vicinity of $\alpha \approx 10°$, a ratio of $\alpha/\beta \approx 25$ is obtained, implying that the methyl twist, β, must be small. If the crude $V_H(R)$ function of Bartell[4] is inserted into eq 3, the equation is satisfied for $\alpha \approx 18°$.

If the next most important H···H interactions (set B with six H···H pairs) are introduced into the calculation, the angle α is reduced to 16° at equilibrium, at which point the hydrogens of set A are 2.6 Å apart (a distance 0.5 Å *longer* than at $\alpha = \beta = 0°$). The hydrogens of set B resist a larger twist than 16° and nestle down to a 2.6-Å distance, also, at equilibrium (a distance 1.1 Å *shorter* than at $\alpha = \beta = 0°$). The remaining hydrogens play a much smaller role. In essence, then, the cooperative displacements just described have the effect of rotating the $Si(CH_3)_3$ groups until the hydrogen bumps on any given group are centered on the hollows between the methyls of the adjacent groups.

According to the model, the equilibrium structure is governed more by the interhydrogen interactions than by the relatively weak bond torsional potential function, $V(\alpha)$. This is underscored by comparing the total effective torsional force constant for concerted rotations, $(\partial^2 V(\alpha)/\partial\alpha^2)_{16°} \approx 34 \times 10^{-12}$ ergs/radian², including H···H interactions, with the "intrinsic" contribution $\partial^2 V_t(\alpha)/\partial\alpha^2 \approx 18 V_\alpha^0(\alpha = 16°) = 1.3 \times 10^{-12}$ ergs/radian², excluding H···H interactions. Such a large value of $\partial^2 V(\alpha)/\partial\alpha^2$ implies that thermal amplitudes of torsional oscillations are small.[16] The model also yields a potential energy lowering of 6.9 kcal/mol upon deformation from T_d symmetry, a value much larger than thermal disordering energy. It stems almost entirely from the decrease in $V_H(R)$ for the closest 12 hydrogens. Although the methyl–methyl interactions appreciably reduce the torsional freedom, they do not restrict the internal rotation so severely that the proton nmr signal is split.

The above experimental and calculated results are rather rough, at best. Nevertheless, they both suggest that the trimethylsilyl groups twist in a correlated manner, by perhaps 14°, in order to relieve intermethyl repulsions.

Acknowledgments.—We wish to thank Professor H. Gilman of Iowa State University for donating the sample of $Si[Si(CH_3)_3]_4$ used in the present investigation. We are also pleased to acknowledge the generous allowance of computing time provided by the University of Michigan Computing Center.

(16) Hence it seems reasonable to interpret the results of Figure 3 in terms of a torsional deformation instead of "torsional shrinkage effects" of the sort discussed by L. S. Bartell and D. A. Kohl, *J. Chem. Phys.*, **39**, 3097 (1963).

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Electron Diffraction Determination of the Molecular Structure of Dimethylaminodichloroborane[1]

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Dimethylaminodichloroborane, $(CH_3)_2NBCl_2$, was found to have a planar C_2NBCl_2 skeleton. The B–N distance of 1.379 ± 0.006 Å is the shortest B–N bond so far measured and suggests that the boron and nitrogen are linked by a double bond. The Cl–B–N and C–N–B angles were 122.1 ± 0.3 and 123.2 ± 0.4°, respectively. Root-mean-square amplitudes of vibration were determined. The structural parameters are discussed in the light of results for related molecules.

Introduction

Dimethylaminodichloroborane and its bromide analog were first prepared by Brown and Osthoff.[3] The dichloride is a colorless liquid with a freezing point of −43° and a vapor pressure of about 20 Torr at 20°. Above its melting point the compound spontaneously dimerizes to form an insoluble solid with a low vapor pressure (about 1 Torr at 91°)[4] and was the first known example of self-association of an aminoborane.[5] The crystal structure of the cyclic dimer has been determined[6] and the monomer has been studied in the infrared and Raman regions by Whitmer.[7]

An electron diffraction study of monomeric $(CH_3)_2NBCl_2$ was undertaken to investigate the character of the B–N bond.

