Supporting Information for

Structural Information from Hydrazine Radical Cation Optical Absorption Spectra

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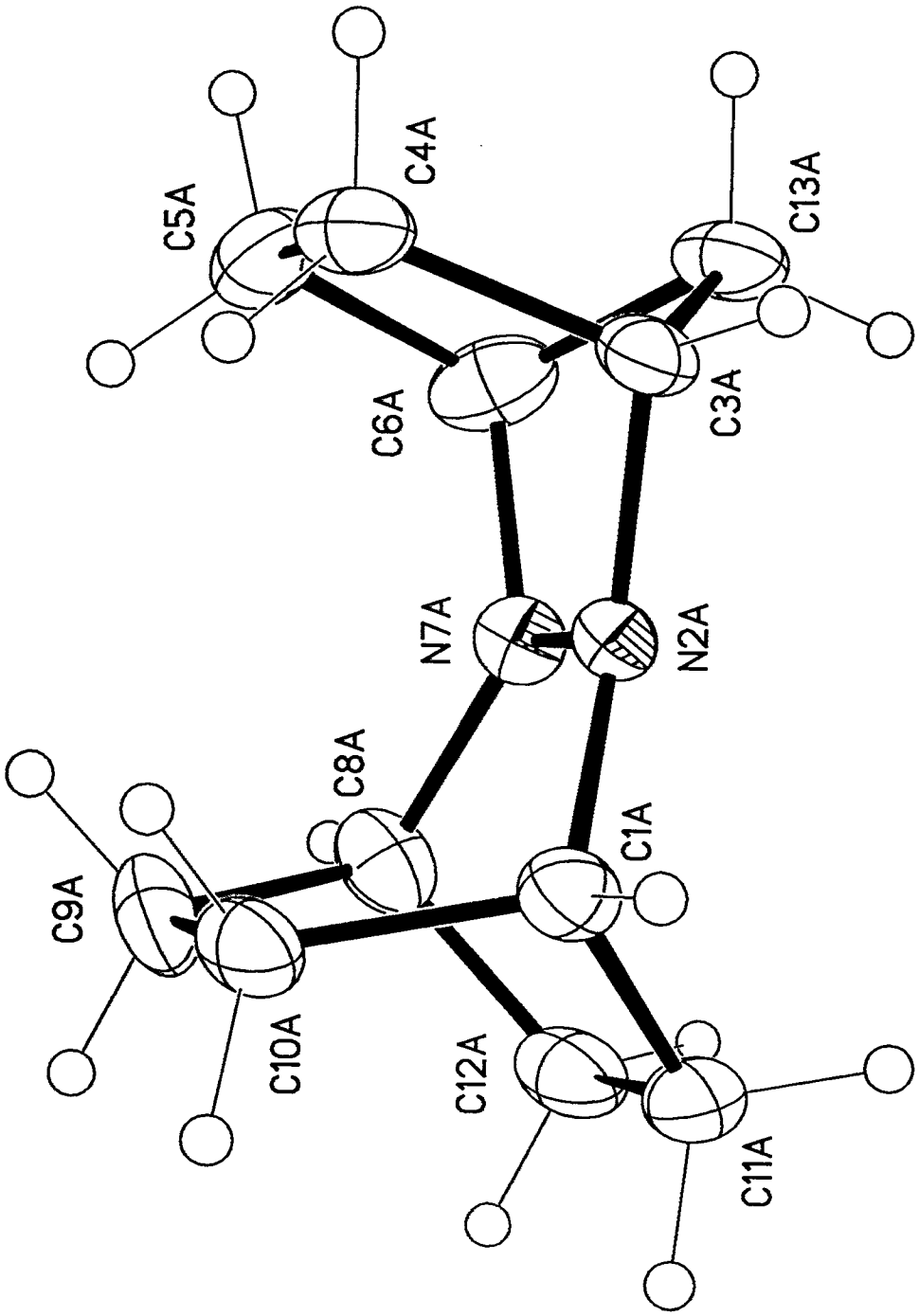
Table 5. Crystal data and structure refinement parameters.

