
0.702	-95.37473401	-95.17792995	-95.38122353	-95.18588867	-95.53265117	-95.32990114	-95.57403811	-95.36355576
0.802	-95.48609977	-95.29309591	-95.49284820	-95.30135140	-95.64405704	-95.44532712	-95.68245648	-95.48381367
0.902	-95.53239471	-95.34366316	-95.53944194	-95.35231655	-95.69091972	-95.49552441	-95.72900986	-95.53426246
1.002	-95.54322490	-95.35968464	-95.55062431	-95.36896428	-95.70330131	-95.51482121	-95.74073956	-95.55191419
1.102	-95.53582342	-95.36074925	-95.54281982	-95.36886983	-95.69880965	-95.51268135	-95.73854302	-95.55065588
1.202	-95.51893456	-95.35457136	-95.52521611	-95.36326895	-95.68401240	-95.51007476	-95.72385890	-95.54817136
1.302	-95.49783681	-95.34997380	-95.50260270	-95.35880559	-95.66481307	-95.50895230	-95.69489473	-95.54427168
1.402	-95.47525774	-95.34946429	-95.48184183	-95.35636271	-95.63745894	-95.50193740	-95.67392641	-95.54392902
1.502	-95.45277440	-95.35182328	-95.45946915	-95.35880512	-95.61615983	-95.50482429	-95.65314995	-95.54695658
1.602	-95.43337163	-95.35434969	-95.43888968	-95.36344836	-95.59587836	-95.50898620	-95.63337997	-95.55111049
1.702	-95.41501274	-95.35980085	-95.42040405	-95.36825284	-95.57715914	-95.51325110	-95.61515728	-95.55529529
1.802	-95.39886166	-95.36460411	-95.40416305	-95.37256521	-95.56029335	-95.51715897	-95.59876150	-95.55907912
1.902	-95.38499051	-95.36865801	-95.39019932	-95.37624482	-95.54541541	-95.52056993	-95.58430785	-95.56233048
2.002	-95.37333185	-95.37199140	-95.37813808	-95.37810167	-95.53255067	-95.52345294	-95.57178039	-95.56501387
2.102	-95.37469907	-95.36372549	-95.38068719	-95.36852444	-95.52583092	-95.52167086	-95.56717739	-95.56113687
2.202	-95.37682546	-95.35595569	-95.38272056	-95.36078640	-95.52774893	-95.51267755	-95.56887656	-95.55225910
2.302	-95.37850949	-95.34979157	-95.38432248	-95.35464790	-95.52927455	-95.50540216	-95.57015698	-95.54489932
2.402	-95.37981720	-95.34498640	-95.38557136	-95.34985845	-95.53047416	-95.49964585	-95.57113351	-95.53924978
2.502	-95.38082848	-95.34129353	-95.38653613	-95.34617558	-95.53140864	-95.49519693	-95.57185079	-95.53441335
2.602	-95.38159417	-95.33849209	-95.38727590	-95.34337833	-95.53213229	-95.49180764	-95.57237317	-95.53088416
2.702	-95.38218518	-95.33639095	-95.38784024	-95.34127528	-95.53269763	-95.48927661	-95.57275154	-95.52824234
2.802	-95.38263497	-95.33482873	-95.38826965	-95.33970710	-95.53313855	-95.48741836	-95.57303180	-95.52609580
2.902	-95.38296462	-95.33367605	-95.38859622	-95.33854530	-95.53348632	-95.48607304	-95.57323301	-95.52447543
3.002	-95.38322233	-95.33283136	-95.38884458	-95.33768863	-95.53376368	-95.48511083	-95.57337835	-95.52339395
3.102	-95.38341661	-95.33221436	-95.38903331	-95.33705887	-95.53398485	-95.48443516	-95.57349942	-95.52252671
3.202	-95.38356435	-95.33176389	-95.38917626	-95.33659647	-95.53416212	-95.48396582	-95.57357946	-95.52189753
3.302	-95.38366054	-95.33142984	-95.38928386	-95.33625674	-95.53430469	-95.48364349	-95.57364416	-95.52145532
3.402	-95.38374363	-95.33118787	-95.38936411	-95.33600664	-95.53441844	-95.48342557	-95.57370070	-95.52115004
3.502	-95.38380477	-95.33100575	-95.38942328	-95.33582192	-95.53450950	-95.48328275	-95.57374088	-95.52090032
3.602	-95.38384808	-95.33086570	-95.38946633	-95.33568497	-95.53458233	-95.48318923	-95.57376915	-95.52073176
4.602	-95.38393574	-95.33041496	-95.38956080	-95.33529921	-95.53476488	-95.48303817	-95.57380392	-95.52033968
5.602	-95.38389242	-95.33035181	-95.38954952	-95.33526716	-95.53476427	-95.48305307	-95.57379277	-95.52033741
7.602	-95.38386981	-95.33030539	-95.38953741	-95.33525593	-95.53476097	-95.48305566	-95.57378768	-95.52033852

