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Gérard VERGOTEN

CONTRIBUTION A L'ETUDE STRUCTURALE DE LA STASE MESOMORPHE NEMATIQUE

BIBLIOTHEQUE UNIVERSITAIRE
Section de SCIENCES
LILLE

SPECTRES DE VIBRATION DE LA N (p. methoxy) BENZYLIDENE (p.n butyl) ANILINE

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ANNEXES

ANNEXES

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A.I.3, A.I.4, A.I.5, A.I.6, A.I.7 — distribution d'énergie potentielle suivant les constantes de force.

A.II. Benzène d_6

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A.II.3, A.II.4, A.II.5, A.II.6, A.II.7 — distribution d'énergie potentielle suivant les constantes de force.

A.III. Benzène d_3

A.III.1, A.III.2 — distribution d'énergie potentielle suivant les coordonnées de symétrie.

A.III.3, A.III.4, A.III.5, A.III.6, A.III.7 — distribution d'énergie potentielle suivant les constantes de force.

A.IV. Valeurs propres et vecteurs propres de la matrice J.W.J.

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A.V.3 matrice de corrélation

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distribution d'énergie potentielle suivant les coordonnées de symétrie.

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distribution d'énergie potentielle suivant les constantes de force.

A.VII. Géométrie de la benzylidène-aniline

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AI 1

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO, 1- 1 SYM. BLOCK NO, 1

		FREQUENCIES	3072.321	3067.535	3067.515	3056.418	3054.327	3054.320	1598.545	1596.544	1482.837	1482.828
S 1	ST1		16.69	0.0	33.45	16.85	0.0	33.77	0.00	0.0	0.0	0.00
S 2	ST16		0.0	0.01	0.0	0.0	0.01	0.0	0.0	9.18	23.01	0.0
S 3	ST2		0.00	0.0	33.36	67.17	0.0	0.00	0.00	0.0	0.0	0.00
S 4	ST4		66.97	0.0	0.00	0.00	0.0	33.86	0.00	0.0	0.0	0.00
S 5	ST5		0.00	0.0	0.00	0.00	0.0	0.16	72.80	0.0	0.0	0.00
S 6	ST6		0.00	0.0	0.58	0.00	0.0	0.00	0.00	0.0	0.0	37.34
S 7	ST7		0.00	0.0	0.00	0.00	0.0	0.04	28.63	0.0	0.0	0.00
S 8	ST8		0.00	0.0	0.04	0.00	0.0	0.00	0.00	0.0	0.0	69.96
S 9	ST9		0.00	0.0	0.00	1.00	0.0	0.00	0.00	0.0	0.0	0.00
S10	ST10		0.87	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00
S11	ST11		0.00	0.0	0.00	0.00	0.0	0.50	11.41	0.0	0.0	0.00
S12	ST12		0.0	100.97	0.0	0.0	0.00	0.0	0.0	0.00	0.00	0.0
S13	ST13		0.0	0.00	0.0	0.0	100.68	0.0	0.0	0.00	0.00	0.0
S14	ST14		0.0	0.00	0.0	0.0	0.16	0.0	0.0	72.80	0.00	0.0
S15	ST15		0.0	0.58	0.0	0.0	0.00	0.0	0.0	0.00	37.34	0.0
S16	ST17		0.0	0.00	0.0	0.0	0.00	0.0	0.0	0.00	0.00	0.0
S17	ST18		0.0	0.00	0.0	0.0	0.01	0.0	0.0	9.16	0.00	0.0
S18	ST19		0.0	0.01	0.0	0.0	0.00	0.0	0.0	0.00	21.86	0.0
S19	ST21		0.0	0.00	0.0	0.0	0.50	0.0	0.0	11.41	0.00	0.0
S20	ST20		0.0	0.01	0.0	0.0	0.01	0.0	0.0	9.18	23.02	0.0
S21	ST3		16.67	0.0	33.47	16.87	0.0	33.75	0.00	0.0	0.0	0.00

		FREQUENCIES	1353.980	1298.755	1191.793	1191.792	1156.453	1024.458	1024.451	1013.333	989.105	601.309
S 1	ST1		0.0	0.0	0.01	0.0	0.0	0.0	0.03	0.02	0.00	0.0
S 2	ST16		17.06	4.36	0.0	23.34	14.55	10.04	0.0	0.0	0.0	0.11
S 3	ST2		0.0	0.0	0.00	0.0	0.0	0.0	0.03	0.08	0.00	0.0
S 4	ST4		0.0	0.0	0.01	0.0	0.0	0.0	0.00	0.00	0.00	0.0
S 5	ST5		0.0	0.0	16.15	0.0	0.0	0.0	0.00	0.00	0.00	0.0
S 6	ST6		0.0	0.0	0.00	0.0	0.0	0.0	63.66	0.00	0.00	0.0
S 7	ST7		0.0	0.0	72.79	0.0	0.0	0.0	0.00	0.00	0.00	0.0
S 8	ST8		0.0	0.0	0.00	0.0	0.0	0.0	30.51	0.00	0.00	0.0
S 9	ST9		0.0	0.0	0.00	0.0	0.0	0.0	0.00	59.42	0.00	0.0
S10	ST10		0.0	0.0	0.00	0.0	0.0	0.0	0.00	0.00	100.04	0.0
S11	ST11		0.0	0.0	2.21	0.0	0.0	0.0	0.00	0.00	0.00	0.0
S12	ST12		0.00	0.00	0.0	0.00	0.00	0.09	0.0	0.0	0.0	0.00
S13	ST13		0.00	0.00	0.0	0.04	0.00	0.00	0.0	0.0	0.0	0.01
S14	ST14		0.00	0.00	0.0	16.15	0.00	0.00	0.0	0.0	0.0	12.98
S15	ST15		0.00	0.00	0.0	0.00	0.00	63.66	0.0	0.0	0.0	0.00
S16	ST17		0.00	95.00	0.0	0.00	9.12	0.00	0.0	0.0	0.0	0.00
S17	ST18		68.09	0.00	0.0	23.29	0.00	0.00	0.0	0.0	0.0	0.10
S18	ST19		0.00	16.56	0.0	0.00	55.26	9.53	0.0	0.0	0.0	0.00
S19	ST21		0.00	0.00	0.0	2.21	0.00	0.00	0.0	0.0	0.0	86.33
S20	ST20		17.06	4.36	0.0	23.34	14.55	10.04	0.0	0.0	0.0	0.11
S21	ST3		0.0	0.0	0.01	0.0	0.0	0.0	0.03	0.02	0.00	0.0