Compound number	**15**	**15**$^+$TsO$^-$	**2**$^+$$NO_3^-$	**31**$^+$$Ar_4B^-$ [a]
Abbreviation	**AdN)$_2$**	**AdN)$_2$**$^+$TsO$^-$	**21/22**$^+$$NO_3^-$	**cHx$_2$N)$_2$**Ar_4B^-
Empirical formula	$C_{18}H_{28}N_2$	$(C_{18}H_{28}N_2)^+$	$(C_{11}H_{18}N_2)^+$	$(C_{24}H_{44}N_2)^+$
		$(C_7H_7O_3S)^-$	$(NO_3)^-$	$(C_{32}H_{12}BF_{24})^-$
Temperature, K	113(2)	113(2)	133(2)	133(2)
Space group	$P2_1/n$	$P\bar{1}$	$I4_1/a$	P4/ncc
Z	2	2	32	4
a, Å	6.9342(7)	6.922(2)	20.836(3)	15.0828(3)
b, Å	10.7103(7)	10.564(3)	20.836(3)	15.0828(3)
c, Å	9.7133(8)	16.255(6)	21.1447(6)	24.8230(7)
α, deg.	90	85.48(2)	90	90
β, deg.	91.925(9)	79.09(2)	90	90
γ, deg.	90	73.62(2)	90	90
Volume, Å^3	720.97(11)	1119.4(6)	9179.7(3)	5647.0(2)
Density, (calcd), Mg/m^3	1.255	1.316	1.391	1.440
F(000)	300	478	4128	2508
crystal size, mm	0.5×0.4×0.4	0.5×0.4×0.1	0.4×0.3×0.04	0.42×0.38×0.02

Table 5. (continued)