Experimental Section

Dimethylaminodichloroborane was prepared by the procedure of Brown and Osthoff[3] and Whitmer,[7] and the purity was checked by infrared spectroscopy. Except while being used, the sample container was stored at −78° to prevent formation of the unwanted dimer.

The diffraction apparatus and the procedure for obtaining the experimental leveled intensity from the 21- and 11-cm camera

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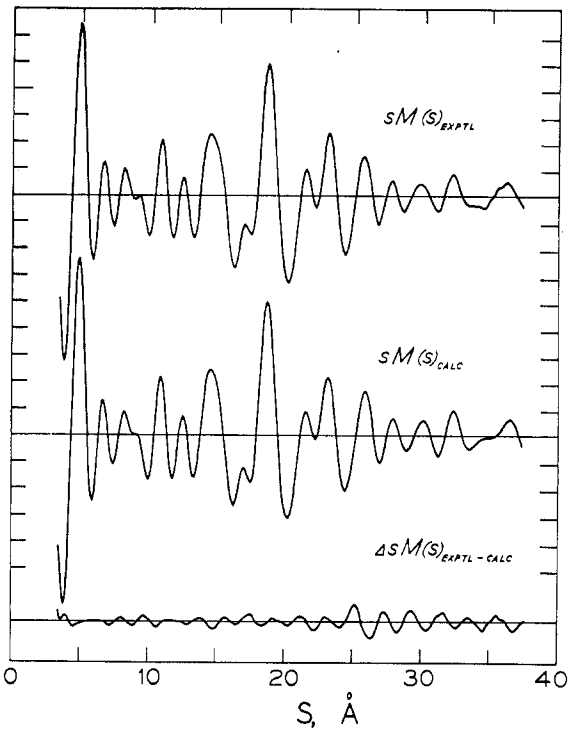

Figure 1.—Molecular intensity curves for $(CH_3)_2NBCl_2$: $\Delta sM(s) = sM(s)_{\text{exptl}} - sM(s)_{\text{calcd}}$.

range data (taken with an r^3 sector) have been described elsewhere.[8,9]

Analysis of Data

Leveled experimental intensities were converted to reduced molecular intensities and fitted by a theoretical reduced intensity function according to a least-squares procedure. Experimental intensity curves were interpolated to convenient values of the scattering variable, and the resultant smoothing was taken into account in error analysis. Comparisons between experimental and theoretical points were carried out using a weighting function

$$W(s) = C - \exp\{-\alpha[(10s/\pi) - 10]^2\} \quad (1)$$

with $\alpha = 0.005$ and $C = 1.2$ for merged[10] 21- and 11-cm camera range data.

Experimental radial distribution functions were calculated by the usual procedure[9,11-14] with theoretical data from $s = 0$ to 4.5 Å^{-1} blended into experimental data from $s = 3.5$ to 37 Å^{-1}. The value of b in the damping factor e^{-bs^2} was taken to be 0.00125.

Asymmetry constants a were estimated[15] to be 2.5, 1.9, 1.8, and 1.6 Å^{-1} for the H–C, B–N, C–N, and B–Cl bonded distances, respectively, and were taken to be 1.0 Å^{-1} for all nonbonded distances. No correction was made for the Bastiansen–Morino shrinkage effect.[16]