		FREQUENCIES	601.307
S 1	ST1		0.00
S 2	ST16		0.0
S 3	ST2		0.00
S 4	ST4		0.00
S 5	ST5		12.99
S 6	ST6		0.00
S 7	ST7		0.33
S 8	ST8		0.00
S 9	ST9		0.00
S10	ST10		0.00
S11	ST11		86.33
S12	ST12		0.0
S13	ST13		0.0
S14	ST14		0.0
S15	ST15		0.0
S16	ST17		0.0
S17	ST18		0.0
S18	ST19		0.0
S19	ST21		0.0
S20	ST20		0.0
S21	ST3		0.00

BUS LILLE

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO. 1- 1 SYM. BLOCK NO. 2

AI_2

	FREQUENCIES	991.205	966.657	966.651	847.025	847.020	705.799	674.176	396.892	396.891	0.0
S 1	ST29	14.56	0.0	27.41	0.0	24.31	4.70	16.45	0.0	6.36	0.
S 2	ST22	0.0	84.10	0.0	0.0	0.0	0.0	0.0	19.51	0.0	0.
S 3	ST23	0.0	0.0	0.0	73.77	0.0	0.0	0.0	0.0	0.0	0.
S 4	ST24	0.0	36.60	0.0	0.0	0.0	0.0	0.0	67.00	0.0	0.
S 5	ST RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.
S 6	ST RED2	0.0	0.0	0.0	32.36	0.0	0.0	0.0	0.0	0.0	0.
S 7	ST RED3	0.00	0.0	0.0	0.0	32.36	0.00	0.00	0.0	0.0	0.
S 8	ST26	0.00	0.0	27.86	0.0	0.00	0.00	66.87	0.0	6.46	0.
S 9	ST25	55.25	0.0	0.00	0.0	23.07	17.83	0.00	0.0	0.00	0.
S10	ST28	50.03	0.0	0.00	0.0	0.00	55.99	0.00	0.0	0.00	0.
S11	ST30	0.00	0.0	36.60	0.0	0.00	0.00	0.00	0.0	67.00	0.
S12	ST27	14.56	0.0	27.41	0.0	24.31	4.70	16.44	0.0	6.36	0.

	FREQUENCIES	0.0	0.0
S 1	ST29	0.0	0.0
S 2	ST22	0.0	0.0
S 3	ST23	0.0	0.0
S 4	ST24	0.0	0.0
S 5	ST RED1	0.0	0.0
S 6	ST RED2	0.0	0.0
S 7	ST RED3	0.0	0.0
S 8	ST26	0.0	0.0
S 9	ST25	0.0	0.0
S10	ST28	0.0	0.0
S11	ST30	0.0	0.0
S12	ST27	0.0	0.0

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 1 SYM. BLOCK NO. 1

AI 3

	FREQUENCIES	3072.321	3067.535	3067.515	3056.418	3054.327	3054.320	1598.545	1598.544	1482.837	1482.828
	ASSIGNMENT (PED)	ST4	ST12	ST3	ST2	ST13	ST4	ST5	ST14	ST15	ST8
	ASSIGNMENT (PED)	ST1		ST1	ST3		ST1	ST7	ST21	ST20	ST6
1 K(CH)	4.6740	90.378	90.651	90.651	91.310	91.440	91.441	0.002	0.002	0.003	0.003
2 K(CD)	4.8082	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3 O(CH)	0.0240	0.928	0.465	0.465	-0.938	-0.470	-0.470	-0.000	-0.000	0.000	0.000
4 O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5 M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6 M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7 P(CH)	-0.0060	-0.116	0.116	0.116	0.117	-0.117	-0.117	-0.000	-0.000	0.000	0.000
8 P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9 H(CCH)	0.1701	0.000	0.031	0.031	0.129	0.093	0.093	19.165	19.165	44.696	44.696
10 O(CCH)	0.0015	0.000	0.000	0.000	-0.000	-0.000	-0.000	-0.151	-0.151	0.378	0.378
11 M(CCH)	-0.0070	0.000	0.001	0.001	0.000	0.001	0.001	0.725	0.725	1.817	1.817
12 P(CCH)	0.0049	-0.000	-0.001	-0.001	0.000	0.001	0.001	0.511	0.511	-1.280	-1.280
13 K(CC)	5.2499	0.606	0.419	0.419	0.000	0.137	0.137	62.758	62.759	26.917	26.917
14 O(CC)	0.4954	0.114	0.040	0.040	0.000	-0.013	-0.013	-5.922	-5.922	2.540	2.540
15 M(CC)	-0.2115	-0.049	0.017	0.017	-0.000	0.006	0.006	2.528	2.528	1.084	1.084
16 P(CC)	0.3528	0.041	-0.028	-0.028	0.000	0.009	0.009	4.217	4.217	-1.809	-1.809
17 H(CCC)	0.4189	0.000	0.033	0.033	0.637	0.327	0.327	7.428	7.428	2.148	2.147
18 O(CCC)	-0.0090	0.000	-0.001	-0.001	0.041	0.011	0.011	0.239	0.239	-0.069	-0.069
19 M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20 P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21 F(CH)	0.3845	8.014	8.233	8.233	8.584	8.536	8.536	7.900	7.900	22.090	22.090
22 F(CC)	0.2417	0.084	0.023	0.023	0.119	0.039	0.039	0.600	0.600	1.487	1.487
23 A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24 B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25 C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26 D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27 AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28 AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29 AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30 BO	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31 BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32 BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PEDSUM		100.000	100.000	100.000	100.000	100.000	100.000	100.001	100.001	100.000	100.001