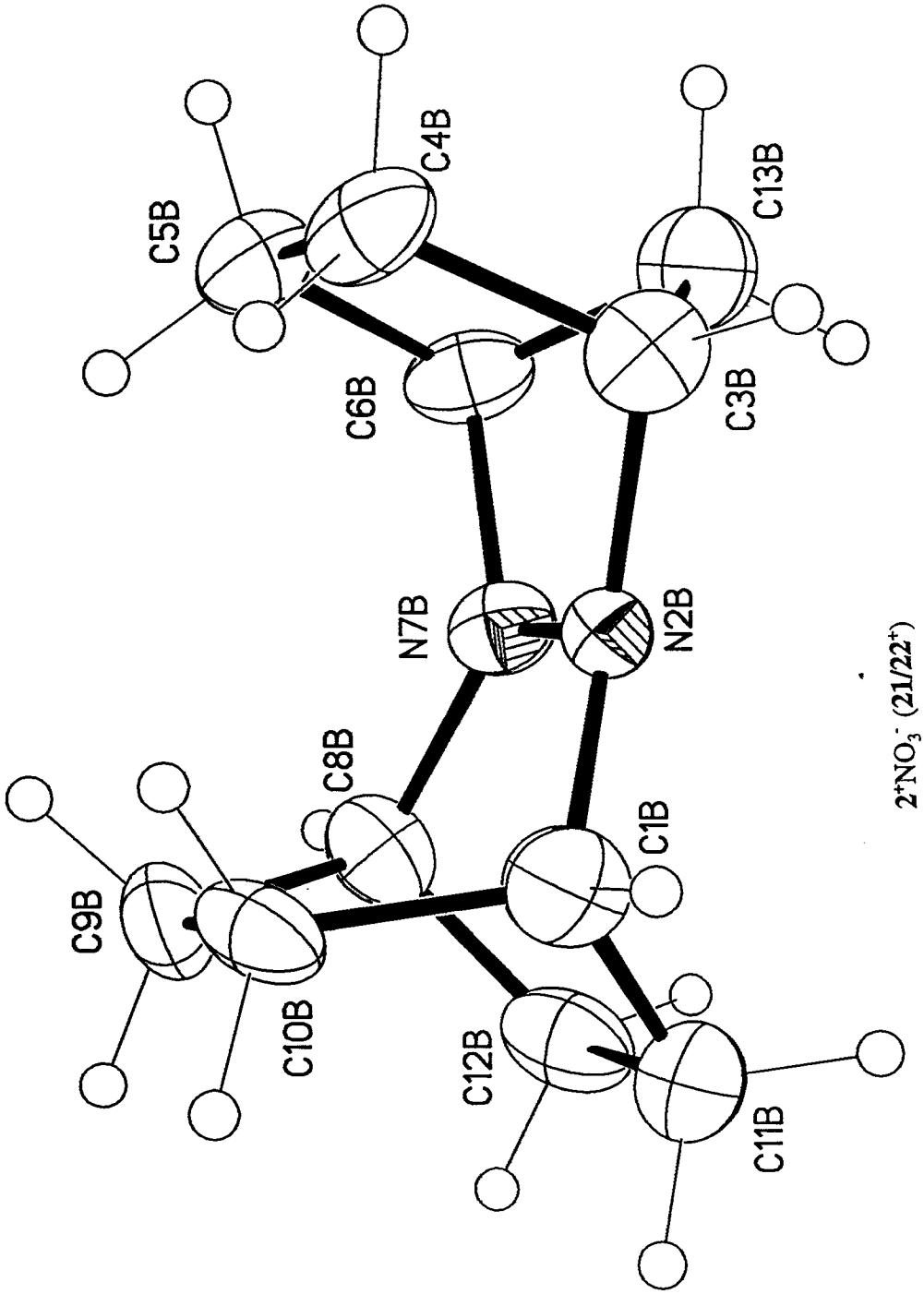
Compound number	**15**	**15**$^{+}$TsO^{-}	**2**$^{+}$$NO_3^{-}$	**31**$^{+}$$Ar_4B^{-}$ [a]
Reflections collected	2128	5842	20703	23269
Independent reflections[b]	978(0.0322)	2926(0.0353)	4519(0.0479)	3383(0.0585)
Final R index[c]	0.0343	0.0513	0.0740	0.0844
wR index (all data)	0.0866	0.1575	0.2186	0.2237
Abbreviation	**AdN)$_2$**	**AdN)$_2$**$^{+}$TsO^{-}	**21/22**$^{+}$$NO_3^{-}$	**cHx$_2$N)$_2$**Ar_4B^{-}
Goodness-of-fit on F^2	1.091	1.132	1.045	1.045
Data/restraints/parameters	978/0/92	2915/0/281	4516/54[d]/363	3382/72[e]/213
Largest diff. Map peaks[f]	0.141,-0.147	0.399,-0.305	0.852,-0.279	0.449,-0.606

a. Ar = m,m'-bistrifluoro-methylphenyl. b. In parentheses: R_{int}. c. $R_1[I>2\sigma(I)]$. Full-matrix least-squares refinement on F^2. d. The oxygens of the two anions were modeled as disordered with two orientations each. The occupancies were refined to 0.82(2), 0.17(2), 0.54(8), and 0.46(8) for the atoms O(1)-O(3), O(1')-O(3'), and O(4)-O(6), O(4')-O(6'), respectively. e. The cation sits on a four-fold axis. The anion sits on a site of 222 crystallographic symmetry. The fluorines were disordered and modelled in two orientations of both CF_3 groups. The occupancies refined to 0.623(17), 0.377(17), 0.941(6), 0.059(6) for the groups F(16)-F(18), F(16')-F(18'), F(20)-F(22), F(20')-F(22'), respectively. f. Unit: $e\text{Å}^{-3}$.



