

# **N Lone-pair $\cdots\pi$ Interaction: A Rotational Study of Chlorotrifluoroethylene $\cdots$ Ammonia**

## **Electronic Supplementary Information**

### **Content:**

- 1) Table of transition frequencies.
- 2) MP2/aug-cc-pVDZ geometry of the observed conformer.
- 3) Tables of the changes of the quadrupole coupling constants as functions of the two angles.

**1) Table 1S:** Experimental transition frequencies ( $\nu$ , MHz) and observed minus calculated values ( $\Delta\nu$ , kHz) of the four isotopologues

$J'(K'_aK'_c)-J''(K''_aK''_c)$	$F_1'+1/2, F'$ $F_1''+1/2, F''$		$C_2F_3^{35}Cl-^{14}NH_3$		$C_2F_3^{37}Cl-^{14}NH_3$		$C_2F_3^{35}Cl-^{14}ND_3$		$F_1'+1/2, F_1''+1/2,$		$C_2F_3^{35}Cl-^{15}NH_3$	
			$\nu$ /MHz	$\Delta\nu$ /kHz	$\nu$ /MHz	$\Delta\nu$ /kHz	$\nu$ /MHz	$\Delta\nu$ /kHz			$\nu$ /MHz	$\Delta\nu$ /kHz
$3_{0,3}-2_{0,2}$	5 6	4 5	7581.6504	0.3	7445.2468	2.1	7091.0957	2.3	5	4	7452.1613	1.6
	5 5	4 4	7581.6262	-2.1	7445.2221	-0.8	7091.0382	-2.7	4	3	7451.2625	0.3
	5 4	4 3	7581.6504	4.6	7445.2468	6.6	7091.0773	-0.9	3	2	7450.2652	3.0
	4 5	3 4	7580.7670	-1.1	7444.5819	-2.3	7090.1832	0.5	2	1	7451.2354	-1.1
	4 4	3 3	7580.7187	2.7	7444.5362	4.0	7090.0524	-6.5				
	4 3	3 2	7580.7802	2.2	7444.5939	0.0	7090.2097	3.0				
	3 4	2 3	7579.6441	-4.0	7443.6002	-3.6	7089.5407	-1.6				
	3 3	2 2	7579.5722	-0.8	7443.5331	4.6	7089.3690	4.1				
	3 2	2 1	7579.6793	-0.5	7443.6312	-4.4	7089.6221	4.2				
	2 3	1 2	7580.6156	2.2	7444.3161	-3.2	7090.5494	-0.2				
	2 2	1 1	7580.5192	-0.5	7444.2340	8.1						
$3_{1,3}-2_{1,2}$	5 6	4 5	7460.4778	2.2	7323.8277	0.5	6971.7076	1.8	5	4	7332.2024	0.3
	5 5	4 4	7460.4331	1.7	7323.7882	5.3	6971.6012	0.6	4	3	7330.7870	-1.6
	5 4	4 3	7460.4778	0.4	7323.8277	-1.4	6971.7076	0.3	3	2	7329.2340	0.0
	4 5	3 4	7458.9428	-2.6	7322.5302	-1.2	6970.6524	-1.6	2	1	7330.7105	5.7
	4 4	3 3	7458.8779	0.0	7322.4673	3.3	6970.4906	-2.9				
	4 3	3 2	7458.9583	-1.5	7322.5449	-1.1	6970.6888	3.2				
	3 4	2 3	7457.4019	0.2	7321.3547	-1.9	6969.0858	0.2				
	3 3	2 2	7457.3093	-4.8	7321.2698	0.8	6968.8702	-2.3				
	3 2	2 1	7457.4334	-5.8	7321.3940	-0.4						