## (2) N-H2 bond fission of eclipsed conformation

R <sub>N-H</sub> (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-rIPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
0.603	-95.14663717	-94.94683391	-95.15096127	-94.95057934	-95.30553862	-95.09993585	-95.34438500	-95.13902925
0.703	-95.37618873	-95.18005620	-95.38064878	-95.18397038	-95.53403612	-95.33217459	-95.57549932	-95.36595498
0.803	-95.48660842	-95.29419661	-95.49125018	-95.29835291	-95.64451124	-95.44650884	-95.68291501	-95.48498808
0.903	-95.53249511	-95.34413523	-95.53736877	-95.34864419	-95.69096130	-95.49597841	-95.72903725	-95.53473519
1.003	-95.54322444	-95.35968409	-95.54837472	-95.36472425	-95.70289030	-95.51333939	-95.74073680	-95.55190939
1.103	-95.53589438	-95.36012826	-95.54045618	-95.36368919	-95.69874540	-95.51184952	-95.73848690	-95.54982440
1.203	-95.51915885	-95.35293125	-95.52274910	-95.35440194	-95.68408016	-95.50805215	-95.72393668	-95.54610050
1.303	-95.49829355	-95.34710630	-95.50206306	-95.34741353	-95.65907636	-95.49964808	-95.69507827	-95.54104703
1.403	-95.47599470	-95.34576294	-95.48045855	-95.34787068	-95.63790699	-95.49828106	-95.67436552	-95.54023509
1.503	-95.45368757	-95.34763992	-95.45911766	-95.35219292	-95.61685139	-95.50110100	-95.65384244	-95.54319582
1.603	-95.43444537	-95.35036231	-95.43907362	-95.35753513	-95.59677930	-95.50530035	-95.63428677	-95.54739003
1.703	-95.41626097	-95.35585077	-95.42092303	-95.36269257	-95.57823308	-95.50959915	-95.61623641	-95.55162041
1.803	-95.40024326	-95.36068433	-95.40494174	-95.36724560	-95.56150218	-95.51352810	-95.59997415	-95.55543318
1.903	-95.38645945	-95.36476086	-95.39119571	-95.37109426	-95.54671909	-95.51694604	-95.58560996	-95.55869832
2.003	-95.37485261	-95.36811188	-95.37961766	-95.37426388	-95.53391133	-95.51982655	-95.57313935	-95.56138867
2.103	-95.37081820	-95.36525072	-95.37682727	-95.37005638	-95.52588668	-95.52476160	-95.56717719	-95.56113705
2.203	-95.37297501	-95.35747678	-95.37887177	-95.36230862	-95.52668939	-95.51687605	-95.56887670	-95.55225927
2.303	-95.37467352	-95.35128863	-95.38048398	-95.35614164	-95.52822670	-95.50955983	-95.57015698	-95.54489932
2.403	-95.37599416	-95.34644336	-95.38174288	-95.35131258	-95.52943972	-95.50374623	-95.57113412	-95.53924980
2.503	-95.37700716	-95.34270613	-95.38271760	-95.34758540	-95.53038944	-95.49923109	-95.57185093	-95.53441363
2.603	-95.37779666	-95.33985196	-95.38346728	-95.34474395	-95.53112695	-95.49577467	-95.57237341	-95.53088421
2.703	-95.37840057	-95.33770834	-95.38404147	-95.34259991	-95.53170556	-95.49318252	-95.57275165	-95.52824315
2.803	-95.37886145	-95.33610870	-95.38448056	-95.34099568	-95.53159112	-95.49388441	-95.57303150	-95.52609608
2.903	-95.37921488	-95.33492486	-95.38481649	-95.33980339	-95.53251735	-95.48987718	-95.57323284	-95.52447599
3.003	-95.37948208	-95.33405360	-95.38507375	-95.33892168	-95.53280399	-95.48887507	-95.57337805	-95.52339401
3.103	-95.37967298	-95.33341646	-95.38527077	-95.33827186	-95.53303206	-95.48816744	-95.57349906	-95.52252668
3.203	-95.37982582	-95.33295072	-95.38542129	-95.33779369	-95.53321403	-95.48767161	-95.57357906	-95.52189788
3.303	-95.37994367	-95.33261030	-95.38553566	-95.33744175	-95.53336038	-95.48732723	-95.57364372	-95.52145567
3.403	-95.38002815	-95.33235335	-95.38562184	-95.33718232	-95.53347788	-95.48709212	-95.57370023	-95.52115039
3.503	-95.38009356	-95.33216814	-95.38568611	-95.33699052	-95.53357079	-95.48693635	-95.57374090	-95.52090105
3.603	-95.38014213	-95.33202488	-95.38573346	-95.33684825	-95.53364489	-95.48683316	-95.57376908	-95.52073214
4.603	-95.38024490	-95.33155861	-95.38584339	-95.33644781	-95.53384707	-95.48667606	-95.57380376	-95.52033946
5.603	-95.38019038	-95.33149312	-95.38583386	-95.33641585	-95.53384565	-95.48669024	-95.57379270	-95.52033772
7.603	-95.38016651	-95.33144689	-95.38582281	-95.33640508	-95.53383516	-95.48668596	-95.57378763	-95.52033884

## (3) staggered conformation

R <sub>N-H</sub> (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
0.616	-95.17633535	-94.97524908	-95.18280783	-94.98380007	-95.33867879	-95.13390867	-95.37807846	-95.17391290
0.716	-95.38598919	-95.18898794	-95.39262409	-95.19761416	-95.54743375	-95.34696928	-95.58661453	-95.38669659
0.816	-95.48543252	-95.29280387	-95.49227946	-95.30162737	-95.64698190	-95.45125625	-95.68596699	-95.49067004
0.916	-95.52510033	-95.33769721	-95.53213950	-95.34662454	-95.68699720	-95.49648782	-95.72579653	-95.53581066
1.016	-95.53201973	-95.35345432	-95.53947447	-95.36064847	-95.69661801	-95.50931609	-95.73689540	-95.54755035
1.116	-95.52247378	-95.35298443	-95.52945970	-95.36045045	-95.68882333	-95.51159156	-95.72924651	-95.54987556
1.216	-95.50451264	-95.34848907	-95.51055551	-95.35672757	-95.67287672	-95.50997156	-95.71343480	-95.54861838
1.316	-95.48252253	-95.34117761	-95.48949636	-95.35297185	-95.64807957	-95.50330345	-95.68510265	-95.54531682
1.416	-95.46020311	-95.34453009	-95.46646566	-95.35482799	-95.62597850	-95.50413130	-95.66335943	-95.54670420
1.516	-95.43853869	-95.35057755	-95.44421049	-95.35944299	-95.60460390	-95.50820439	-95.64252071	-95.55087023
1.616	-95.41845042	-95.35681086	-95.42385965	-95.36497728	-95.58440518	-95.51294615	-95.62283605	-95.55558277
1.716	-95.40050572	-95.36241431	-95.40578189	-95.37006872	-95.56587600	-95.51746958	-95.60481059	-95.56000538
1.816	-95.38512679	-95.36695737	-95.38979014	-95.37268916	-95.54921882	-95.52134428	-95.58870702	-95.56374113
1.916	-95.37433744	-95.36830568	-95.38045033	-95.37255550	-95.53466991	-95.52328101	-95.57578782	-95.56509272
2.016	-95.37547338	-95.35925067	-95.38160273	-95.36344830	-95.53054165	-95.51994741	-95.57228925	-95.56029029
2.116	-95.37839135	-95.35009768	-95.38385862	-95.35466396	-95.53176335	-95.51071187	-95.57344163	-95.55104349
2.216	-95.38048121	-95.34293516	-95.38578484	-95.34749995	-95.53344154	-95.50236315	-95.57489128	-95.54272131
2.316	-95.38211573	-95.33727073	-95.38732778	-95.34184384	-95.53488448	-95.49556475	-95.57611435	-95.53581105
2.416	-95.38338576	-95.33287633	-95.38853596	-95.33746689	-95.53604442	-95.49021240	-95.57704082	-95.53039774
2.516	-95.38436060	-95.32954180	-95.38946900	-95.33413187	-95.53695580	-95.48610689	-95.57774514	-95.52606081
2.616	-95.38510177	-95.32703343	-95.39018229	-95.33162176	-95.53766810	-95.48301111	-95.57825915	-95.52275353
2.716	-95.38565173	-95.32517315	-95.39072354	-95.32975061	-95.53822666	-95.48072663	-95.57863975	-95.52029946
2.816	-95.38604407	-95.32380198	-95.39113212	-95.32836600	-95.53866539	-95.47906880	-95.57890442	-95.51834282
2.916	-95.38636708	-95.32279124	-95.39143943	-95.32734697	-95.53901096	-95.47787820	-95.57912325	-95.51700955
3.016	-95.38665682	-95.32205649	-95.39166983	-95.32659966	-95.53928630	-95.47704016	-95.57928073	-95.51588840
3.116	-95.38685817	-95.32151982	-95.39184184	-95.32605265	-95.53950405	-95.47645501	-95.57939574	-95.51522687
3.216	-95.38697630	-95.32112723	-95.39196944	-95.32565228	-95.53967505	-95.47605357	-95.57948123	-95.51466005
3.316	-95.38706121	-95.32083801	-95.39206327	-95.32535879	-95.53981008	-95.47577759	-95.57954655	-95.51424918
3.416	-95.38712610	-95.32062277	-95.39213145	-95.32514301	-95.53991621	-95.47559358	-95.57959499	-95.51397561
3.516	-95.38715350	-95.32044944	-95.39218033	-95.32498375	-95.54000029	-95.47547322	-95.57963149	-95.51378401
3.616	-95.38718855	-95.32032672	-95.39221482	-95.32486571	-95.54006772	-95.47539391	-95.57966045	-95.51362816
4.116	-95.38724316	-95.32002753	-95.39227753	-95.32459828	-95.54021826	-95.47528046	-95.57971276	-95.51335108
5.116	-95.38722002	-95.31989859	-95.39227413	-95.32451097	-95.54023422	-95.47527344	-95.57968723	-95.51329492
7.116	-95.38715697	-95.31983874	-95.39225728	-95.32449164	-95.54024355	-95.47529437	-95.57969510	-95.51330928