$2^{+}NO_3^{-}$

$21/22^{+}NO_3^{-}$

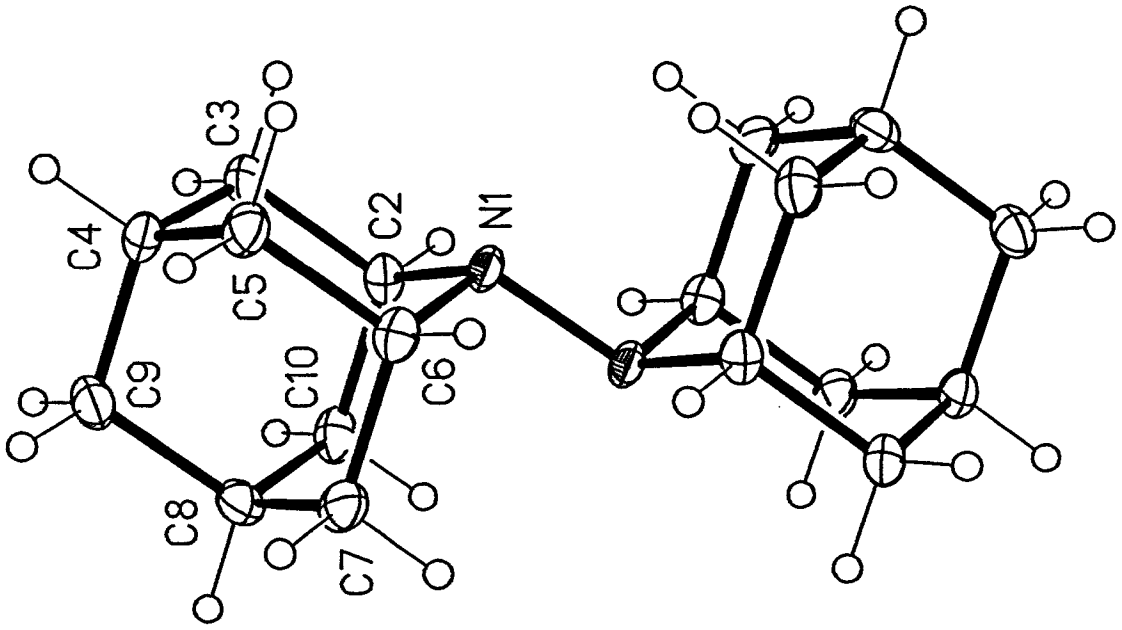


$2^{+}NO_3^{-}$ (21/22^{+})

$2^+NO_3^-$ (21/22$^+$) Atomic coordinates and equivalent isotropic displacement parameters [Å^2 U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