	2 3	1 2	7458.9892	-3.4	7322.6915	3.7						
	2 2	1 1	7458.8779	-5.8	7322.5779	-1.4	6969.9923	1.0				
$3_{1,2}-2_{1,1}$	5 6	4 5	7752.1358	1.7	7615.3318	0.7	7259.5691	0.4	5	4	7620.8066	2.7
	5 5	4 4	7752.1038	3.1	7615.2984	0.7	7259.4929	-1.2	4	3	7619.3771	1.3
	5 4	4 3	7752.1455	4.1	7615.3318	-6.2	7259.5894	2.8	3	2	7620.9989	2.3
	4 5	3 4	7750.5821	1.3	7614.0142	-4.9	7258.4600	-0.3	2	1	7622.4718	-9.5
	4 4	3 3	7750.5597	0.0	7613.9943	-3.7	7258.4130	-2.8				
	4 3	3 2	7750.5821	-4.8	7614.0278	2.5	7258.4745	-0.4				
	3 4	2 3	7752.1827	-1.4	7615.2378	3.2	7260.1233	-0.9				
	3 3	2 2	7752.1610	-6.6	7615.2257	7.7	7260.0921	0.2				
	3 2	2 1	7752.1827	-8.6	7615.2378	-3.8	7260.1371	-2.6				
	2 3	1 2	7753.7917	2.7	7616.5832	-2.0	7261.2435	2.3				
	2 2	1 1	7753.7686	-2.8	7616.5692	2.0	7261.2067	3.4				
$3_{2,2}-2_{2,1}$	5 6	4 5	7611.9746	1.4								
	5 5	4 4	7611.8600	-2.0								
	5 4	4 3	7612.0101	2.1								
	4 5	3 4	7606.4666	0.8								
	4 4	3 3	7606.4241	2.4								
	4 3	3 2	7606.4882	5.6								
	3 4	2 3	7610.3971	-2.0								
	3 3	2 2	7610.3971	-3.6								
	3 2	2 1	7610.3971	-1.0								
	2 3	1 2	7615.7656	2.8								
2 2	1 1	7753.7686	-2.8									
$3_{2,1}-2_{2,0}$	5 6	4 5	7640.7866	2.2								
	5 5	4 4	7640.6845	1.6								
	5 4	4 3	7640.8198	2.7								
	4 5	3 4	7636.1808	0.2								
	4 4	3 3	7636.1465	1.7								
	4 3	3 2	7636.1993	3.8								
	3 4	2 3	7639.8397	-4.2								
	3 3	2 2	7639.8544	0.3								
	3 2	2 1	7639.8397	0.6								
	2 3	1 2	7644.3058	-0.6								
2 2	1 1	7644.3205	2.7									
$4_{0,4}-3_{0,3}$	6 7	5 6	10076.1194	-0.3	9894.6843	-2.4	9422.1509	-0.9	6	5	9903.8493	-1.3
	6 6	5 5	10076.0981	-2.1	9894.6713	4.0	9422.1026	-1.2	5	4	9902.7139	-0.4
	6 5	5 4	10076.1194	2.2	9894.6843	0.2	9422.1408	-3.9	4	3	9902.3494	0.3
	5 6	4 5	10074.9988	0.9	9893.8458	0.0	9420.9857	-1.6	3	2	9903.4910	-3.6
	5 5	4 4	10074.9685	3.8	9893.8113	-1.3	9420.9056	-1.6				
	5 4	4 3	10074.9988	-0.2	9893.8458	-1.0	9420.9857	-6.1				
	4 5	3 4	10074.5750	-0.5	9893.4616	-1.4	9420.7886	-3.7				
	4 4	3 3	10074.5363	3.0	9893.4185	-2.1	9420.6895	-1.1				
	4 3	3 2	10074.5750	-3.5	9893.4616	-4.4	9420.8063	4.2				