AI4

	FREQUENCIES		1353.980	1298.755	1191.793	1191.792	1156.453	1024.458	1024.451	1013.333	989.105	601.309
	ASSIGNMENT (PED)		ST18	ST17	ST7	ST20	ST19	ST15	ST6	ST9	ST10	ST21
	ASSIGNMENT (PED)		ST16	ST19	ST5	ST16	ST16	ST16	ST8			ST14
1	K(CH)	4.6740	0.000	0.000	0.034	0.034	0.000	0.083	0.083	0.112	0.000	0.008
2	K(CD)	4.8082	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	C(CH)	0.0240	0.000	0.000	-0.000	-0.000	-0.000	0.000	0.000	-0.001	0.000	-0.000
4	C(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	0.000	0.000	-0.000	-0.000	-0.000	0.000	0.000	0.000	-0.000	-0.000
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	F(CCH)	0.1701	65.622	16.767	45.184	45.185	55.950	20.046	20.046	12.867	0.000	11.608
10	C(CCH)	0.0015	1.120	-0.286	-0.383	-0.383	-0.955	0.165	0.165	-0.000	0.000	-0.002
11	M(CCH)	-0.0070	-5.386	-1.376	1.842	1.842	-4.593	0.792	0.792	0.000	0.000	0.008
12	P(CCH)	0.0049	1.897	-0.485	1.298	1.298	-1.618	-0.558	-0.558	0.000	-0.000	0.006
13	K(CC)	5.2499	0.000	122.615	13.922	13.922	11.776	45.886	45.886	0.000	69.986	11.193
14	C(CC)	0.4954	-0.000	-23.142	-1.314	-1.314	-2.223	4.330	4.330	-0.000	13.209	-1.056
15	M(CC)	-0.2115	-0.000	-9.878	0.561	0.561	-0.949	1.848	1.848	0.000	-5.638	0.451
16	P(CC)	0.3528	-0.000	-8.239	0.936	0.936	-0.791	-3.083	-3.083	0.000	4.703	0.752
17	H(CCC)	0.4189	0.000	0.000	1.441	1.441	0.000	3.661	3.661	63.381	0.000	56.186
18	O(CCC)	-0.0090	-0.000	0.000	0.046	0.046	0.000	-0.118	-0.118	4.086	-0.000	1.811
19	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	F(CH)	0.3845	36.747	4.590	36.299	36.299	43.456	24.413	24.413	7.670	8.074	4.963
22	F(CC)	0.2417	0.000	-0.565	0.134	0.134	-0.054	2.535	2.535	11.886	5.666	14.071
23	A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25	C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26	D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29	AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	BO	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31	BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32	BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	PEDSUM		100.000	100.000	100.000	100.000	100.000	100.001	100.000	100.000	100.000	100.000

AI5

	FREQUENCIES	601.307	
	ASSIGNMENT (PED)	ST11	
	ASSIGNMENT (PED)	ST5	
1	K(CH)	4.6740	0.008
2	K(CD)	4.8082	0.0
3	D(CH)	0.0240	-0.000
4	D(CD)	0.0420	0.0
5	M(CH)	0.0	0.0
6	M(CD)	0.0060	0.0
7	P(CH)	-0.0060	-0.000
8	P(CD)	-0.0080	0.0
9	H(CCH)	0.1701	11.608
10	C(CCH)	0.0015	-0.002
11	M(CCH)	-0.0070	0.008
12	P(CCH)	0.0049	0.006
13	K(CC)	5.2499	11.193
14	C(CC)	0.4954	-1.056
15	M(CC)	-0.2115	0.451
16	P(CC)	0.3528	0.752
17	H(CCC)	0.4189	56.186
18	C(CCC)	-0.0090	1.811
19	M(CCC)	0.0	0.0
20	P(CCC)	0.0	0.0
21	F(CH)	0.3845	4.963
22	F(CC)	0.2417	14.071
23	A	0.3850	0.0
24	B	0.4238	0.0
25	C	0.0377	0.0
26	D	-0.0067	0.0
27	AO	0.0054	0.0
28	AM	-0.0066	0.0
29	AP	0.0076	0.0
30	BC	0.0732	0.0
31	BM	0.0761	0.0
32	BP	0.0365	0.0
	PEDSUM		100.000

BBS UTSE

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 1 SYM. BLOCK NO. 2

AI6

	FREQUENCIES	991.205	966.657	966.651	847.025	847.020	705.799	674.176	396.892	396.891	0.0
	ASSIGNMENT (PED)	ST25	ST22	ST30	ST23	ST RED3	ST28	ST26	ST24	ST30	
	ASSIGNMENT (PED)	ST28	ST24	ST26	ST RED2	ST27	ST25	ST29	ST22		
1 K(CH)	4.6740	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2 K(CD)	4.8082	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3 C(CH)	0.0240	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4 C(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5 M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6 M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7 P(CH)	-0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8 P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9 H(CCH)	0.1701	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10 C(CCH)	0.0015	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11 M(CCH)	-0.0070	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12 P(CCH)	0.0049	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13 K(CC)	5.2499	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14 C(CC)	0.4954	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15 M(CC)	-0.2115	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16 P(CC)	0.3528	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17 H(CCC)	0.4189	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18 C(CCC)	-0.0090	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19 M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20 P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21 F(CH)	0.3845	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
22 F(CC)	0.2417	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
23 A	0.3850	87.337	82.215	82.216	72.933	72.933	28.189	98.670	19.069	19.069	0.0
24 B	0.4238	53.929	49.878	49.878	35.686	35.686	60.351	0.000	91.304	91.304	0.0
25 C	0.0377	-25.621	-20.703	-20.703	-9.523	-9.523	15.398	0.000	13.490	13.490	0.0
26 D	-0.0067	-4.563	0.0	-0.000	3.392	3.392	2.742	0.000	0.0	0.000	0.0
27 AO	0.0054	-2.454	-1.155	-1.155	1.025	1.025	-0.792	2.772	-0.268	-0.268	0.0
28 AM	-0.0066	-3.004	1.414	1.414	1.254	1.254	-0.970	-3.394	0.328	0.328	0.0
29 AP	0.0076	-1.727	1.626	1.626	-1.443	-1.443	-0.558	1.952	0.377	0.377	0.0
30 BC	0.0732	-18.625	-8.613	-8.613	6.163	6.163	-20.843	-0.000	-15.767	-15.767	0.0
31 BM	0.0761	19.377	-8.961	-8.961	-6.411	-6.411	21.684	0.000	-16.403	-16.403	0.0
32 BP	0.0365	-4.648	4.299	4.299	-3.076	-3.076	-5.202	-0.000	7.870	7.870	0.0
PEDSUM		100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	0.0