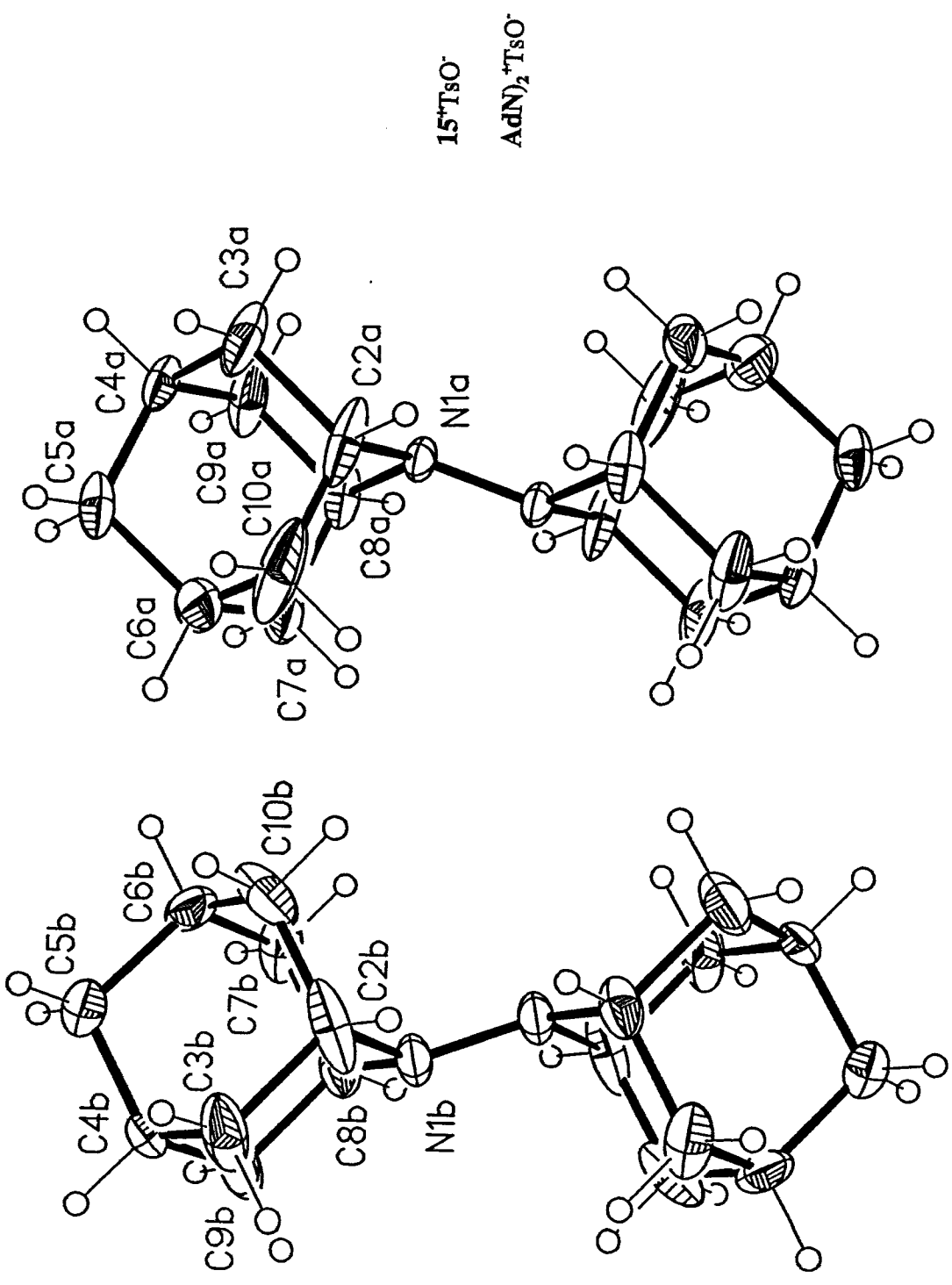
	x	y	z	U(eq)
C(1A)	0.8923(2)	0.6831(2)	0.58883(14)	0.0246(7)
N(2A)	0.91011(11)	0.66438(11)	0.52451(11)	0.0198(5)
C(3A)	0.8941(2)	0.6916(2)	0.46205(13)	0.0242(7)
C(4A)	0.8281(2)	0.6643(2)	0.44216(14)	0.0287(7)
C(5A)	0.8420(2)	0.5920(2)	0.4322(2)	0.0350(8)
C(6A)	0.9142(2)	0.5875(2)	0.4485(2)	0.0354(8)
N(7A)	0.92170(12)	0.60154(12)	0.51692(11)	0.0229(6)
C(8A)	0.9108(2)	0.5633(2)	0.5739(2)	0.0296(7)
C(9A)	0.8419(2)	0.5743(2)	0.5975(2)	0.0338(8)
C(10A)	0.8309(2)	0.6463(2)	0.6082(2)	0.0284(7)
C(11A)	0.9474(2)	0.6608(2)	0.6305(2)	0.0343(8)
C(12A)	0.9574(2)	0.5895(2)	0.6235(2)	0.0364(8)
C(13A)	0.9409(2)	0.6530(2)	0.42117(14)	0.0317(8)
C(1B)	0.7093(2)	0.3662(2)	0.4173(2)	0.0384(9)
N(2B)	0.64867(12)	0.34949(12)	0.44988(12)	0.0246(6)
C(3B)	0.5791(2)	0.3542(2)	0.4314(2)	0.0393(9)
C(4B)	0.5571(2)	0.4237(2)	0.4425(2)	0.0383(9)
C(5B)	0.5632(2)	0.4299(2)	0.5167(2)	0.0433(9)
C(6B)	0.5847(2)	0.3616(2)	0.5372(2)	0.0377(8)