## (4) H6-C4-N1-H3 dihedral angle equaling 95°

$R_{N-H}$ (Å)	MS-CASPT2		XMS-CASPT2		SI- $\rho$ PBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
0.616	-95.17688607	-94.97687925	-95.18312897	-94.98369492	-95.33890661	-95.13376750	-95.37807670	-95.16396513
0.716	-95.38652124	-95.19056021	-95.39294446	-95.19750643	-95.54762590	-95.34671222	-95.58661654	-95.37677174
0.816	-95.48593507	-95.29434625	-95.49259731	-95.30150964	-95.64701973	-95.45053135	-95.68604822	-95.49019432
0.916	-95.52551365	-95.33899961	-95.53246135	-95.34649319	-95.68793362	-95.49294661	-95.72624358	-95.52692307
1.016	-95.53248982	-95.35251597	-95.53980943	-95.36049659	-95.69680807	-95.50931032	-95.73061900	-95.54648522
1.116	-95.52199741	-95.35156680	-95.52981716	-95.36026608	-95.68900341	-95.51157419	-95.72692437	-95.54510653
1.216	-95.50248831	-95.34714346	-95.51094127	-95.35649116	-95.67300261	-95.50996897	-95.71107798	-95.54422257
1.316	-95.48319779	-95.34535434	-95.48966786	-95.35235253	-95.65001158	-95.50537096	-95.69050195	-95.54455270
1.416	-95.46063841	-95.34316381	-95.46529190	-95.35074266	-95.62645093	-95.50373597	-95.66031038	-95.54207050
1.516	-95.43899027	-95.34911790	-95.44365257	-95.35638860	-95.60507839	-95.50759735	-95.63934256	-95.54630185
1.616	-95.41901833	-95.35591758	-95.42364902	-95.36219517	-95.58495474	-95.51217131	-95.61970512	-95.55104990
1.716	-95.40123589	-95.36128978	-95.40591858	-95.36728976	-95.56657346	-95.51649208	-95.60186689	-95.55539326
1.816	-95.38622723	-95.36538564	-95.39115196	-95.37098607	-95.55025876	-95.51995159	-95.58628326	-95.55874449
1.916	-95.37619461	-95.36595769	-95.38228388	-95.37035591	-95.53657412	-95.52116695	-95.57435852	-95.55935889
2.016	-95.37597530	-95.35837672	-95.38206489	-95.36260541	-95.53099579	-95.51834541	-95.56963945	-95.55496660
2.116	-95.37839711	-95.34971316	-95.38385560	-95.35427857	-95.53168892	-95.50997195	-95.57010566	-95.54660937
2.216	-95.38028790	-95.34273436	-95.38559105	-95.34730219	-95.53317833	-95.50195045	-95.57133662	-95.53861827
2.316	-95.38181713	-95.33715875	-95.38703466	-95.34174496	-95.53452899	-95.49531219	-95.57244934	-95.53189008
2.416	-95.38302643	-95.33282048	-95.38818434	-95.33742726	-95.53563953	-95.49004993	-95.57332087	-95.52662968
2.516	-95.38396332	-95.32952641	-95.38908067	-95.33413027	-95.53652282	-95.48600605	-95.57398886	-95.52229541
2.616	-95.38467973	-95.32705401	-95.38977013	-95.33164538	-95.53721794	-95.48295151	-95.57447405	-95.51907655
2.716	-95.38521380	-95.32520447	-95.39029557	-95.32979126	-95.53776562	-95.48069361	-95.57483793	-95.51664413
2.816	-95.38558908	-95.32384643	-95.39069356	-95.32841827	-95.53819861	-95.47905541	-95.57508616	-95.51468891
2.916	-95.38590637	-95.32285025	-95.39099374	-95.32740722	-95.53854195	-95.47787671	-95.57529346	-95.51339305
3.016	-95.38619617	-95.32212106	-95.39121923	-95.32666549	-95.53881593	-95.47704593	-95.57544319	-95.51231055
3.116	-95.38637516	-95.32158839	-95.39138853	-95.32612189	-95.53903369	-95.47646743	-95.57555352	-95.51162526
3.216	-95.38649955	-95.32119822	-95.39151482	-95.32572347	-95.53920584	-95.47607074	-95.57563485	-95.51108048
3.316	-95.38658571	-95.32091063	-95.39160707	-95.32543194	-95.53934321	-95.47579857	-95.57569593	-95.51066979
3.416	-95.38665218	-95.32069643	-95.39167438	-95.32521738	-95.53945163	-95.47561726	-95.57574323	-95.51040233
3.516	-95.38670104	-95.32052483	-95.39172285	-95.32505882	-95.53953733	-95.47549866	-95.57577762	-95.51021201
3.616	-95.38673283	-95.32040238	-95.39175715	-95.32494121	-95.53960578	-95.47542344	-95.57580602	-95.51005713
4.116	-95.38678295	-95.32010274	-95.39181982	-95.32467450	-95.53975880	-95.47531470	-95.57585323	-95.50978688
5.116	-95.38675685	-95.31997470	-95.39181668	-95.32458725	-95.53977883	-95.47530892	-95.57582701	-95.50973272
7.116	-95.38669729	-95.31991394	-95.39179996	-95.32456772	-95.53979258	-95.47532765	-95.57583749	-95.50974995