	FREQUENCIES		0.0	0.0
	ASSIGNMENT (PED)			
	ASSIGNMENT (PED)			
1	K(CH)	4.6740	0.0	0.0
2	K(CD)	4.8082	0.0	0.0
3	C(CH)	0.0240	0.0	0.0
4	C(CD)	0.0420	0.0	0.0
5	M(CH)	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0
7	P(CH)	-0.0060	0.0	0.0
8	P(CD)	-0.0080	0.0	0.0
9	H(CCH)	0.1701	0.0	0.0
10	O(CCH)	0.0015	0.0	0.0
11	M(CCH)	-0.0070	0.0	0.0
12	P(CCH)	0.0049	0.0	0.0
13	K(CC)	5.2499	0.0	0.0
14	O(CC)	0.4954	0.0	0.0
15	M(CC)	-0.2115	0.0	0.0
16	P(CC)	0.3528	0.0	0.0
17	H(CCC)	0.4189	0.0	0.0
18	C(CCC)	-0.0090	0.0	0.0
19	M(CCC)	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0
21	F(CH)	0.3845	0.0	0.0
22	F(CC)	0.2417	0.0	0.0
23	A	0.3850	0.0	0.0
24	B	0.4238	0.0	0.0
25	C	0.0377	0.0	0.0
26	D	-0.0067	0.0	0.0
27	AO	0.0054	0.0	0.0
28	AM	-0.0066	0.0	0.0
29	AP	0.0076	0.0	0.0
30	BO	0.0732	0.0	0.0
31	BM	0.0761	0.0	0.0
32	BP	0.0365	0.0	0.0
	PEDSUM		0.0	0.0

BIBS LILLE

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO. 1- 2 SYM. BLOCK NO. 1

AII1

	FREQUENCIES	2293.172	2289.546	2284.887	2284.887	2280.212	2280.206	1557.114	1557.114	1341.305	1341.297
S 1	ST1	16.55	16.54	33.31	0.0	33.36	0.0	0.0	0.28	0.19	0.0
S 2	ST16	0.0	0.0	0.0	0.08	0.0	0.09	4.57	0.0	0.0	12.95
S 3	ST2	0.00	66.01	33.19	0.0	0.00	0.0	0.0	0.00	0.19	0.0
S 4	ST4	66.36	0.00	0.00	0.0	33.49	0.0	0.0	0.28	0.00	0.0
S 5	ST5	0.00	0.00	0.00	0.0	1.31	0.0	0.0	82.27	0.00	0.0
S 6	ST6	0.00	0.00	2.80	0.0	0.00	0.0	0.0	0.00	66.03	0.0
S 7	ST7	0.00	0.00	0.00	0.0	0.28	0.0	0.0	14.25	0.00	0.0
S 8	ST8	0.00	0.00	0.25	0.0	0.00	0.0	0.0	0.00	39.36	0.0
S 9	ST9	0.00	3.96	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0
S10	ST10	3.46	0.00	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0
S11	ST11	0.00	0.00	0.00	0.0	2.19	0.0	0.0	11.16	0.00	0.0
S12	ST12	0.0	0.0	0.0	100.46	0.0	0.00	0.00	0.0	0.0	0.58
S13	ST13	0.0	0.0	0.0	0.00	0.0	99.52	0.85	0.0	0.0	0.00
S14	ST14	0.0	0.0	0.0	0.00	0.0	1.31	82.27	0.0	0.0	0.00
S15	ST15	0.0	0.0	0.0	2.80	0.0	0.00	0.00	0.0	0.0	66.03
S16	ST17	0.0	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.0	0.00
S17	ST18	0.0	0.0	0.0	0.00	0.0	0.09	4.56	0.0	0.0	0.00
S18	ST19	0.0	0.0	0.0	0.08	0.0	0.00	0.00	0.0	0.0	12.30
S19	ST21	0.0	0.0	0.0	0.00	0.0	2.19	11.16	0.0	0.0	0.00
S20	ST20	0.0	0.0	0.0	0.08	0.0	0.09	4.57	0.0	0.0	12.95
S21	ST3	16.54	16.58	33.29	0.0	33.36	0.0	0.0	0.28	0.19	0.0

	FREQUENCIES	1290.778	1053.162	969.454	949.568	857.865	857.865	823.171	800.037	800.035	582.413
S 1	ST1	0.0	0.0	0.31	0.14	0.01	0.0	0.0	0.00	0.0	0.0
S 2	ST16	1.06	17.06	0.0	0.0	0.0	27.82	17.24	0.0	20.03	0.17
S 3	ST2	0.0	0.0	1.23	0.00	0.00	0.0	0.0	0.00	0.0	0.0
S 4	ST4	0.0	0.0	0.00	0.58	0.01	0.0	0.0	0.00	0.0	0.0
S 5	ST5	0.0	0.0	0.00	0.00	6.55	0.0	0.0	0.00	0.0	0.0
S 6	ST6	0.0	0.0	0.00	0.00	0.00	0.0	0.0	32.71	0.0	0.0
S 7	ST7	0.0	0.0	0.00	0.00	86.73	0.0	0.0	0.00	0.0	0.0
S 8	ST8	0.0	0.0	0.00	0.00	0.00	0.0	0.0	60.90	0.0	0.0
S 9	ST9	0.0	0.0	96.45	0.00	0.00	0.0	0.0	0.00	0.0	0.0
S10	ST10	0.0	0.0	0.00	97.42	0.00	0.0	0.0	0.00	0.0	0.0
S11	ST11	0.0	0.0	0.00	0.00	0.48	0.0	0.0	0.00	0.0	0.0
S12	ST12.	0.00	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00
S13	ST13	0.00	0.00	0.0	0.0	0.0	0.03	0.00	0.0	0.00	0.32
S14	ST14	0.00	0.00	0.0	0.0	0.0	6.55	0.00	0.0	0.00	11.96
S15	ST15	0.00	0.00	0.0	0.0	0.0	0.00	0.00	0.0	32.71	0.00
S16	ST17	103.37	0.00	0.0	0.0	0.0	0.00	1.05	0.0	0.00	0.00
S17	ST18	0.00	68.09	0.0	0.0	0.0	27.75	0.00	0.0	0.00	0.17
S18	ST19	6.31	0.00	0.0	0.0	0.0	0.00	65.51	0.0	19.03	0.00
S19	ST21	0.00	0.00	0.0	0.0	0.0	0.48	0.00	0.0	0.00	86.60
S20	ST20	1.06	17.06	0.0	0.0	0.0	27.82	17.24	0.0	20.03	0.17
S21	ST3	0.0	0.0	0.31	0.14	0.01	0.0	0.0	0.00	0.0	0.0

	FREQUENCIES	582.412
S 1	ST1	0.11
S 2	ST16	0.0
S 3	ST2	0.00
S 4	ST4	0.11
S 5	ST5	11.96
S 6	ST6	0.00
S 7	ST7	0.52
S 8	ST8	0.00
S 9	ST9	0.00
S10	ST10	0.00
S11	ST11	86.60
S12	ST12	0.0
S13	ST13	0.0
S14	ST14	0.0
S15	ST15	0.0
S16	ST17	0.0
S17	ST18	0.0
S18	ST19	0.0
S19	ST21	0.0
S20	ST20	0.0
S21	ST3	0.11