N(7B)	0.65133(13)	0.35366(13)	0.51284(13)	0.0304(6)
C(8B)	0.7153(2)	0.3723(2)	0.5381(2)	0.0371(8)
C(9B)	0.7349(2)	0.4364(2)	0.5103(2)	0.0397(9)
C(10B)	0.7275(2)	0.4340(2)	0.4377(2)	0.0360(8)
C(11B)	0.7583(2)	0.3187(2)	0.4409(2)	0.0467(10)
C(12B)	0.7603(2)	0.3223(2)	0.5147(2)	0.0434(9)
C(13B)	0.5519(2)	0.3195(2)	0.4884(2)	0.0457(10)
N(8)	0.65191(13)	0.62891(13)	0.52677(11)	0.0266(6)
O(1)	0.5950(4)	0.6150(4)	0.5269(4)	0.050(2)
O(2)	0.6695(4)	0.6866(2)	0.5329(2)	0.050(2)
O(3)	0.6951(5)	0.5885(4)	0.5185(4)	0.063(2)
O(1')	0.603(2)	0.588(2)	0.519(2)	0.046(7)
O(2')	0.630(2)	0.6846(11)	0.5323(9)	0.050(5)
O(3')	0.696(2)	0.601(2)	0.540(2)	0.064(8)
N(9)	1.09152(11)	0.61148(12)	0.51984(11)	0.0213(6)
O(4)	1.0901(13)	0.604(2)	0.4620(12)	0.039(4)
O(5)	1.082(2)	0.665(2)	0.544(2)	0.041(4)
O(6)	1.102(2)	0.5637(14)	0.555(2)	0.040(4)
O(4')	1.086(2)	0.589(2)	0.464(2)	0.038(4)
O(5')	1.078(2)	0.669(2)	0.529(2)	0.041(5)
O(6')	1.111(2)	0.577(2)	0.563(2)	0.047(5)