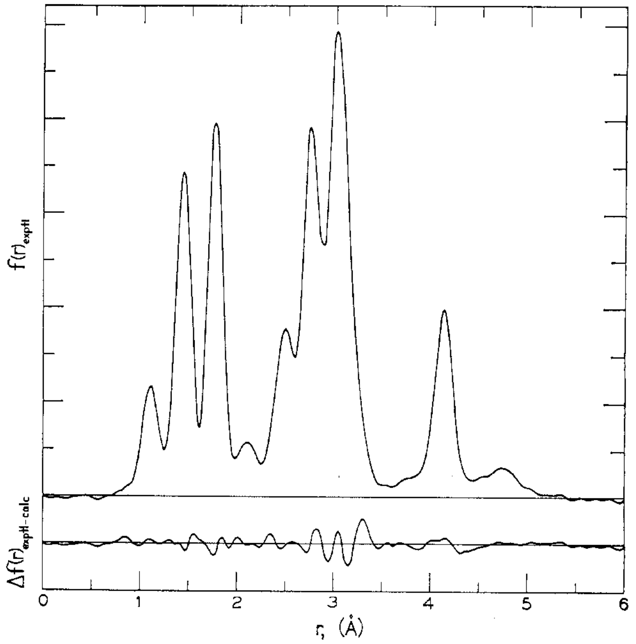

Figure 2.—Radial distribution function for $(CH_3)_2NBCl_2$: $\Delta f(r) = f(r)_{\text{exptl}} - f(r)_{\text{calcd}}$.

TABLE I

MOLECULAR PARAMETERS DETERMINED FOR $(CH_3)_2NBCl_2$[a]

Parameter	r_g	l_g
C–H	1.119 ± 0.006	0.079 ± 0.008
B–N	1.379 ± 0.006	0.035 ± 0.015
C–N	1.465 ± 0.004	0.038 ± 0.005
Cl–B	1.770 ± 0.004	0.048 ± 0.003
∠out-of-plane[b]	0.0 ± 3	
∠Cl–B–N	122.1 ± 0.3	
∠H–C–N	109.7 ± 1	
∠C–N–B	123.2 ± 0.4	
C···C	2.450	0.067 ± 0.010
B···C[c]	2.502	0.067 ± 0.010
Cl···Cl	3.000	0.065 ± 0.005
N···Cl	2.762	0.056 ± 0.008
$(C\cdots Cl)_{\text{short}}$[d]	3.134	0.066 ± 0.008
$(C\cdots Cl)_{\text{long}}$[d]	4.144	0.068 ± 0.010

[a] Distances in ångströms. Angles in degrees. Estimated uncertainties include the effects of known systematic errors and random errors inferred from least-squares analyses according to L. S. Bartell in "Physical Methods in Chemistry," A. Weissberger and B. W. Rossiter, Ed., 4th ed, Interscience, New York, N. Y., in press. The interaction between random and systematic errors as expressed in terms of eq 27 in this reference has not, however, been included. Hence, the standard errors listed are probably overoptimistic, particularly for the angles. See, for example, Figure 3. [b] Angle between the planes C–N–B and Cl_2-BN. [c] $l_g(B\cdots C)$ constrained to equal $l_g(C\cdots C)$. [d] $l_g(C\cdots Cl)_{\text{short}}$ and $l_g(C\cdots Cl)_{\text{long}}$ constrained to equal $l_g(N\cdots Cl)$ plus 0.010 and 0.012 Å, respectively.

Results

Figure 1 shows the molecular intensity curve[10] determined for $(CH_3)_2NBCl_2$. The mean index of resolution $R = M(s)_{\text{exptl}}/M(s)_{\text{calcd}}$ was 1.04 for both the 21- and 11-cm camera ranges. The experimental radial distribution function is illustrated in Figure 2. The

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TABLE II

ERROR MATRIX FOR $(CH_3)_2NBCl_2$[a]

	r(C–H)	r(B–N)	r(C–N)	r(Cl–B)	∠OOP[b]	∠Cl–B–N	∠H–C–N	∠C–N–B	l(C–H)	l(N–B)	l(N–C)	l(Cl–B)	l(C···C)[c]	l(Cl···Cl)	l(N···Cl)[d]	R
r(C–H)	31.1	5.8	13.5	−4.2	28.6	2.0	−40.3	−15.0	−12.9	−22.1	12.1	9.3	16.8	3.3	8.6	29.0
r(B–N)		28.5	−18.7	−14.8	−40.5	−17.2	4.2	7.5	−5.6	33.9	23.5	1.8	10.3	7.7	3.3	14.3
r(C–N)			20.5	10.6	50.6	12.0	−17.5	−16.7	−9.2	36.0	20.8	6.3	12.7	4.9	6.3	23.4
r(Cl–B)				11.4	6.2	10.5	20.0	−7.8	5.0	18.0	11.8	2.4	5.1	2.9	3.4	11.3
∠OOP[b]					300.4	22.2	−70.2	−60.8	−26.3	93.6	54.9	24.7	7.1	25.3	13.6	91.3
∠Cl–B–N						12.9	12.5	−9.0	3.4	21.5	14.5	2.3	5.2	3.4	6.4	3.2
∠H–C–N							110.7	18.9	19.4	37.2	24.2	16.0	34.8	17.7	12.2	44.6
∠C–N–B								26.3	9.3	29.9	16.4	8.7	16.2	14.0	5.4	33.0
l(C–H)									38.1	23.7	12.8	4.4	7.9	2.2	5.3	17.9
l(N–B)										81.9	43.5	12.6	23.0	7.8	13.3	47.7
l(N–C)											32.6	9.6	13.9	5.5	8.8	28.1
l(Cl–B)												16.7	6.9	2.2	5.8	20.8
l(C···C)[c]													40.3	12.4	6.2	19.4
l(Cl···Cl)														21.4	12.0	12.2
l(N···Cl)[d]															16.5	22.1
R																77.9