	67	56	12703.8875	0.0				
	66	55	12703.8411	0.7				
	65	54	12703.9033	5.8				
	56	45	12704.6840	-3.0				
	55	44	12704.6429	-1.4				
	54	43	12704.7010	1.9				
	45	34	12706.9471	-1.0				
	44	33	12706.9049	4.5				
	43	32	12706.9650	-2.8				
	78	67	12713.2955	-0.1				
	77	66	12713.2415	0.9				
	76	65	12713.3077	1.7				
	67	56	12711.1743	-3.2				
	66	55	12711.1312	-0.7				
	65	54	12711.1887	1.3				
	56	45	12711.9405	-1.0				
	55	44	12711.8992	-1.3				
	54	43	12711.9578	4.6				
	45	34	12714.0530	-1.8				
	44	33	12714.0083	0.0				
	43	32	12714.0789	4.9				
	89	78	14998.3458	-0.2				
	88	77	14998.3268	-1.8				
	87	76	14998.3458	1.1				
	78	67	14997.1364	-0.2				
	77	66	14997.1104	-4.1				
	76	65	14997.1364	0.7				
	67	56	14996.9950	-0.8				
	66	55	14996.9700	-1.2				
	65	54	14996.9950	0.7				
	56	45	14998.2096	5.9				
	55	44	14998.1828	1.4				
	54	43	14998.1911	-6.5				
	89	78	14877.0640	1.4				
	88	77	14877.0499	-0.8				
	87	76	14877.0640	4.1				
	78	67	14876.5717	-0.8				
	77	66	14876.5504	-3.9				
	76	65	14876.5717	1.3				
	67	56	14876.1361	-3.2				
	66	55	14876.1114	-6.8				
	65	54	14876.1361	0.0				
	56	45	14876.6324	3.6				
	55	44	14876.6069	-4.1				
	54	43	14876.6264	6.2				
	89	78	15442.7970	1.7				
	88	77	15442.7826	-1.6				
	87	76	15442.7970	0.1				
	78	67	15442.0357	-3.2				
	77	66	15442.0238	1.7				
	76	65	15442.0529	1.9				
	67	56	15442.2441	0.6				
	66	55	15442.2161	1.5				
	65	54	15442.2441	6.0				
	56	45	15442.9895	-1.2				
	55	44	15442.9755	-2.8				
	54	43	15442.9895	0.4				
	910	89	17434.6953	-0.9	17118.6565	-0.5		
	99	88	17434.6764	-4.5	17118.6360	-5.7		
	98	87	17434.6953	0.4	17118.6565	0.8		
	89	78	17433.6272	0.0	17117.8474	2.4		
	88	77	17433.6080	-0.6	17117.8230	-3.4		
	87	76	17433.6272	1.1	17117.8474	3.5		
	78	67	17433.4983	-1.3	17117.7326	0.3		
	77	66	17433.4753	-4.2	17117.7078	-4.4		
	76	65	17433.4983	0.4	17117.7326	2.0		
	67	56	17434.5648	-2.5	17118.5431	-0.3		
	66	55	17434.5408	-8.2	17118.5158	-9.3		
	65	54	17434.5648	1.8	17118.5431	4.0		