BUS LILLE

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO. 1- 2 SYM. BLOCK NO. 2

A_{II_2}

	FREQUENCIES	827.991	787.427	787.423	658.842	658.841	597.737	495.025	344.687	344.686	0.0
S 1	ST29	19.25	0.0	31.34	24.31	0.0	0.01	16.44	2.42	0.0	0.0
S 2	ST22	0.0	96.18	0.0	0.0	0.0	0.0	0.0	0.0	7.43	0.0
S 3	ST23	0.0	0.0	0.0	0.0	73.77	0.0	0.0	0.0	0.0	0.0
S 4	ST24	0.0	20.32	0.0	0.0	0.0	0.0	0.0	0.0	83.29	0.0
S 5	ST RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S 6	ST RED2	0.0	0.0	0.0	0.0	32.36	0.0	0.0	0.0	0.0	0.0
S 7	ST RED3	0.00	0.0	0.00	32.36	0.0	0.00	0.0	0.00	0.0	0.0
S 8	ST26	0.00	0.0	31.86	0.0	0.0	0.00	66.87	2.46	0.0	0.0
S 9	ST25	73.05	0.0	0.00	23.07	0.0	0.04	0.0	0.00	0.0	0.0
S10	ST28	4.99	0.0	0.00	0.00	0.0	101.03	0.0	0.00	0.0	0.0
S11	ST30	0.00	0.0	20.32	0.00	0.0	0.00	0.00	83.29	0.0	0.0
S12	ST27	19.24	0.0	31.34	24.31	0.0	0.01	16.44	2.42	0.0	0.0

	FREQUENCIES	0.0	0.0
S 1	ST29	0.0	0.0
S 2	ST22	0.0	0.0
S 3	ST23	0.0	0.0
S 4	ST24	0.0	0.0
S 5	ST RED1	0.0	0.0
S 6	ST RED2	0.0	0.0
S 7	ST RED3	0.0	0.0
S 8	ST26	0.0	0.0
S 9	ST25	0.0	0.0
S10	ST28	0.0	0.0
S11	ST30	0.0	0.0
S12	ST27	0.0	0.0

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 2 SYM. BLOCK NO. 1

AII3

	FREQUENCIES	2293.172	2289.546	2284.887	2284.887	2280.212	2280.206	1557.114	1557.114	1341.305	1341.297
	ASSIGNMENT (PED)	ST4	ST2	ST1	ST12	ST4	ST13	ST14	ST5	ST6	ST15
	ASSIGNMENT (PED)	ST1	ST3	ST3		ST1		ST21	ST7	ST8	ST20
1	K(CH)	4.6740	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	K(CD)	4.8082	89.843	89.959	90.451	90.451	90.621	90.621	0.770	0.770	0.518	0.518
3	C(CH)	0.0240	0.897	-0.898	0.451	0.451	-0.452	-0.452	-0.004	-0.004	0.003	0.003
4	O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	-0.112	0.112	0.113	0.113	-0.113	-0.113	-0.001	-0.001	0.001	0.001
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	H(CCH)	0.1701	0.000	0.513	0.192	0.192	0.463	0.463	10.266	10.267	25.672	25.672
10	O(CCH)	0.0015	-0.000	-0.000	0.001	0.001	-0.001	-0.001	-0.075	-0.075	0.212	0.212
11	M(CCH)	-0.0070	0.000	0.000	0.007	0.007	0.007	0.007	0.361	0.361	1.022	1.022
12	P(CCH)	0.0049	0.000	0.000	-0.005	-0.005	0.005	0.005	0.254	0.254	-0.720	-0.720
13	K(CC)	5.2499	2.422	0.000	2.022	2.022	1.128	1.128	70.922	70.922	47.600	47.601
14	O(CC)	0.4954	0.457	0.000	0.191	0.191	-0.106	-0.106	-6.693	-6.693	4.492	4.492
15	M(CC)	-0.2115	-0.195	-0.000	0.081	0.081	0.045	0.045	2.857	2.857	1.917	1.917
16	P(CC)	0.3528	0.163	0.000	-0.136	-0.136	0.076	0.076	4.766	4.766	-3.199	-3.199
17	F(CCC)	0.4189	0.000	2.526	0.161	0.161	1.428	1.428	7.267	7.267	3.798	3.798
18	O(CCC)	-0.0090	0.000	0.163	-0.005	-0.005	0.046	0.046	0.234	0.234	-0.122	-0.122
19	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	F(CH)	0.3845	6.192	7.151	6.365	6.365	6.714	6.714	8.394	8.394	16.177	16.177
22	F(CC)	0.2417	0.335	0.474	0.112	0.112	0.142	0.142	0.683	0.683	2.630	2.630
23	A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25	C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26	D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29	AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	BC	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31	BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32	BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	PEDSUM		100.000	100.000	100.001	100.000	100.001	100.001	100.001	100.001	100.001	100.001

AII4

	FREQUENCIES	1290.778	1053.162	969.454	949.568	857.865	857.865	823.171	800.037	800.035	582.413
	ASSIGNMENT (PED)	ST17	ST18	ST9	ST10	ST7	ST16	ST19	ST8	ST15	ST21
	ASSIGNMENT (PED)		ST16				ST20	ST16	ST6	ST20	ST14
1	K(CH)	4.6740	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	K(CD)	4.8082	0.000	0.000	1.682	0.779	0.024	0.024	0.000	0.003	0.288
3	C(CH)	0.0240	-0.000	-0.000	-0.017	0.008	-0.000	-0.000	-0.000	0.000	-0.001
4	O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	-0.000	-0.000	0.002	-0.001	-0.000	-0.000	-0.000	0.000	0.000
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	H(CCH)	0.1701	6.390	65.622	12.482	0.000	53.557	53.557	66.326	38.909	38.910	11.764
10	O(CCH)	0.0015	-0.109	1.120	-0.000	0.000	-0.456	-0.456	-1.132	0.329	0.329	0.003
11	M(CCH)	-0.0070	-0.525	-5.386	0.000	0.000	2.195	2.195	-5.444	1.581	1.581	0.013
12	P(CCH)	0.0049	-0.185	1.897	0.000	-0.000	1.547	1.547	-1.918	-1.114	1.114	0.009
13	K(CC)	5.2499	133.035	0.000	0.000	68.154	5.645	5.645	1.356	23.580	23.580	10.310
14	O(CC)	0.4954	-25.108	-0.000	0.000	12.863	-0.533	-0.533	-0.256	2.225	2.225	-0.973
15	M(CC)	-0.2115	-10.717	0.000	-0.000	-5.490	0.227	0.227	-0.109	0.950	0.950	0.415
16	P(CC)	0.3528	-8.940	0.000	0.000	4.580	0.379	0.379	-0.091	-1.585	-1.585	0.693
17	H(CCC)	0.4189	0.000	0.000	61.484	0.000	0.315	0.315	0.000	1.881	1.881	56.365
18	O(CCC)	-0.0090	0.000	0.000	3.963	-0.000	0.010	0.010	-0.000	-0.061	-0.061	1.817
19	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	F(CH)	0.3845	6.772	36.747	8.873	9.695	37.025	37.025	41.274	31.998	31.998	5.349
22	F(CC)	0.2417	-0.612	0.000	11.531	9.413	0.065	0.065	-0.006	1.303	1.303	13.954
23	A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25	C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26	D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29	AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	BO	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31	BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32	BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	PEDSUM		100.001	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000