[a] Values are $\times 10^4$. Based on 109 intensity values interpolated from 278 data points. Units for distances and amplitudes are ångströms, and for angles they are radians; the index of resolution R is dimensionless. Matrix elements are given by $\sigma_{ij} = \text{sign}[B_{ij}^{-1}] \cdot \{|B_{ij}^{-1}|\mathbf{v}'\mathbf{w}\mathbf{v}/(n - m)\}^{1/2}$, where the notation corresponds to that of O. Bastiansen, L. Hedberg, and K. Hedberg, *J. Chem. Phys.*, **27,** 1311 (1957). See also K. Hedberg and M. Iwasaki, *Acta Crystallogr.*, **17,** 529 (1964). Since the elements are based on a diagonal (nonoptimum) weight matrix, they do not represent *bona fide* standard errors. [b] Angle between the planes C–N–B and the plane Cl_2BN. [c] l(B···C) was constrained to equal l(C···C). [d] $l(C\cdots Cl)_{short}$ and $l(C\cdots Cl)_{long}$ were constrained to equal l(N···Cl) plus 0.010 and 0.012 Å, respectively.

TABLE III

EXPERIMENTAL LEVELED INTENSITY AND BACKGROUND DATA FOR $(CH_3)_2NBCl_2$[a]

S	I_0(S)	B(S)	S	I_0(S)	B(S)	S	I_0(S)	B(S)	S	I_0(S)	B(S)	S	I_0(S)	B(S)	S	I_0(S)	B(S)
3.339	1.8920		9.497	2.1154	2.1202	15.581	2.1633	2.1654	8.406	5.0743		19.856	4.8104	4.8732	30.787	5.0622	5.0683
3.463	1.8196	2.0649	9.619	2.1067	2.1197	15.701	2.1567	2.1677	8.638	4.9880	5.0205	20.081	4.7949	4.8742	30.999	5.0669	5.0758
3.586	1.7629	2.0804	9.742	2.0978	2.1194	15.822	2.1496	2.1699	8.871	4.9788	5.0052	20.305	4.7942	4.8752	31.210	5.0741	5.0835
3.710	1.7402	2.0949	9.864	2.0904	2.1195	15.943	2.1446	2.1722	9.103	4.9859	4.9908	20.529	4.8087	4.8763	31.421	5.0852	5.0914
3.833	1.7503	2.1083	9.987	2.0860	2.1197	16.063	2.1416	2.1745	9.335	4.9819	4.9769	20.753	4.8326	4.8774	31.632	5.1009	5.0997
3.957	1.8049	2.1206	10.109	2.0864	2.1195	16.183	2.1404	2.1768	9.567	4.9500	4.9654	20.977	4.8633	4.8786	31.843	5.1171	5.1081
4.080	1.8984	2.1317	10.232	2.0923	2.1190	16.304	2.1425	2.1792	9.799	4.9022	4.9566	21.201	4.8892	4.8799	32.053	5.1285	5.1167
4.204	2.0076	2.1412	10.354	2.1064	2.1186	16.424	2.1475	2.1816	10.030	4.8748	4.9495	21.424	4.9033	4.8812	32.263	5.1400	5.1255
4.327	2.1360	2.1495	10.476	2.1230	2.1190	16.544	2.1543	2.1841	10.262	4.9048	4.9416	21.647	4.9027	4.8826	32.472	5.1437	5.1344
4.451	2.2433	2.1568	10.599	2.1389	2.1195	16.665	2.1613	2.1866	10.493	4.9477	4.9347	21.870	4.8884	4.8841	32.682	5.1484	5.1435