7 <sub>1,7</sub> -6 <sub>1,6</sub>	9 10	8 9	17336.9909	2.5								
	9 9	8 8	17336.9783	-0.5								
	9 8	8 7	17336.9909	4.9								
	8 9	7 8	17336.5462	-1.1								
	8 8	7 7	17336.5315	-2.1								
	8 7	7 6	17336.5462	0.9								
	7 8	6 7	17336.2282	0.7								
	7 7	6 6	17336.2075	-4.4								
	7 6	6 5	17336.2282	3.7								
	6 7	5 6	17336.6701	1.5								
	6 6	5 5	17336.6551	-0.3								
6 5	5 4	17336.6701	7.7									
7 <sub>1,6</sub> -6 <sub>1,5</sub>	9 10	8 9	17977.4510	4.2								
	9 9	8 8	17977.4327	-1.2								
	9 8	8 7	17977.4510	4.4								
	8 9	7 8	17977.5968	3.6								
	8 8	7 7	17977.5801	-1.1								
	8 7	7 6	17977.5801	1.9								
	7 8	6 7	17976.7549	-2.0								
	7 7	6 6	17976.7549	-3.6								
	7 6	6 5	17976.7549	-4.2								
	6 7	5 6	17977.6072	1.1								
	6 6	5 5	17977.6072	1.2								
3 <sub>2,2</sub> -2 <sub>1,1</sub>	5 6	4 5	10367.9379	1.6								
	5 5	4 4	10367.9379	7.9								
	5 4	4 3	10367.9379	0.5								
	4 5	3 4	10364.3350	4.8								
	4 4	3 3	10364.3350	5.7								
	4 3	3 2	10364.3350	5.2								
	3 4	2 3	10366.8922	-1.3								
	3 3	2 2	10366.8922	-0.6								
	3 2	2 1	10366.8922	-1.4								
	2 3	1 2	10370.5448	2.7								
	2 2	1 1	10370.5448	2.8								
3 <sub>2,1</sub> -2 <sub>1,2</sub>	5 6	4 5	10692.9214	1.6								
	5 5	4 4	10693.0519	-1.7								
	5 4	4 3	10692.8823	1.4								
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	3 4	2 3	10696.3197	-2.4								
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	3 2	2 1	10696.3197	-0.9								
	2 3	1 2	10695.8034	1.2								
	2 2	1 1	10695.8179	5.8								
3 <sub>3,1</sub> -2 <sub>2,0</sub>	5 6	4 5	12444.4254	2.0								
	5 5	4 4	12444.4649	2.3								
	5 4	4 3	12444.4254	2.1								
	4 5	3 4	12445.3328	1.3								
	4 4	3 3	12445.3945	-0.7								
	4 3	3 2	12445.3135	-5.4								
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	3 3	2 2	12446.4995	0.4								
	3 2	2 1	12446.3818	3.0								
	2 3	1 2	12445.4349	4.0								
	2 2	1 1	12445.5334	-0.3								
3 <sub>3,0</sub> -2 <sub>2,1</sub>	5 6	4 5	12451.9447	-0.1								
	5 5	4 4	12451.9890	-1.0								
	5 4	4 3	12451.9447	1.4								
	4 5	3 4	12453.4955	2.2								
	4 4	3 3	12453.5584	-1.3								
	4 3	3 2	12453.4771	-2.4								
	3 4	2 3	12454.1256	0.8								
	3 3	2 2	12454.2082	-1.0								
	3 2	2 1	12454.0939	4.1								
	2 3	1 2	12452.5062	0.3								
	2 2	1 1	12452.6099	0.5								
4 <sub>0,4</sub> -3 <sub>1,3</sub>	6 7	5 6	9367.7202	1.9	9174.9427	5.7	8734.5648	-1.6	6	5	9201.8954	-0.8
	6 6	5 5	9367.7202	-1.7	9174.9427	1.6	8734.5800	-0.2	5	4	9204.5638	0.4