AII5

	FREQUENCIES		582.412
	ASSIGNMENT (PED)		ST11
	ASSIGNMENT (PED)		ST5
1	K(CH)	4.6740	0.0
2	K(CD)	4.8082	0.288
3	C(CH)	0.0240	-0.001
4	C(CD)	0.0420	0.0
5	M(CH)	0.0	0.0
6	M(CD)	0.0060	0.0
7	P(CH)	-0.0060	-0.000
8	P(CD)	-0.0080	0.0
9	H(CCH)	0.1701	11.763
10	C(CCH)	0.0015	-0.003
11	M(CCH)	-0.0070	0.013
12	P(CCH)	0.0049	0.009
13	K(CC)	5.2499	10.310
14	C(CC)	0.4954	-0.973
15	M(CC)	-0.2115	0.415
16	P(CC)	0.3528	0.693
17	H(CCC)	0.4189	56.365
18	C(CCC)	-0.0090	1.817
19	M(CCC)	0.0	0.0
20	P(CCC)	0.0	0.0
21	F(CH)	0.3845	5.349
22	F(CC)	0.2417	13.954
23	A	0.3850	0.0
24	B	0.4238	0.0
25	C	0.0377	0.0
26	D	-0.0067	0.0
27	AC	0.0054	0.0
28	AM	-0.0066	0.0
29	AP	0.0076	0.0
30	BC	0.0732	0.0
31	BM	0.0761	0.0
32	BP	0.0365	0.0
	PEDSUM		100.000

ЭГЛИТ БИБ

AII6

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 2 SYM. BLOCK NO. 2

	FREQUENCIES	827.991	787.427	787.423	658.842	658.841	597.737	495.025	344.687	344.686	0.0
	ASSIGNMENT (PED)	ST25	ST22	ST26	ST RED3	ST23	ST28	ST26	ST30	ST24	
	ASSIGNMENT (PED)	ST29	ST24	ST27	ST29	ST RED2		ST29			
1 K(CH)	4.6740	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2 K(CD)	4.8082	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3 C(CH)	0.0240	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4 C(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5 M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6 M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7 P(CH)	-0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8 P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9 H(CCH)	0.1701	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10 C(CCH)	0.0015	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11 M(CCH)	-0.0070	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12 P(CCH)	0.0049	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13 K(CC)	5.2499	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14 C(CC)	0.4954	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15 M(CC)	-0.2115	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16 P(CC)	0.3528	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17 H(CCC)	0.4189	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18 C(CCC)	-0.0090	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19 M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20 P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21 F(CH)	0.3845	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
22 F(CC)	0.2417	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
23 A	0.3850	115.471	94.022	94.022	72.933	72.933	0.055	98.670	7.263	7.263	0.0
24 B	0.4238	5.381	27.687	27.687	35.686	35.686	108.898	0.000	113.495	113.495	0.0
25 C	0.0377	-9.306	-16.495	-16.495	-9.523	-9.523	-0.917	0.0	9.282	9.282	0.0
26 D	-0.0067	-1.657	0.0	-0.000	3.392	3.392	-0.163	0.0	0.000	0.0	0.0
27 AO	0.0054	-3.244	-1.321	-1.321	1.025	1.025	-0.002	2.772	-0.102	-0.102	0.0
28 AM	-0.0066	-3.972	1.617	1.617	1.254	1.254	-0.002	-3.394	0.125	0.125	0.0
29 AP	0.0076	-2.284	1.860	1.860	1.443	1.443	-0.001	1.952	0.144	0.144	0.0
30 BO	0.0732	-1.359	-4.781	-4.781	6.163	6.163	-37.610	-0.000	-19.599	-19.599	0.0
31 BM	0.0761	1.934	-4.974	-4.974	-6.411	-6.411	39.128	-0.000	-20.390	-20.390	0.0
32 BP	0.0365	-0.464	2.386	2.386	-3.076	-3.076	-9.386	0.000	9.782	9.782	0.0
PEDSUM		100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.001	100.001	0.0

AII7

	FREQUENCIES		0.0	0.0
	ASSIGNMENT (PED)			
	ASSIGNMENT (PED)			
1	K(CH)	4.6740	0.0	0.0
2	K(CD)	4.8082	0.0	0.0
3	C(CH)	0.0240	0.0	0.0
4	C(CD)	0.0420	0.0	0.0
5	M(CH)	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0
7	P(CH)	-0.0060	0.0	0.0
8	P(CD)	-0.0080	0.0	0.0
9	H(CCH)	0.1701	0.0	0.0
10	C(CCH)	0.0015	0.0	0.0
11	M(CCH)	-0.0070	0.0	0.0
12	P(CCH)	0.0049	0.0	0.0
13	K(CC)	5.2499	0.0	0.0
14	C(CC)	0.4954	0.0	0.0
15	M(CC)	-0.2115	0.0	0.0
16	P(CC)	0.3528	0.0	0.0
17	H(CCC)	0.4189	0.0	0.0
18	O(CCC)	-0.0090	0.0	0.0
19	M(CCC)	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0
21	F(CH)	0.3845	0.0	0.0
22	F(CC)	0.2417	0.0	0.0
23	A	0.3850	0.0	0.0
24	B	0.4238	0.0	0.0
25	C	0.0377	0.0	0.0
26	D	-0.0067	0.0	0.0
27	AO	0.0054	0.0	0.0
28	AM	-0.0066	0.0	0.0
29	AP	0.0076	0.0	0.0
30	BO	0.0732	0.0	0.0
31	BM	0.0761	0.0	0.0
32	BP	0.0365	0.0	0.0
	PEDSUM		0.0	0.0