4.574	2.3637	2.1632	10.721	2.1518	2.1199	16.785	2.1692	2.1891	10.725	5.0107	4.9292	22.092	4.8780	4.8857	32.891	5.1520	5.1527
4.698	2.4320	2.1687	10.843	2.1603	2.1198	16.905	2.1752	2.1917	10.956	5.0218	4.9243	22.315	4.8783	4.8874	33.099	5.1585	5.1619
4.821	2.4802	2.1737	10.965	2.1609	2.1196	17.025	2.1803	2.1943	11.187	4.9807	4.9198	22.537	4.8949	4.8892	33.308	5.1656	5.1711
4.945	2.4754	2.1774	11.088	2.1537	2.1193	17.145	2.1830	2.1970	11.418	4.9118	4.9159	22.759	4.9186	4.8911	33.516	5.1745	5.1804
5.068	2.4347	2.1788	11.210	2.1401	2.1192	17.265	2.1839	2.1997	11.649	4.8572	4.9121	22.980	4.9419	4.8931	33.723	5.1845	5.1899
5.191	2.3681	2.1774	11.332	2.1236	2.1192	17.385	2.1841	2.2025	11.880	4.8491	4.9081	23.202	4.9456	4.8953	33.931	5.1935	5.1996
5.315	2.2928	2.1746	11.454	2.1095	2.1195	17.505	2.1857	2.2054	12.110	4.8798	4.9050	23.423	4.9362	4.8976	34.138	5.2030	5.2094
5.438	2.2087	2.1708	11.576	2.0970	2.1199	17.625	2.1893	2.2084	12.341	4.9166	4.9021	23.644	4.9111	4.9000	34.345	5.2133	5.2194
5.561	2.1460	2.1666	11.698	2.0906	2.1205	17.744	2.1953	2.2114	12.571	4.9279	4.8988	23.864	4.8872	4.9027	34.551	5.2226	5.2297
5.685	2.0942	2.1631	11.820	2.0908	2.1210	17.864	2.2045	2.2144	12.801	4.8990	4.8962	24.085	4.8691	4.9055	34.757	5.2352	5.2403
5.808	2.0697	2.1610	11.942	2.0958	2.1215	17.984	2.2162	2.2175	13.031	4.8585	4.8937	24.305	4.8626	4.9084	34.963	5.2497	5.2511
5.931	2.0680	2.1593	12.064	2.1062	2.1217	18.103	2.2315	2.2206	13.261	4.8336	4.8914	24.525	4.8693	4.9115	35.168	5.2620	5.2622
6.055	2.0831	2.1573	12.185	2.1162	2.1220	18.223	2.2477	2.2237	13.491	4.8404	4.8892	24.745	4.8844	4.9148	35.374	5.2764	5.2734
6.178	2.1108	2.1552	12.307	2.1260	2.1225	18.342	2.2625	2.2268	13.721	4.8726	4.8871	24.964	4.9082	4.9182	35.578	5.2901	5.2849
6.301	2.1417	2.1531	12.429	2.1327	2.1233	18.462	2.2752	2.2299	13.950	4.9154	4.8852	25.183	4.9294	4.9219	35.783	5.3019	5.2967
6.424	2.1681	2.1511	12.551	2.1353	2.1242	18.581	2.2842	2.2331	14.180	4.9493	4.8834	25.402	4.9477	4.9257	35.987	5.3154	5.3086
6.547	2.1864	2.1492	12.673	2.1326	2.1251	18.701	2.2890	2.2363	14.409	4.9609	4.8816	25.621	4.9575	4.9297	36.191	5.3291	5.3207
6.671	2.1897	2.1473	12.794	2.1266	2.1262	18.820	2.2892	2.2394	14.638	4.9574	4.8799	25.839	4.9616	4.9338	36.394	5.3399	5.3329
6.794	2.1809	2.1455	12.916	2.1185	2.1273	18.939	2.2858	2.2425	14.867	4.9472	4.8783	26.057	4.9579	4.9382	36.598	5.3492	5.3454