	6 5	5 4	9367.7078	-2.7	9174.9247	-4.6	8734.5470	0.6	4	3	9202.4172	-1.6
	5 6	4 5	9370.2472	1.0	9176.7556	-3.0	8737.6018	1.9	3	2	9199.7676	-0.1
	5 5	4 4	9370.2290	1.6	9176.7380	-2.3	8737.5628	2.0				
	5 4	4 3	9370.2472	4.2	9176.7556	0.1	8737.5841	-4.9				
	4 5	3 4	9368.1171	-1.9	9175.1281	-4.6	8735.4431	0.4				
	4 4	3 3	9368.0892	0.6	9175.1050	2.6	8735.3754	0.3				
	4 3	3 2	9368.1171	0.1	9175.1281	-2.6	8735.4431	6.8				
	3 4	2 3	9365.6140	0.9	9173.3245	-1.9	8732.4562	-2.7				
	3 3	2 2	9365.5888	0.3	9173.3000	-1.7	8732.4043	2.2				
	3 2	2 1	9365.5888	5.4	9173.3000	2.9	8732.3939	7.2				
	6 7	5 6	10646.9918	2.1	10476.3686	5.1	9974.6369	-3.9	6	5	10469.6549	3.0
	6 6	5 5	10646.9446	2.4	10476.3105	-5.3	9974.5234	2.0	5	4	10465.0895	-0.8
	6 5	5 4	10646.9918	-0.2	10476.3686	2.7	9974.6515	4.9	4	3	10465.9292	-0.8
	5 6	4 5	10642.5374	-1.9	10473.0436	1.4	9969.8297	1.5	3	2	10470.4948	-1.2
	5 5	4 4	10642.4820	-2.5	10472.9834	-3.5	9969.6901	-0.8				
	5 4	4 3	10642.5450	-0.4	10473.0436	-4.5	9969.8433	-3.7				
	4 5	3 4	10643.2854	-1.0	10473.5318	1.1	9970.9148	-0.2				
	4 4	3 3	10643.2264	2.2	10473.4664	-1.6	9970.7644	4.2				
	4 3	3 2	10643.2979	2.6	10473.5318	-7.6	9970.9482	7.3				
	3 4	2 3	10647.7435	-0.5	10476.8544	-1.7	9975.7396	6.6				
	3 3	2 2	10647.6798	0.2	10476.7908	-0.7	9975.5724	-2.5				
	3 2	2 1	10647.7435	6.3	10476.8544	5.1	9975.7155	-3.0				
	6 7	5 6	12757.8439	0.4	12610.9455	0.9						
	6 6	5 5	12757.8174	0.6	12610.9163	-1.6						
	6 5	5 4	12757.8439	-3.2	12610.9455	-2.6						
	5 6	4 5	12753.4616	-1.5	12607.7991	3.9						
	5 5	4 4	12753.4369	-2.3	12607.7674	-3.3						
	5 4	4 3	12753.4616	-4.4	12607.7991	1.3						
	4 5	3 4	12755.2349	-1.5	12609.0392	4.4						
	4 4	3 3	12755.2101	-2.3	12609.0081	-2.6						
	4 3	3 2	12755.2349	-5.8	12609.0392	0.5						
	3 4	2 3	12759.6053	-2.1	12612.1835	4.5						
	3 3	2 2	12759.5795	-0.3	12612.1481	-3.4						
	3 2	2 1	12759.6141	1.5	12612.1835	-0.1						
	6 7	5 6	13445.1339	-3.5								
	6 6	5 5	13445.2773	2.5								
	6 5	5 4	13445.1029	-1.7								
	5 6	4 5	13446.0983	-1.6								
	5 5	4 4	13445.1895	-1.3								
	5 4	4 3	13445.0691	-5.1								
	4 5	3 4	13451.0036	-2.1								
	4 4	3 3	13451.0711	-1.7								
	4 3	3 2	13450.9768	0.2								
	3 4	2 3	13440.0983	0.9								
	3 3	2 2	13440.1850	0.6								
	3 2	2 1	13440.0252	4.9								
	6 7	5 6	16919.1648	1.1								
	6 6	5 5	16919.1890	-2.1								
	6 5	5 4	16919.1648	-0.7								
	5 6	4 5	16919.9068	-2.1								
	5 5	4 4	16919.9455	-4.9								
	5 4	4 3	16919.9068	-0.1								
	4 5	3 4	16920.4640	-1.5								
	4 4	3 3	16920.5162	-1.2								
	4 3	3 2	16920.4640	2.8								
	3 4	2 3	16919.6859	-0.6								
	3 3	2 2	16919.7373	0.0								
	3 2	2 1	16919.7039	0.8								
	6 7	5 6	16919.5203	3.4								
	6 6	5 5	16919.5447	0.0								
	6 5	5 4	16919.5203	1.5								
	5 6	4 5	16920.2835	-2.1								
	5 5	4 4	16920.3247	-1.7								
	5 4	4 3	16920.2835	0.8								
	4 5	3 4	16920.8284	-2.2								
	4 4	3 3	16920.8802	-2.3								
	4 3	3 2	16920.8284	2.2								
	3 4	2 3	16920.0351	5.3								
	7 8	6 7	11767.7386	0.4					7	6	11767.0097	1.7