BIBS UCLA

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO. 1- 3 SYM. BLOCK NO. 1

AIII 1

	FREQUENCIES	3064.404	3060.940	3060.931	2291.344	2282.816	2282.811	1579.500	1579.498	1425.043	1425.043
S 1	ST1	0.00	0.0	0.00	33.07	66.63	0.0	0.38	0.0	0.15	0.0
S 2	ST16	0.0	0.02	0.0	0.0	0.0	0.00	0.0	3.34	0.0	10.46
S 3	ST2	33.47	0.0	17.18	33.10	16.12	0.0	0.10	0.0	0.02	0.0
S 4	ST4	34.32	0.0	17.01	32.28	16.74	0.0	0.08	0.0	0.05	0.0
S 5	ST5	0.00	0.0	0.08	0.00	0.67	0.0	75.05	0.0	4.44	0.0
S 6	ST6	0.00	0.0	0.30	0.00	1.41	0.0	0.20	0.0	42.95	0.0
S 7	ST7	0.00	0.0	0.02	0.00	0.19	0.0	22.05	0.0	3.04	0.0
S 8	ST8	0.00	0.0	0.02	0.00	0.17	0.0	2.11	0.0	54.19	0.0
S 9	ST9	0.49	0.0	0.00	2.00	0.00	0.0	0.00	0.0	0.00	0.0
S10	ST10	0.44	0.0	0.00	1.71	0.00	0.0	0.00	0.0	0.00	0.0
S11	ST11	0.00	0.0	0.25	0.00	1.11	0.0	10.87	0.0	0.85	0.0
S12	ST12	0.0	51.79	0.0	0.0	0.0	48.83	0.0	0.32	0.0	0.06
S13	ST13	0.0	50.34	0.0	0.0	0.0	49.81	0.0	0.25	0.0	0.16
S14	ST14	0.0	0.08	0.0	0.0	0.0	0.67	0.0	75.05	0.0	4.44
S15	ST15	0.0	0.30	0.0	0.0	0.0	1.41	0.0	0.20	0.0	42.95
S16	ST17	0.0	0.00	0.0	0.0	0.0	0.00	0.0	0.00	0.0	0.00
S17	ST18	0.0	0.01	0.0	0.0	0.0	0.06	0.0	7.05	0.0	0.97
S18	ST19	0.0	0.01	0.0	0.0	0.0	0.05	0.0	0.66	0.0	16.93
S19	ST21	0.0	0.25	0.0	0.0	0.0	1.11	0.0	10.87	0.0	0.85
S20	ST20	0.0	0.00	0.0	0.0	0.0	0.23	0.0	12.19	0.0	27.15
S21	ST3	33.67	0.0	67.08	0.00	0.00	0.0	0.00	0.0	0.01	0.0

	FREQUENCIES	1308.554	1271.754	1098.186	1098.186	1003.906	956.823	908.478	824.113	824.113	591.820
S 1	ST1	0.0	0.0	0.01	0.0	0.08	0.37	0.0	0.0	0.01	0.0
S 2	ST16	0.01	4.65	0.0	6.51	0.0	0.0	31.31	44.86	0.0	0.12
S 3	ST2	0.0	0.0	0.00	0.0	0.16	0.48	0.0	0.0	0.00	0.0
S 4	ST4	0.0	0.0	0.00	0.0	0.03	0.28	0.0	0.0	0.02	0.0
S 5	ST5	0.0	0.0	7.50	0.0	0.00	0.00	0.0	0.0	1.83	0.0
S 6	ST6	0.0	0.0	34.21	0.0	0.00	0.00	0.0	0.0	22.48	0.0
S 7	ST7	0.0	0.0	46.27	0.0	0.00	0.00	0.0	0.0	29.85	0.0
S 8	ST8	0.0	0.0	4.55	0.0	0.00	0.00	0.0	0.0	39.47	0.0
S 9	ST9	0.0	0.0	0.00	0.0	72.40	25.53	0.0	0.0	0.00	0.0
S10	ST10	0.0	0.0	0.00	0.0	26.98	71.76	0.0	0.0	0.00	0.0
S11	ST11	0.0	0.0	0.69	0.0	0.00	0.00	0.0	0.0	0.28	0.0
S12	ST12	0.00	0.00	0.0	0.00	0.0	0.0	0.00	0.01	0.0	0.05
S13	ST13	0.00	0.00	0.0	0.01	0.0	0.0	0.00	0.05	0.0	0.11
S14	ST14	0.00	0.00	0.0	7.50	0.0	0.0	0.00	1.83	0.0	12.52
S15	ST15	0.00	0.00	0.0	34.21	0.0	0.0	0.00	22.48	0.0	0.02
S16	ST17	51.83	51.17	0.0	0.00	0.0	0.0	1.12	0.00	0.0	0.00
S17	ST18	23.23	29.50	0.0	14.81	0.0	0.0	15.35	9.55	0.0	0.12
S18	ST19	20.45	1.20	0.0	1.42	0.0	0.0	50.16	12.33	0.0	0.00
S19	ST21	0.00	0.00	0.0	0.69	0.0	0.0	0.00	0.28	0.0	86.41
S20	ST20	22.40	10.77	0.0	25.77	0.0	0.0	2.80	0.26	0.0	0.12
S21	ST3	0.0	0.0	0.00	0.0	0.01	0.01	0.0	0.0	0.03	0.0

	FREQUENCIES	591.818
S 1	ST1	0.11
S 2	ST16	0.0
S 3	ST2	0.02
S 4	ST4	0.04
S 5	ST5	12.52
S 6	ST6	0.02
S 7	ST7	0.37
S 8	ST8	0.00
S 9	ST9	0.00
S10	ST10	0.00
S11	ST11	86.41
S12	ST12	0.0
S13	ST13	0.0
S14	ST14	0.0
S15	ST15	0.0
S16	ST17	0.0
S17	ST18	0.0
S18	ST19	0.0
S19	ST21	0.0
S20	ST20	0.0
S21	ST3	0.00