6.917	2.1652	2.1437	13.037	2.1106	2.1284	19.058	2.2798	2.2457	15.095	4.9299	4.8769	26.275	4.9482	4.9427	36.800	5.3598	5.3581
7.040	2.1427	2.1421	13.159	2.1056	2.1296	19.177	2.2717	2.2488	15.324	4.9078	4.8755	26.493	4.9362	4.9473	37.003	5.3699	5.3711
7.163	2.1208	2.1404	13.280	2.1029	2.1309	19.296	2.2623	2.2519	15.552	4.8753	4.8743	26.710	4.9313	4.9522	37.205	5.3801	5.3843
7.286	2.1064	2.1388	13.402	2.1065	2.1322	19.415	2.2539	2.2550	15.780	4.8375	4.8731	26.927	4.9386	4.9572	37.407	5.3916	5.3978
7.409	2.1007	2.1371	13.523	2.1121	2.1336	19.534	2.2460	2.2581	16.008	4.8007	4.8720	27.144	4.9532	4.9625	37.609	5.4089	
7.532	2.1043	2.1354	13.645	2.1218	2.1351	19.653	2.2400	2.2612	16.236	4.7852	4.8711	27.361	4.9687	4.9678	37.810	5.4275	
7.655	2.1134	2.1337	13.766	2.1338	2.1366	19.772	2.2360	2.2643	16.464	4.7922	4.8702	27.577	4.9820	4.9733	38.011	5.4456	
7.778	2.1268	2.1320	13.887	2.1466	2.1381	19.891	2.2341	2.2674	16.691	4.8144	4.8695	27.793	4.9891	4.9790	38.211	5.4579	
7.901	2.1402	2.1304	14.009	2.1580	2.1397	20.009	2.2346	2.2705	16.919	4.8328	4.8689	28.009	4.9904	4.9847	38.411	5.4715	
8.024	2.1494	2.1287	14.130	2.1675	2.1414	20.128	2.2374	2.2736	17.146	4.8348	4.8684	28.224	4.9888	4.9905	38.611	5.4876	
8.147	2.1530	2.1272	14.251	2.1744	2.1431	20.247	2.2438	2.2767	17.373	4.8259	4.8681	28.439	4.9860	4.9963	38.811	5.5049	
8.270	2.1515	2.1261	14.372	2.1792	2.1449	20.365	2.2508	2.2798	17.600	4.8274	4.8680	28.654	4.9920	5.0022	39.010	5.5252	
8.392	2.1446	2.1251	14.493	2.1814	2.1468	20.484	2.2585	2.2828	17.826	4.8456	4.8681	28.869	5.0012	5.0081			
8.515	2.1363	2.1242	14.614	2.1822	2.1487	20.602	2.2671	2.2859	18.053	4.8886	4.8683	29.083	5.0118	5.0142			
8.638	2.1270	2.1232	14.735	2.1822	2.1506	20.720	2.2756	2.2890	18.279	4.9459	4.8686	29.297	5.0227	5.0204			
8.761	2.1214	2.1225	14.856	2.1819	2.1526	20.839	2.2868	2.2920	18.505	4.9899	4.8690	29.511	5.0327	5.0268			
8.884	2.1179	2.1220	14.977	2.1813	2.1546	20.957	2.2991		18.731	5.0045	4.8695	29.724	5.0407	5.0333			
9.006	2.1183	2.1218	15.098	2.1799	2.1567	21.075	2.3120		18.956	4.9836	4.8701	29.938	5.0474	5.0399			
9.129	2.1195	2.1216	15.219	2.1789	2.1588	21.193	2.3235		19.181	4.9392	4.8707	30.150	5.0526	5.0467			
9.252	2.1210	2.1211	15.339	2.1757	2.1610	21.311	2.3338		19.407	4.8834	4.8715	30.363	5.0563	5.0537			
9.374	2.1196	2.1207	15.460	2.1705	2.1632	21.429	2.3426		19.632	4.8385	4.8723	30.575	5.0580	5.0609			