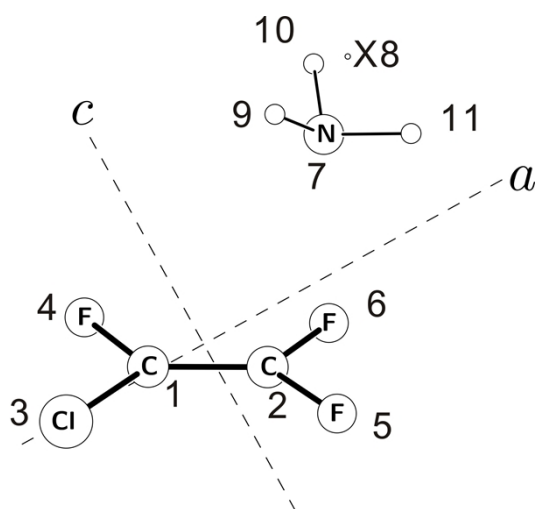
	77	66	11976.7522	4.9			6	5		
	76	65	11976.7280	-3.2			5	4	11767.7994	-3.7
	67	56	11978.8305	0.9			4	3	11765.6377	5.6
	66	55	11978.8229	-2.0						
	65	54	11978.8229	-1.3						
	56	45	11977.4542	2.2						
	55	44	11977.4385	-2.8						
	54	43	11977.4542	8.9						
	45	34	11975.3669	-0.5						
	44	33	11975.3669	3.6						
	43	32	11975.3399	-8.1						
	78	67	12981.8265	2.9			7	6	12763.2989	0.3
	77	66	12981.7814	1.6			6	5	12759.3080	-5.4
	76	65	12981.8265	0.9			5	4	12759.9154	2.0
	67	56	12977.9173	0.9			4	3	12763.8983	4.3
	66	55	12977.8684	-0.5						
	65	54	12977.9173	-2.5						
	56	45	12978.4640	0.8						
	55	44	12978.4102	-2.0						
	54	43	12978.4640	-2.8						
	45	34	12982.3678	0.5						
	44	33	12982.3168	0.2						
	43	32	12982.3678	3.1						
	56	45	8870.7002	-0.5	8746.0475	-3.8				
	55	44	8870.7920	0.6	8746.1416	-0.1				
	54	43	8870.6767	6.1	8746.0194	-1.6				
	45	34	8878.8657	2.7	8752.3881	-1.7				
	44	33	8878.8861	-1.1	8752.4160	1.0				
	43	32	8878.8489	-3.4	8752.3703	-9.3				
	34	23	8873.5106	-1.2	8748.1374	-1.8				
	33	22	8873.4905	-5.1	8748.1292	6.5				
	32	21	8873.5187	-1.2	8748.1446	-3.4				
	23	12	8865.4793	0.2	8741.8838	-3.8				
	22	11	8865.4563	-4.1	8741.8710	2.3				
	56	45	12451.6068	1.8						
	55	44	12451.6527	2.8						
	54	43	12451.6068	3.4						
	45	34	12453.1320	0.5						
	44	33	12453.1986	0.8						
	43	32	12453.1128	-5.0						
	34	23	12453.7744	1.0						
	33	22	12453.8565	-1.2						
	32	21	12453.7411	2.6						
	56	45	12444.7642	0.8						
	55	44	12444.8025	-0.2						
	54	43	12444.7642	1.1						
	45	34	12445.6961	2.8						
	44	33	12445.7559	-1.2						
	43	32	12445.6715	-9.1						
	34	23	12446.7642	-1.4						
	33	22	12446.8479	-2.6						
	32	21	12446.7343	4.2						
	23	12	12445.7559	-5.0						
	22	11	12445.8656	1.6						
	67	56	11615.2611	0.0	11444.7738	-1.5				
	66	55	11615.2563	1.5	11444.8739	5.0				
	65	54	11615.2381	1.0	11444.7496	-1.3				
	56	45	11623.4306	-1.3	11451.0576	-4.3				
	55	44	11623.4915	0.7	11451.1267	4.3				
	54	43	11623.4182	3.6	11451.0440	-1.5				
	45	34	11619.7365	-1.9	11448.1676	-4.1				
	44	33	11619.7785	0.6	11448.2186	7.1				
	43	32	11619.7224	3.5	11448.1531	-0.6				
	34	23	11611.6191	0.2	11441.9207	-1.2				
	33	22	11611.6712	-2.0	11441.9770	1.2				
	32	21	11611.5652	3.7	11441.8690	3.8				