## (5) H6-C4-N1-H3 dihedral angle equaling 100°

$R_{N-H}$ (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
0.616	-95.17862633	-94.97501014	-95.18293654	-94.98084683	-95.33998805	-95.13332063	-95.37550934	-95.16759637
0.716	-95.38837670	-95.18879264	-95.39278233	-95.19467154	-95.54576504	-95.34137618	-95.58416502	-95.38058982
0.816	-95.48794397	-95.29262766	-95.49249808	-95.29860173	-95.64549098	-95.44581036	-95.68716806	-95.48068934
0.916	-95.52773084	-95.33728212	-95.53246400	-95.34341940	-95.68612560	-95.49199954	-95.72410412	-95.53067264
1.016	-95.53441246	-95.35234944	-95.53994083	-95.35711920	-95.69611928	-95.50448468	-95.73237213	-95.54630780
1.116	-95.52508826	-95.35146165	-95.53012217	-95.35622075	-95.68865591	-95.50656782	-95.72334276	-95.54766005
1.216	-95.50728086	-95.34664095	-95.51118627	-95.34842381	-95.67281695	-95.50497480	-95.71273978	-95.54320353
1.316	-95.48577326	-95.34406651	-95.49217163	-95.35096639	-95.65251142	-95.50422083	-95.69232583	-95.54310957
1.416	-95.46347259	-95.34112446	-95.46822008	-95.34869630	-95.62609108	-95.49843727	-95.66300765	-95.54024957
1.516	-95.44229371	-95.34693823	-95.44702889	-95.35353445	-95.60484832	-95.50179949	-95.64219388	-95.54379480
1.616	-95.42291841	-95.35215530	-95.42767999	-95.35849694	-95.58507977	-95.50586869	-95.62298586	-95.54783231
1.716	-95.40609491	-95.35641687	-95.41098541	-95.36242605	-95.56727984	-95.50944623	-95.60584730	-95.55124747
1.816	-95.39267554	-95.35880566	-95.39788481	-95.36436012	-95.55202366	-95.51171352	-95.59145021	-95.55322748
1.916	-95.38405488	-95.35797860	-95.38974244	-95.36293017	-95.54044815	-95.51165384	-95.58092651	-95.55267886
2.016	-95.38089989	-95.35330508	-95.38672322	-95.35792104	-95.53454580	-95.50848708	-95.57566781	-95.54866417
2.116	-95.38089608	-95.34696716	-95.38647979	-95.35158004	-95.53251375	-95.50289376	-95.57358965	-95.54277299
2.216	-95.38172975	-95.34104162	-95.38712598	-95.34565206	-95.53241746	-95.49659799	-95.57334408	-95.53631346
2.316	-95.38265301	-95.33609126	-95.38794478	-95.34068430	-95.53291665	-95.49088937	-95.57360072	-95.53045728
2.416	-95.38293880	-95.33176619	-95.38870739	-95.33672323	-95.53353105	-95.48617109	-95.57402287	-95.52567475
2.516	-95.38361820	-95.32868785	-95.38935071	-95.33365310	-95.53410303	-95.48245609	-95.57436805	-95.52165905
2.616	-95.38472093	-95.32672661	-95.38986869	-95.33131777	-95.53459195	-95.47961557	-95.57464808	-95.51864821
2.716	-95.38457933	-95.32460201	-95.39027506	-95.32956484	-95.53499550	-95.47749787	-95.57487712	-95.51631219
2.816	-95.38548053	-95.32369380	-95.39058930	-95.32826152	-95.53464058	-95.47883797	-95.57504230	-95.51447344
2.916	-95.38573721	-95.32274251	-95.39082998	-95.32729923	-95.53560184	-95.47484093	-95.57517347	-95.51324285
3.016	-95.38595103	-95.32204843	-95.39101328	-95.32659183	-95.53582397	-95.47405651	-95.57526967	-95.51224279
3.116	-95.38612603	-95.32154053	-95.39115150	-95.32607369	-95.53600548	-95.47351207	-95.57534989	-95.51153415
3.216	-95.38625650	-95.32116712	-95.39125504	-95.32569413	-95.53615242	-95.47313722	-95.57541110	-95.51102715
3.316	-95.38633283	-95.32089244	-95.39133177	-95.32541570	-95.53627095	-95.47288312	-95.57544248	-95.51062618
3.416	-95.38638727	-95.32068807	-95.39138793	-95.32521075	-95.53636482	-95.47271237	-95.57547366	-95.51037892
3.516	-95.38641988	-95.32052447	-95.39142789	-95.32505980	-95.53643966	-95.47260347	-95.57550368	-95.51020148
3.616	-95.38644270	-95.32040754	-95.39145659	-95.32494731	-95.53650099	-95.47253576	-95.57552666	-95.51003919
4.116	-95.38646011	-95.32012030	-95.39150620	-95.32469353	-95.53664032	-95.47243558	-95.57555121	-95.50977371
5.116	-95.38643829	-95.31999916	-95.39149977	-95.32460981	-95.53665792	-95.47242954	-95.57551977	-95.50971884
7.116	-95.38637676	-95.31993532	-95.39148291	-95.32459032	-95.53667526	-95.47245397	-95.57553570	-95.50973957