[a] The 21-cm camera data are given above, and the 11-cm data, below. The function M(s) is given by $[(I_0/B) - 1]$.

results of our investigation are summarized in Table I. Experimental data were analyzed by least-squares fittings of the intensity for each camera distance and for a blend of the two camera distances. A representation of the error matrix[17] computed during the final least-squares runs on the blended intensity may be seen in Table II. A listing of the experimental leveled intensity and the background used in data analysis as functions of the scattering variable for the 21- and 11-cm camera distances is given in Table III.

Discussion

The experimental radial distribution excludes the possibility of any appreciable twist about the BN bond and is completely consistent with a planar C_{2v} structure analogous to that of a substituted ethylene. Although it was unnecessary to use a nonplanar skeleton model to fit the diffraction data, an effort was made to establish to what extent models with slightly pyramidal nitrogen atoms are compatible with the data. The necessary calculations were performed for a series of C_s models with nonplanar skeletons in which both methyl groups

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[17] Y. Morino, K. Kuchitsu, and Y. Murata, *Acta Crystallogr.*, **18,** 549 (1965); Y. Murata and Y. Morino, *ibid.*, **20,** 605 (1966).

TABLE IV

COMPARISON OF STRUCTURES[a]

Molecule	B–N or N–N	B–X or N–O	R–N	∠RNB or ∠RNN	∠XBN or ∠ONN	C–H
$(CH_3)_2NBCl_2$[b]	1.379 ± 0.006	1.770 ± 0.004	1.465 ± 0.004	123.2 ± 0.4	122.1 ± 0.3	1.119 ± 0.006
$(SiH_3)_2NBF_2$[c]	1.485 ± 0.022	1.339 ± 0.009	1.747 ± 0.005	117.2 ± 1.3	119.0 ± 1.3	. . .
$(CH_3)_2NNO_2$[d]	1.382 ± 0.003	1.223 ± 0.002	1.460 ± 0.003	116.2 ± 0.3	114.8 ± 0.2	1.121 ± 0.005
BCl_3[e]	. . .	1.742 ± 0.004	. . .	. . .	. . .	. . .
$Cl_3B_3N_3H_3$[f]	1.41 ± 0.02	1.78 ± 0.03	. . .	. . .	. . .	. . .

[a] Distances in ångströms; angles in degrees. [b] This work. [c] See ref 18. [d] See ref 20. [e] S. Konaka, Y. Murata, K. Kuchitsu, and Y. Morino, *Bull. Chem. Soc. Jap.*, **39,** 1134 (1966). [f] K. P. Coffin and S. H. Bauer, *J. Phys. Chem.*, **59,** 193 (1955).

were displaced from the Cl_2BN plane. It is evident from Figure 3 and the error matrix that the answer based on electron diffraction data is indeterminate; distortions less than about 10° cannot be ruled out.

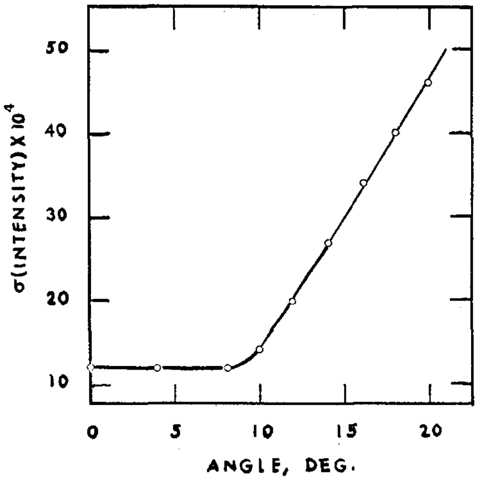
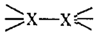
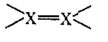
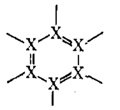


Figure 3.—Minima in standard deviation curve *vs.* angle between the planes C–N–B and the plane Cl_2BN (C_s symmetry model) for $(CH_3)_2NBCl_2$.