2) MP2/aug-cc-pVDZ geometries of the observed conformer of the complex

bond lengths/Å		angles/°		dihedral angles/°	
C2C1	1.339				
Cl3C1	1.709	Cl3C1C2	124.5		
F4C1	1.700	F4C1C2	119.9	F4C1C2C3	-178.0
F5C2	1.326	F5C2C1	123.2	F5C2C1Cl3	-2.0
F6C2	1.328	F6C2C1	123.2	F6C2C1Cl3	179.5
N7C2	3.103 <sup>a</sup>	N7C2C1	101.5 <sup>a</sup>	N7C2C1Cl3	89.0 <sup>a</sup>
X8N7	1.000	X8N7C2	176.2	X8N7C2C1	154.8
H9N7	1.020	H9N7X8	67.4	H9N7X8C2	76.3
H10N7	1.020	H10N7X8	67.4	H10N7X8C2	120.0
H11N7	1.020	H11N7X8	67.4	H11N7X8C2	-120.0

<sup>a</sup>To reproduce the experimental rotational constants of the four isotopologues, the effective values are adjusted to 2.987 Å, 100.9° and 88.3°, respectively.





b. The MP2/aug-cc-pVDZ value of  $(\chi_{bb}-\chi_{cc})/4$  as a function of the orientation angles of  $\text{NH}_3$ .

		$\angle X8N7C2/^\circ \rightarrow$																	
		150	155	160	165	166	166.1	166.11	166.15	166.2	166.25	166.5	167	170	175	176.2	180.1	185	190
	130				-0.173									0.001					
	135			-0.317	-0.158								-0.090	0.013					
	137			-0.306	-0.151	-0.118						-0.101	-0.085	0.017					
	138			-0.301	-0.147	-0.115	-0.111				-0.107	-0.098	-0.082	0.019					
	138.5					-0.113	-0.110			-0.106	-0.105	-0.097							
	138.6					-0.113	-0.109	-0.109	-0.108	-0.106		-0.096							
	138.75					-0.112	-0.109			-0.106									
	139			-0.295	-0.143	-0.111	-0.108			-0.105	-0.103	-0.095	-0.079	0.021					
	139.5					-0.110				-0.101	-0.093								
$\angle X8N7C2C1/^\circ$	140	-0.535	-0.423	-0.290	-0.139	-0.108						-0.092	-0.076	0.024					
↓	145				-0.118								-0.058	0.036					
	150	-0.430	-0.338	-0.226	-0.095								-0.038	0.051	0.207				
	154.8															0.250			
	160	-0.318	-0.246	-0.152	-0.041									0.085	0.223		0.369	0.514	0.661
	170														0.242				
	180														0.265				
	190														0.290				
	200														0.318				
	210														0.347				
	220														0.376				