## Absolute energies (in a.u.) for the PESs of N-H bond fission near LAC

### (1) N-H3 bond fission of eclipsed conformation

$R_{N-H}$ (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
1.922	-95.38248614	-95.36938026	-95.38723337	-95.37566736				
1.932	-95.38126553	-95.36973033	-95.38601705	-95.37599853				
1.942	-95.38006763	-95.37007388	-95.38482248	-95.37632313				
1.952	-95.37889137	-95.37041049	-95.38364950	-95.37664125				
1.962	-95.37773658	-95.37074022	-95.38249796	-95.37695294				
1.972	-95.37660311	-95.37106317	-95.38136768	-95.37725829				
1.982	-95.37549079	-95.37137925	-95.38025850	-95.37755736	-95.53496323	-95.52291839	-95.57413038	-95.56452015
1.992	-95.37439973	-95.37168839	-95.37917025	-95.37785023	-95.53374702	-95.52318821	-95.57294570	-95.56476972
2.002	-95.37333185	-95.37199140	-95.37813816	-95.37810158	-95.53255159	-95.52345306	-95.57178038	-95.56501389
2.012	-95.37229253	-95.37228646	-95.37841782	-95.37705570	-95.53137549	-95.52371333	-95.57063392	-95.56525313
2.022	-95.37257852	-95.37125056	-95.37869260	-95.37602910	-95.53021980	-95.52396833	-95.56950589	-95.56548748
2.032	-95.37286256	-95.37024059	-95.37896154	-95.37502265	-95.52908390	-95.52421819	-95.56839618	-95.56571666
2.042	-95.37314046	-95.36925035	-95.37922470	-95.37403616	-95.52796737	-95.52446289	-95.56730488	-95.56594050
2.052	-95.37341234	-95.36827879	-95.37948217	-95.37306942	-95.52686985	-95.52470274	-95.56623145	-95.56615960
2.062	-95.37367832	-95.36732808	-95.37973403	-95.37212221	-95.52579156	-95.52493776	-95.56637352	-95.56517624
2.072	-95.37393823	-95.36639711	-95.37998038	-95.37119434	-95.52516847	-95.52473224	-95.56658208	-95.56413957
2.082	-95.37419320	-95.36548524	-95.38022130	-95.37028556	-95.52539392	-95.52369236	-95.56678562	-95.56312080
2.092	-95.37444434	-95.36459279	-95.38045687	-95.36939567	-95.52561475	-95.52267192	-95.56698394	-95.56211990
2.102					-95.52583098	-95.52167077	-95.56717739	-95.56113686
2.112					-95.52604251	-95.52068888	-95.56736592	-95.56017183
2.122					-95.52624945	-95.51972567	-95.56754959	-95.55922498
2.132					-95.52645197	-95.51878124	-95.56772845	-95.55829679
2.142					-95.52665011	-95.51785562	-95.56790301	-95.55738670
2.152					-95.52684400	-95.51694823	-95.56807402	-95.55649383

## (2) N-H2 bond fission of eclipsed conformation

R <sub>N-H</sub> (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-rIPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
1.973	-95.37811027	-95.36717800	-95.38287122	-95.37338043				
1.983	-95.37700357	-95.36749595	-95.38176617	-95.37368113				
1.993	-95.37591571	-95.36780708	-95.38068172	-95.37397559				
2.003	-95.37485261	-95.36811188	-95.37961766	-95.37426388				
2.013	-95.37380058	-95.36841001	-95.37857381	-95.37454610				
2.023	-95.37277295	-95.36870185	-95.37754998	-95.37482233	-95.53158673	-95.52034034	-95.57087319	-95.56186218
2.033	-95.37176536	-95.36898742	-95.37654600	-95.37509266	-95.53045359	-95.52059034	-95.56976672	-95.56209130
2.043	-95.37077692	-95.36926679	-95.37556180	-95.37535703	-95.52933943	-95.52083459	-95.56867745	-95.56231518
2.053	-95.36980846	-95.36954004	-95.37561604	-95.37459666	-95.52824450	-95.52107477	-95.56760670	-95.56253440
2.063	-95.36980749	-95.36885838	-95.37586919	-95.37365099	-95.52716859	-95.52130927	-95.56655293	-95.56274756
2.073	-95.37006894	-95.36792826	-95.37611680	-95.37272434	-95.52611087	-95.52153916	-95.56551631	-95.56295706
2.083	-95.37032462	-95.36701708	-95.37635896	-95.37181650	-95.52507340	-95.52176468	-95.56449714	-95.56316076
2.093	-95.37057383	-95.36612462	-95.37659576	-95.37092725	-95.52405452	-95.52198467	-95.56349766	-95.56335677
2.103	-95.37081820	-95.36525072	-95.37682727	-95.37005638	-95.52305441	-95.52220035	-95.56355277	-95.56250988
2.113	-95.37105724	-95.36439505	-95.37705361	-95.36920368	-95.52241248	-95.52207203	-95.56374156	-95.56154258
2.123	-95.37129103	-95.36355743	-95.37727484	-95.36836890	-95.52261830	-95.52110936	-95.56392543	-95.56059246
2.133	-95.37151961	-95.36273776	-95.37749106	-95.36755184	-95.52282054	-95.52016454	-95.56410483	-95.55966180
2.143	-95.37174489	-95.36193566	-95.37770237	-95.36675225	-95.52301843	-95.51923881	-95.56427880	-95.55874990
2.153	-95.37197436	-95.36115242	-95.37790884	-95.36596990	-95.52321156	-95.51833108	-95.56444999	-95.55785601
2.163					-95.52340139	-95.51744049	-95.56461798	-95.55697900
2.173					-95.52358603	-95.51656774	-95.56478289	-95.55611883
2.183					-95.52376664	-95.51571263	-95.56494335	-95.55527395
2.193					-95.52394316	-95.51487432	-95.56510033	-95.55444348
2.203					-95.52411636	-95.51405221	-95.56525313	-95.55362640
2.213					-95.52428488	-95.51324755	-95.56540218	-95.55282166
2.223					-95.52444981	-95.51246048	-95.56554616	-95.55202960
2.233					-95.52461126	-95.51169049	-95.56568576	-95.55125020
2.243					-95.52476891	-95.51093687	-95.56582071	-95.55048436

## (3) staggered conformation

R <sub>N-H</sub> (Å)	MS-CASPT2		XMS-CASPT2		SI-tPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
1.836	-95.38218459	-95.36718135	-95.38292900	-95.36711510				
1.846	-95.38088666	-95.36749930	-95.38164420	-95.36743470				
1.856	-95.37963659	-95.36778663	-95.38041600	-95.36771260				
1.866	-95.37844303	-95.36803276	-95.37925600	-95.36793710				
1.876	-95.37730728	-95.36821857	-95.37818070	-95.36809160	-95.53738813	-95.51937804	-95.57803901	-95.56031275
1.886	-95.37627211	-95.36832947	-95.37721220	-95.36815400	-95.53622562	-95.51953620	-95.57699337	-95.56036482
1.896	-95.37534902	-95.36834018	-95.37637780	-95.36809720	-95.53513275	-95.51971862	-95.57594715	-95.56045047
1.906	-95.37457510	-95.36822369	-95.37570500	-95.36789340	-95.53409286	-95.51992090	-95.57489796	-95.56056567
1.916	-95.37396231	-95.36794809	-95.37521190	-95.36752470	-95.53309245	-95.52012491	-95.57385612	-95.56068605
1.926	-95.37352752	-95.36750656	-95.37489670	-95.36699260	-95.53212838	-95.52030225	-95.57284616	-95.56077627
1.936	-95.37326101	-95.36690996	-95.37473770	-95.36631900	-95.53121012	-95.52042044	-95.57190471	-95.56079966
1.946	-95.37313189	-95.36617983	-95.37470190	-95.36553660	-95.53035861	-95.52044967	-95.57106440	-95.56072073
1.956	-95.37312550	-95.36534106	-95.37475680	-95.36467820	-95.52960014	-95.52036390	-95.57035424	-95.56051487
1.966	-95.37323436	-95.36441305	-95.37487570	-95.36377010	-95.52896059	-95.52014248	-95.56979031	-95.56016664
1.976	-95.37345438	-95.36340266	-95.37503880	-95.36283210	-95.52845689	-95.51977488	-95.56937252	-95.55967599
1.986	-95.37375001	-95.36232819	-95.37523240	-95.36187800	-95.52809203	-95.51926590	-95.56908892	-95.55905679
1.996					-95.52785526	-95.51862965	-95.56891676	-95.55833097
2.006					-95.52772581	-95.51789074	-95.56883226	-95.55752363
2.016					-95.52768096	-95.51707390	-95.56881424	-95.55665736
2.026					-95.52769913	-95.51620287	-95.56884495	-95.55575236
2.036					-95.52776440	-95.51529541	-95.56891217	-95.55482326
2.046					-95.52786365	-95.51436544	-95.56900713	-95.55388136
2.056					-95.52798694	-95.51342323	-95.56912284	-95.55293504
2.066					-95.52812836	-95.51247635	-95.56925391	-95.55199037