15 $(AdN)_2$



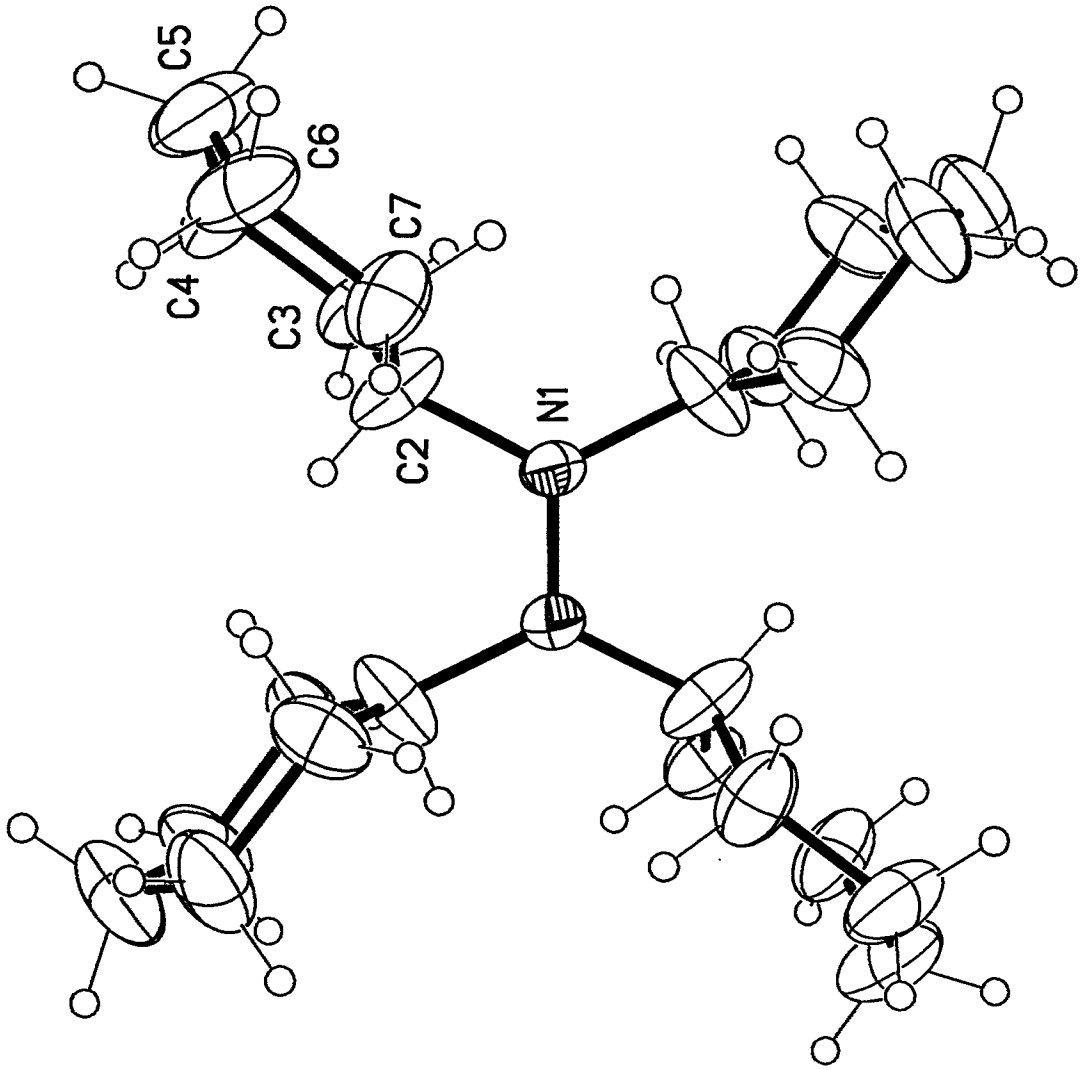
15(AdN)$_2$) **Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.**

	x	y	z	U(eq)
N(1)	247(2)	9332(1)	5185(1)	15(1)
C(2)	1371(2)	9325(1)	6525(1)	17(1)
C(3)	1915(2)	7975(1)	6872(1)	20(1)
C(4)	97(2)	7208(1)	7076(1)	18(1)
C(5)	-1071(2)	7270(1)	5718(1)	20(1)
C(6)	-1575(2)	8631(1)	5386(1)	17(1)
C(7)	-2781(2)	9175(1)	6531(2)	21(1)
C(8)	-1590(2)	9136(1)	7889(1)	21(1)
C(9)	-1064(2)	7776(1)	8237(1)	20(1)
C(10)	252(2)	9897(1)	7704(1)	21(1)



$15^{+}TsO^{-}$. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1A)	-269(4)	637(3)	5114(2)	21(1)
C(2A)	358(8)	1629(3)	4506(2)	45(1)
C(3A)	-1124(9)	2981(4)	4723(3)	58(2)
C(4A)	-1043(6)	3323(3)	5603(2)	29(1)
C(5A)	1112(6)	3309(3)	5663(2)	36(1)
C(6A)	2551(7)	1952(4)	5450(4)	58(1)
C(7A)	1884(7)	914(4)	6052(3)	53(1)
C(8A)	-246(6)	927(3)	5987(2)	29(1)
C(9A)	-1713(7)	2283(4)	6185(3)	44(1)
C(10A)	2511(8)	1623(4)	4574(3)	71(2)
N(1B)	-26(5)	540(3)	9740(2)	29(1)
C(2B)	-2022(7)	1308(4)	9514(3)	47(1)
C(3B)	-1617(9)	1993(4)	8666(3)	53(1)
C(4B)	-316(6)	2916(4)	8714(2)	34(1)
C(5B)	-1406(6)	3936(3)	9379(2)	31(1)
C(6B)	-1780(7)	3227(4)	10229(2)	41(1)
C(7B)	228(7)	2392(4)	10461(3)	42(1)
C(8B)	1311(6)	1384(4)	9793(2)	32(1)
C(9B)	1685(6)	2076(4)	8939(3)	56(1)
C(10B)	-3090(6)	2334(5)	10183(3)	52(1)
S(1)	3582(1)	605(1)	2204(1)	18(1)
O(1)	1372(3)	974(2)	2427(1)	23(1)
O(2)	4578(4)	-440(2)	2741(2)	30(1)
O(3)	4298(4)	369(2)	1315(1)	26(1)
C(1C)	4347(5)	2017(3)	2392(2)	17(1)
C(2C)	6314(5)	1874(3)	2517(2)	20(1)
C(3C)	6940(5)	2966(3)	2642(2)	23(1)
C(4C)	5627(5)	4229(3)	2641(2)	23(1)
C(5C)	3659(5)	4361(3)	2508(2)	26(1)
C(6C)	3018(5)	3278(3)	2378(2)	25(1)
C(7C)	6333(6)	5410(4)	2781(3)	35(1)