Several compounds related to $(CH_3)_2NBCl_2$ are compared in Table IV. The most striking feature is the very large (0.1 ± 0.02 Å) difference between the B–N bond lengths in $(CH_3)_2NBCl_2$ and $(SiH_3)_2NBF_2$.[18] One way of rationalizing this difference is in terms of the postulate of Robiette, *et al.*, that substantial $(p \rightarrow d)\pi$ bonding from nitrogen to silicon occurs in the latter compound, consistent with the known planarity of $N(SiH_3)_3$.[19] An analogous delocalization of the nitrogen lone pair along the C–N bonds in $(CH_3)_2NBCl_2$, of course, is not favorable. The existence of $(p \rightarrow d)\pi$ bonding in the silicon compound would presumably tend to shorten the Si–N bond and lengthen the B–N bond. From the data collected in Tables IV and V it appears that the B–N bond in $(CH_3)_2NBCl_2$ is within the range expected for a normal B–N double bond, and the 1.48 ± 0.02 Å B–N bond reported[18] for $(SiH_3)_2NBF_2$ is intermediate between a single and a double bond.

TABLE V

COMPARISON OF ISOELECTRONIC C–C AND B–N BONDS

Bond	Length of bond, Å	
	Carbon–carbon	Boron–nitrogen
	1.53[a]	1.56–1.60[d]
	1.34[b]	1.38[e]
	1.39[c]	1.44[f]

[a] L. S. Bartell and H. K. Higginbotham, *J. Chem. Phys.*, **42,** 851 (1965). [b] L. S. Bartell, E. A. Roth, C. D. Hollowell, K. Kuchitsu, and J. E. Young, Jr., *ibid.*, **42,** 2683 (1965). [c] I. L. Karle, *ibid.*, **20,** 65 (1952). [d] P. H. Clippard, Ph.D. Thesis, University of Michigan, 1969. B–N bond determined for adducts $(CH_3)_3NBCl_3$, $(CH_3)_3NBBr_3$, and $(CH_3)_3NBI_3$. See also P. H. Clippard, R. C. Taylor, and J. C. Hanson, *Inorg. Chem.*, in press; L. E. Sutton, "Tables of Internuclear Distances and Configurations in Molecules and Ions," Special Publications No. 11 and 18, The Chemical Society, London, 1958 and 1965. The higher (Clippard) values are the most accurate but may be unrepresentatively long because of steric deformation. [e] This work. [f] S. H. Bauer, *J. Amer. Chem. Soc.*, **60,** 524 (1938); W. Harshbarger, G. Lee, R. F. Porter, and S. H. Bauer, *Inorg. Chem.*, **8,** 1683 (1969).

The molecule $(CH_3)_2NNO_2$ recently studied by Stölevik and Rademacher[20] resembles $(CH_3)_2NBCl_2$, being isoelectronic with $(CH_3)_2NBF_2$. No tendency of the bonds around the trivalent nitrogen to deviate from a planar configuration was detected.

In summary, the B–N bond length determined in this work, 1.379 ± 0.006 Å, is the shortest boron–nitrogen distance yet measured. The bond length, the apparent skeletal planarity, and the spontaneous dimerization exhibited by the molecule are all consistent with the characterization of the B–N bond as a double bond. Values of comparable bonds in the isoelectronic C–C and B–N series are listed in Table V, where a marked similarity between the series is apparent.

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(18) A. G. Robiette, G. M. Sheldrick, W. S. Sheldrick, B. Beagley, D. W. J. Cruickshank, J. J. Monaghan, B. J. Aylett, and I. A. Ellis, *Chem. Commun.*, 909 (1968).

(19) K. Hedberg, *J. Amer. Chem. Soc.*, **77,** 6491 (1955).

(20) P. Rademacher and R. Stölevik, *Acta Chem. Scand.*, **23,** 660 (1969); R. Stölevik and P. Rademacher, *ibid.*, **23,** 672 (1969).