## (4) H6-C4-N1-H3 dihedral angle equaling 95°

$R_{N-H}$ (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
1.836	-95.38348044	-95.36542479	-95.38870850	-95.37140473				
1.846	-95.38226985	-95.36565370	-95.38758026	-95.37154411				
1.856	-95.38111671	-95.36583876	-95.38652554	-95.37162571				
1.866	-95.38002816	-95.36597501	-95.38555443	-95.37163936				
1.876	-95.37901306	-95.36604900	-95.38467779	-95.37157416	-95.53875046	-95.51775632	-95.57943235	-95.55861592
1.886	-95.37808185	-95.36605250	-95.38390613	-95.37141956	-95.53749275	-95.51787203	-95.57828685	-95.55865281
1.896	-95.37724595	-95.36597418	-95.38324790	-95.37116705	-95.53629356	-95.51797816	-95.57717570	-95.55867896
1.906	-95.37651628	-95.36580265	-95.38270751	-95.37081216	-95.53515862	-95.51807321	-95.57610474	-95.55869001
1.916	-95.37590155	-95.36553383	-95.38228391	-95.37035588	-95.53409373	-95.51814942	-95.57508186	-95.55867885
1.926	-95.37540261	-95.36515452	-95.38197030	-95.36980493	-95.53310559	-95.51819537	-95.57411981	-95.55863318
1.936	-95.37502464	-95.36467450	-95.38175537	-95.36917057	-95.53219771	-95.51819608	-95.57323251	-95.55853872
1.946	-95.37476171	-95.36409334	-95.38162525	-95.36846657	-95.53137820	-95.51813628	-95.57243427	-95.55838048
1.956	-95.37462238	-95.36342331	-95.38156561	-95.36770719	-95.53065321	-95.51800057	-95.57173571	-95.55814590
1.966	-95.37456571	-95.36266659	-95.38156310	-95.36690568	-95.53002938	-95.51777642	-95.57114287	-95.55782521
1.976	-95.37460410	-95.36183991	-95.38160609	-95.36607359	-95.52950990	-95.51745671	-95.57065733	-95.55741412
1.986	-95.37473059	-95.36096855	-95.38168487	-95.36522051	-95.52909453	-95.51704054	-95.57027500	-95.55691448
1.996	-95.37491210	-95.36004905	-95.38179157	-95.36435422	-95.52877714	-95.51653149	-95.56998635	-95.55633285
2.006	-95.37514182	-95.35909770	-95.38191991	-95.36348090	-95.52854884	-95.51593900	-95.56977909	-95.55567951
2.016	-95.37539600	-95.35814307	-95.38206490	-95.36260530	-95.52839755	-95.51527483	-95.56963977	-95.55496608
2.026	-95.37566331	-95.35719299	-95.38222250	-95.36173160	-95.52831061	-95.51455234	-95.56955625	-95.55420465
2.036					-95.52827772	-95.51378372	-95.56951983	-95.55340592
2.046					-95.52828706	-95.51298091	-95.56952082	-95.55258049
2.056					-95.52833018	-95.51215269	-95.56955224	-95.55173658
2.066					-95.52839951	-95.51130754	-95.56960804	-95.55088208
2.076					-95.52848958	-95.51045220	-95.56968297	-95.55002287
2.086					-95.52859627	-95.50959195	-95.56977325	-95.54916338