$3I^{+}Ar_4B^{-}$

$cHx_2N)_2Ar_4B^{-}$

$31^{+}Ar_4B^{-}$ $(cHx_2N)_2^{+}$. Atomic coordinates and equivalent isotropic displacement parameters [$Å^2$] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	0.2340(7)	0.2088(4)	0.3342(2)	0.0338(13)
C(2)	0.3002(3)	0.1334(2)	0.3341(2)	0.0535(11)
C(3)	0.2972(3)	0.0851(3)	0.2828(2)	0.0495(10)
C(4)	0.3493(4)	0.0021(3)	0.2833(2)	0.0653(13)
C(5)	0.3445(4)	-0.0509(3)	0.3335(2)	0.079(2)
C(6)	0.3450(4)	-0.0004(3)	0.3846(2)	0.0670(14)
C(7)	0.2940(3)	0.0836(3)	0.3848(2)	0.0547(11)
B(8)	0.7500	0.2500	0.5000	0.030(2)
C(9)	0.7594(2)	0.1610(2)	0.46216(12)	0.0300(7)
C(10)	0.7092(2)	0.1508(2)	0.41486(13)	0.0340(7)
C(11)	0.7109(2)	0.0733(2)	0.38446(14)	0.0371(8)
C(12)	0.7643(2)	0.0035(2)	0.39903(14)	0.0364(8)
C(13)	0.8147(2)	0.0115(2)	0.44536(14)	0.0335(7)
C(14)	0.8124(2)	0.0884(2)	0.47573(13)	0.0318(7)
C(15)	0.6551(3)	0.0677(3)	0.3353(2)	0.0506(10)
F(16)	0.6857(5)	0.1278(7)	0.2965(2)	0.072(2)
F(17)	0.5706(4)	0.0897(6)	0.3461(3)	0.053(2)
F(18)	0.6579(5)	-0.0080(4)	0.3108(3)	0.064(2)
F(16')	0.5786(8)	0.1120(7)	0.3354(5)	0.050(3)
F(17')	0.6304(6)	-0.0229(5)	0.3244(3)	0.046(3)
F(18')	0.6938(8)	0.0925(9)	0.2918(5)	0.068(3)
C(19)	0.8737(3)	-0.0631(2)	0.4622(2)	0.0446(9)
F(20)	0.8466(2)	-0.1417(2)	0.4448(2)	0.0853(14)
F(21)	0.8827(3)	-0.0695(2)	0.51527(12)	0.096(2)
F(22)	0.9556(2)	-0.0553(2)	0.44422(14)	0.0717(11)
F(20')	0.824(2)	-0.120(2)	0.4894(13)	0.043(11)
F(21')	0.939(2)	-0.041(3)	0.493(2)	0.07(2)
F(22')	0.902(3)	-0.102(3)	0.4181(12)	0.09(2)