## (5) H6-C4-N1-H3 dihedral angle equaling 100°

$R_{N-H}$ (Å)	MS-CASPT2		XMS-CASPT2		SI-IPBE		SI-ftPBE	
	E0	E1	E0	E1	E0	E1	E0	E1
1.836	-95.39030921	-95.35847158	-95.39581499	-95.36438859				
1.846	-95.38929559	-95.35849656	-95.39485939	-95.36434754				
1.856	-95.38833417	-95.35848467	-95.39395855	-95.36426761				
1.866	-95.38741389	-95.35843391	-95.39311358	-95.36414764	-95.54585052	-95.51179756	-95.58627504	-95.55281861
1.876	-95.38656374	-95.35834396	-95.39232534	-95.36398676	-95.54473396	-95.51178348	-95.58524878	-95.55274766
1.886	-95.38577030	-95.35821234	-95.39159429	-95.36378443	-95.54366609	-95.51174226	-95.58426631	-95.55264902
1.896	-95.38503457	-95.35803878	-95.39092048	-95.36354056	-95.54264842	-95.51167480	-95.58332835	-95.55252260
1.906	-95.38435821	-95.35782735	-95.39030348	-95.36325549	-95.54168258	-95.51157777	-95.58243555	-95.55236796
1.916	-95.38374267	-95.35756834	-95.38974248	-95.36293012	-95.54076877	-95.51145384	-95.58158893	-95.55218474
1.926	-95.38318676	-95.35726625	-95.38923582	-95.36256561	-95.53990901	-95.51129918	-95.58078805	-95.55197172
1.936	-95.38268567	-95.35692384	-95.38878190	-95.36216391	-95.53910237	-95.51111534	-95.58003343	-95.55172762
1.946	-95.38223726	-95.35654134	-95.38837837	-95.36172713	-95.53834978	-95.51089974	-95.57932446	-95.55145207
1.956	-95.38183752	-95.35612090	-95.38802262	-95.36125780	-95.53765153	-95.51065206	-95.57866248	-95.55114525
1.966	-95.38149312	-95.35566625	-95.38771179	-95.36075869	-95.53700686	-95.51037195	-95.57804687	-95.55080679
1.976	-95.38120278	-95.35517901	-95.38744283	-95.36023274	-95.53641469	-95.51005934	-95.57747881	-95.55043675
1.986	-95.38095783	-95.35466196	-95.38721261	-95.35968299	-95.53587403	-95.50971426	-95.57695757	-95.55003646
1.996	-95.38074875	-95.35411822	-95.38701798	-95.35911247	-95.53538344	-95.50933692	-95.57648264	-95.54960691
2.006	-95.38057991	-95.35356259	-95.38685583	-95.35852417	-95.53494000	-95.50892806	-95.57605329	-95.54914909
2.016	-95.38044717	-95.35297652	-95.38672318	-95.35792098	-95.53454250	-95.50849060	-95.57566790	-95.54866584
2.026	-95.38034807	-95.35237179	-95.38661717	-95.35730562	-95.53418830	-95.50802150	-95.57532325	-95.54815618
2.036	-95.38027785	-95.35175302	-95.38653510	-95.35668067	-95.53387466	-95.50752911	-95.57501671	-95.54762327
2.046	-95.38023223	-95.35112501	-95.38647447	-95.35604849	-95.53359875	-95.50700901	-95.57474414	-95.54706707
2.056	-95.38020703	-95.35048908	-95.38643298	-95.35541126	-95.53335899	-95.50646827	-95.57450445	-95.54649274
2.066	-95.38020142	-95.34984777	-95.38640850	-95.35477096	-95.53315151	-95.50590770	-95.57429294	-95.54590127
2.076	-95.38021213	-95.34920311	-95.38639910	-95.35412939	-95.53297425	-95.50532980	-95.57410779	-95.54529486
2.086	-95.38023762	-95.34855975	-95.38640304	-95.35348815	-95.53282407	-95.50473716	-95.57394644	-95.54467635
2.096	-95.38027589	-95.34791869	-95.38641872	-95.35284867	-95.53269877	-95.50413201	-95.57380726	-95.54404831
2.106	-95.38032494	-95.34728084	-95.38644473	-95.35221223	-95.53259577	-95.50351693	-95.57368843	-95.54341316
2.116					-95.53251306	-95.50289391	-95.57358912	-95.54277293
2.126					-95.53244872	-95.50226490	-95.57350850	-95.54212929
2.136					-95.53240010	-95.50163155	-95.57344573	-95.54148355

## Natural orbitals of SA-CASSCF calculations with equilibrium geometry (only active orbitals are shown)

### (1) eclipsed conformation

#### \* ORBITAL 1 7

9.55481545851503E-02 -2.15572136627055E-01 -2.28967218586476E-01 5.59669685726644E-02 -9.11534272276254E-04  
 -3.84445188844512E-04 1.12576902260415E-03 -9.74663359873427E-08 1.56790561449910E-06 3.70631763977641E-07  
 4.29372779483094E-01 2.42457526602965E-01 -3.64459853889286E-02 -1.00114559577660E-07 -9.48571104302540E-07  
 -2.02160994029975E-02 7.32968892032582E-04 4.88276260731508E-03 5.66656185795388E-02 4.67543105515929E-02  
 2.41261262249070E-02 -3.39728432708932E-03 2.65951377701836E-07 5.61033833399816E-03 5.62551562557934E-02  
 4.43099691782894E-02 2.55596855422946E-02 3.57932795045290E-03 2.69857862072923E-07 5.52629674333058E-03  
 5.68520814834723E-02 -1.19944609505252E-01 5.32952515337700E-03 -7.66864021484878E-02 -1.08157040130127E-02  
 -6.06615476362318E-03 -3.71944845556400E-03 -1.56623995857290E-05 -4.91500071100468E-06 2.91440485242595E-06  
 -3.60325270295304E-01 -9.70203129670936E-02 -3.43926684085835E-02 -1.28169690182813E-06 1.54263710429824E-06  
 -3.67152388965471E-02 -4.39337759465620E-04 3.34220692384300E-04 4.25959262307501E-02 3.74615039026584E-02  
 3.98013289626493E-03 -8.26868365069269E-04 1.23031416798564E-03 -3.68240442704115E-03 4.40117888899710E-02  
 4.10319011119433E-02 -3.93800988241914E-03 1.00251783012962E-03 -7.04548145768688E-07 -3.62387081315814E-03  
 4.25695967387177E-02 3.74387294603196E-02 3.97443811796087E-03 -8.26632755708346E-04 -1.22885868486675E-03  
 -3.68304609863649E-03

#### \* ORBITAL 1 8

1.18069860722597E-05 -3.91649538230648E-05 -1.86117446295831E-05 1.55780274778675E-05 -9.14036852441189E-08  
 6.09544020526067E-07 2.43940840592836E-06 -6.00128105402143E-01 -4.66720827773001E-01 -1.31264183500111E-01  
 -1.17559537536028E-05 -3.37334552003520E-06 -1.42216083881822E-05 1.17985315348957E-03 5.66866092181322E-05  
 1.26496956428026E-06 1.80213764341074E-08 3.34876888898622E-06 7.94666996779449E-06 -3.40074665986128E-06  
 2.17557463048116E-06 -7.93711480978145E-07 -1.85734670920755E-02 -8.56179244770280E-07 7.77364020456519E-06  
 -1.01854698125097E-06 4.64080798787653E-06 7.47842455965309E-07 -1.88323130197707E-02 -8.99916394958748E-07  
 -7.49174879828376E-07 1.66508014917732E-06 1.70641307733719E-06 -1.58802216494838E-05 -3.60525703502979E-07  
 -1.38367812071162E-06 -4.83010776038923E-06 1.03821694841433E-01 7.42420739019572E-02 3.63966799139542E-02  
 1.37040481577362E-06 -5.12791063269798E-06 -6.14511907977196E-06 1.09309888293599E-02 -3.32548385284702E-02  
 -1.04892746773502E-06 -4.68453759240540E-08 9.77450982664863E-06 -1.05146561199124E-01 -1.49295002039088E-01  
 -9.48943717945166E-03 2.10664705906309E-03 -1.89520057693280E-03 -4.55984586718798E-04 3.63404082639786E-05  
 4.47965974048959E-05 -3.55548704362414E-06 1.57295473875939E-06 1.98938895582040E-03 3.90537692374815E-08  
 1.05112012219350E-01 1.49236880485105E-01 9.49297526198977E-03 -2.10828362678281E-03 -1.89308980909284E-03  
 4.55625203089270E-04

#### \* ORBITAL 1 9

9.82356001846593E-05 -5.63287274457070E-04 -7.20757478679694E-05 9.79194176498762E-06 -5.81686869305776E-06  
 7.15121341818313E-06 6.96675505002170E-06 8.55560360683011E-01 -5.66411335525909E-01 -5.83414474554775E-01  
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 -2.34959059035082E-04 5.44847445079532E-08 -9.14337925848101E-05 -1.06143840316645E-04 -2.74790832771591E-04  
 7.07402004291846E-05 -1.82415701239280E-06 -1.77853397069055E-02 1.31942808385273E-05 -1.02416187170050E-04  
 -2.57583759520885E-04 6.84127240410402E-05 2.25250750957656E-06 -1.86621679349035E-02 1.25913769188804E-05  
 -1.68093417479946E-04 5.75902858024100E-04 4.65858653641385E-04 -1.16554902099652E-04 2.88277340217935E-05  
 -7.50490803334649E-06 -4.38126179388060E-06 -1.12466818716441E-01 -1.32792670063972E-01 2.34784692536648E-01  
 1.08217150965888E-03 4.44156556876984E-04 2.27200876528556E-05 8.90710173639262E-03 -7.21691076723097E-02  
 9.82101469102196E-05 6.26897317914106E-06 -6.21028721018565E-06 -8.75500061356073E-02 -3.19853487088098E-01  
 7.16208432674002E-02 4.82010480789593E-04 9.52994127601759E-04 1.07230677498025E-02 2.83956112960141E-06  
 -1.83749351352586E-06 1.00846885448696E-05 4.26622325911939E-06 1.74730460690355E-03 9.76432318141878E-06  
 8.74285196611145E-02 3.19574347049566E-01 -7.15228604847774E-02 -4.78710657699679E-04 9.55470314609926E-04  
 -1.06813420728430E-02

#### \* ORBITAL 1 10

2.50213331426640E-04 -5.88870408059672E-04 -6.11769524962638E-04 1.00652589542874E-04 -2.62238708161195E-07  
 1.01513808591635E-06 1.48303132585123E-06 -1.49780375625341E-01 -7.44538055949973E-02 -2.99899171161392E-03  
 -4.01844087698008E-04 -1.92127867326865E-04 -1.26045990675986E-05 -1.32922381170625E-03 1.24125808500901E-02  
 4.79663460342482E-06 1.41644039969335E-07 -2.19567543487186E-05 -2.99492991087831E-04 -6.85554785090252E-05  
 -1.81166168759947E-05 3.19955492842914E-05 -4.01323012671879E-03 1.18794072020780E-05 -2.99763153638134E-04  
 -6.62577430887228E-05 -1.81066601216121E-05 -3.18448419681621E-05 -4.31263473320112E-03 1.18358006506530E-05  
 -3.84010659179830E-05 8.88296979357027E-05 1.21581082026402E-04 -6.81092105771634E-05 -4.01139539325363E-06  
 -4.52228612791591E-06 -2.12838777317580E-06 -4.33353292725904E-01 -2.13286211888140E-01 1.06804413254203E-02

2.39505124319850E-05 3.50018768793855E-05 -1.39213132662513E-05 -2.20811977897360E-02 1.04803552607817E-02  
-5.29533080849701E-06 1.77549663148956E-07 -1.92504122054233E-05 2.24655530555013E-01 1.68819344913171E-01  
2.77404402957439E-02 -6.87396029297253E-03 6.31155943446853E-03 5.95642458723732E-03 -5.16653568570718E-05  
-6.22842497834464E-05 -2.62042971977079E-06 -3.50712047999069E-06 -6.78947020573713E-03 -5.83818592367717E-07  
-2.24542809931495E-01 -1.68766759219436E-01 -2.77133067919515E-02 6.87792227084634E-03 6.30089835858046E-03  
-5.95174974598638E-03

\* ORBITAL 1 11

8.70288433809271E-02 -5.71143836204871E-01 -8.35803083932215E-03 -8.63746595727339E-03 -3.59824332382553E-03  
3.07446251909810E-03 3.84726790081557E-03 -1.42376531696594E-03 9.64097943195651E-04 9.65818569271137E-04  
7.93371781095499E-01 -5.21412272161878E-03 2.47733297690106E-02 2.87990255870923E-07 1.25844372963163E-04  
-7.26971271236172E-02 2.44813010547474E-04 4.71427134046297E-02 3.37417103636617E-03 -4.45097440923715E-02  
-6.54927760187786E-02 1.01304420696008E-03 3.31280511882836E-05 8.28793265919311E-03 5.37365508488086E-03  
-3.66796858231475E-02 -6.51736303684358E-02 -8.18069792651366E-04 3.45756311517879E-05 7.84980452196849E-03  
-1.02081397390383E-01 3.28654063482053E-01 3.15055463922876E-01 1.63201898090504E-01 1.66787272342168E-02  
-3.27088006418067E-03 -7.31371327446370E-03 1.47978761855874E-04 2.13238371746284E-04 -3.78831372770733E-04  
6.39231461097952E-01 2.68015852114565E-01 8.30423230110666E-03 -1.58370126600049E-05 1.01384077521926E-04  
5.96642734269202E-02 3.20554578220991E-03 -7.29980284658140E-03 -2.74855710375902E-02 -5.35909206444786E-02  
-2.93338393827131E-02 3.97625406354940E-04 -4.22917744182477E-04 1.00840422456068E-02 -2.24178113946073E-02  
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## (2) staggered conformation

## \* ORBITAL 1 7

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## \* ORBITAL 1 8

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## \* ORBITAL 1 9

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## \* ORBITAL 1 10

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## \* ORBITAL 1 7

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## \* ORBITAL 1 8

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## \* ORBITAL 1 9

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## \* ORBITAL 1 10

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## (4) H6-C4-N1-H3 dihedral angle equaling 100°

## \* ORBITAL 1 7

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## \* ORBITAL 1 8

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## \* ORBITAL 1 10

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-1.31116806155701E-03

## Natural orbitals of SA-CASSCF calculations near LAC (only active orbitals are shown)

### (1) eclipsed conformation with N-H3 bond fission

#### \* ORBITAL 1 7

1.16170440631055E-01 -2.59447387804259E-01 -2.76789783903110E-01 6.68864370059539E-02 1.25478276035925E-01  
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## (2) eclipsed conformation with N-H3 bond fission

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## (3) staggered conformation

## \* ORBITAL 1 7

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## \* ORBITAL 1 8

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## \* ORBITAL 1 10

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## (4) H6-C4-N1-H3 dihedral angle equaling 95°

## \* ORBITAL 1 7

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## \* ORBITAL 1 8

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## \* ORBITAL 1 9

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## (5) H6-C4-N1-H3 dihedral angle equaling 95°

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