BUS LILLE

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO. 1- 3 SYM. BLOCK NO. 2

AIII2

	FREQUENCIES	924.159	924.153	916.854	707.496	707.494	700.303	529.607	369.518	369.515	0.0
S 1	ST29	0.0	5.31	8.48	0.0	50.92	11.73	15.49	1.84	0.0	0.0
S 2	ST22	66.71	0.0	0.0	24.93	0.0	0.0	0.0	0.0	11.97	0.0
S 3	ST23	16.38	0.0	0.0	55.73	0.0	0.0	0.0	0.0	1.15	0.0
S 4	ST24	25.92	0.0	0.0	2.42	0.0	0.0	0.0	0.0	75.27	0.0
S 5	ST RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S 6	ST RED2	7.41	0.0	0.0	24.45	0.0	0.0	0.0	0.0	0.51	0.0
S 7	ST RED3	0.0	7.41	0.00	0.0	24.45	0.00	0.00	0.51	0.0	0.0
S 8	ST26	0.0	22.10	4.49	0.0	8.26	10.09	52.29	3.96	0.0	0.0
S 9	ST25	0.0	5.28	59.64	0.0	17.43	12.98	0.46	0.36	0.0	0.0
S10	ST28	0.0	0.00	31.74	0.0	0.00	51.27	23.00	0.00	0.0	0.0
S11	ST30	0.0	25.92	0.00	0.0	2.42	0.00	0.00	75.27	0.0	0.0
S12	ST27	0.0	49.30	25.15	0.0	2.06	0.08	10.47	6.71	0.0	0.0

	FREQUENCIES	0.0	0.0
S 1	ST29	0.0	0.0
S 2	ST22	0.0	0.0
S 3	ST23	0.0	0.0
S 4	ST24	0.0	0.0
S 5	ST RED1	0.0	0.0
S 6	ST RED2	0.0	0.0
S 7	ST RED3	0.0	0.0
S 8	ST26	0.0	0.0
S 9	ST25	0.0	0.0
S10	ST28	0.0	0.0
S11	ST30	0.0	0.0
S12	ST27	0.0	0.0

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 3 SYM. BLOCK NO. 1

AIII3

	FREQUENCIES	3064.404	3060.940	3060.931	2291.344	2282.816	2282.811	1579.500	1579.498	1425.043	1425.043
	ASSIGNMENT (PED)	ST4	ST12	ST3	ST2	ST1	ST13	ST5	ST14	ST8	ST15
	ASSIGNMENT (PED)	ST3	ST13	ST2	ST1	ST4	ST12	ST7	ST20	ST6	ST20
1	K(CH)	4.6740	90.838	91.043	91.043	0.006	0.005	0.005	0.002	0.002	0.010	0.010
2	K(CD)	4.8082	0.002	0.002	0.002	89.899	90.454	90.454	0.515	0.515	0.197	0.197
3	C(CH)	0.0240	0.008	0.004	0.004	-0.014	-0.007	-0.007	0.000	0.000	-0.000	-0.000
4	O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	-0.001	0.001	0.001	0.002	-0.002	-0.002	0.000	0.000	-0.000	0.000
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	H(CCH)	0.1701	0.063	0.058	0.058	0.259	0.388	0.388	16.367	16.368	36.775	36.775
10	O(CCH)	0.0015	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.105	-0.105	0.277	0.277
11	M(CCH)	-0.0070	0.000	0.001	0.001	0.000	0.009	0.009	0.613	0.613	1.484	1.484
12	P(CCH)	0.0049	0.000	0.000	0.000	0.000	0.000	0.000	0.355	0.355	-0.937	-0.937
13	K(CC)	5.2499	0.311	0.281	0.281	1.158	1.594	1.594	64.840	64.840	34.792	34.792
14	O(CC)	0.4954	0.059	0.014	0.014	0.226	0.041	0.041	-6.092	-6.092	2.560	2.560
15	M(CC)	-0.2115	-0.025	0.011	0.011	-0.096	0.064	0.064	2.612	2.612	1.401	1.401
16	P(CC)	0.3528	0.021	-0.010	-0.010	0.080	-0.029	-0.029	4.338	4.338	1.823	-1.823
17	H(CCC)	0.4189	0.310	0.177	0.177	1.277	0.805	0.805	7.084	7.084	3.021	3.021
18	O(CCC)	-0.0090	0.020	0.005	0.005	0.082	0.021	0.021	0.228	0.228	-0.062	-0.062
19	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	F(CH)	0.3845	8.294	8.384	8.384	6.678	6.529	6.529	8.617	8.617	20.559	20.559
22	F(CC)	0.2417	0.101	0.031	0.031	0.405	0.128	0.128	0.627	0.627	1.748	1.748
23	A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25	C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26	D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29	AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	BC	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31	BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32	BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	PEDSUM		100.000	100.000	100.000	100.000	100.001	100.001	100.001	100.002	100.001	100.001

BIBS LILLE

A III 4

	FREQUENCIES		1308.554	1271.794	1098.186	1098.186	1003.906	956.823	908.478	824.113	824.113	591.820
	ASSIGNMENT (PED)		ST17	ST17	ST7	ST15	ST9	ST10	ST19	ST16	ST8	ST21
	ASSIGNMENT (PED)		ST18	ST18	ST6	ST20	ST10	ST9	ST16	ST15	ST7	ST14
1	K(CH)	4.6740	0.000	0.000	0.001	0.001	0.039	0.018	0.000	0.045	0.045	0.004
2	K(CD)	4.8082	0.000	0.000	0.014	0.014	0.216	1.016	0.000	0.009	0.009	0.147
3	O(CH)	0.0240	-0.000	-0.000	-0.000	-0.000	-0.002	-0.003	0.000	-0.000	-0.000	-0.000
4	O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	-0.000	-0.000	-0.000	-0.000	0.000	0.000	0.000	-0.000	-0.000	-0.000
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	H(CCH)	0.1701	43.098	29.653	31.908	31.908	9.370	3.303	65.587	43.682	43.683	11.644
10	O(CCH)	0.0015	0.029	0.465	-0.219	-0.219	-0.000	0.000	-0.614	0.056	0.056	-0.002
11	M(CCH)	-0.0070	-3.538	-2.434	1.289	1.289	0.000	0.000	-5.384	1.781	1.781	0.009
12	P(CCH)	0.0049	0.049	0.787	0.742	0.742	0.000	-0.000	-1.041	-0.190	-0.190	0.007
13	K(CC)	5.2499	66.899	66.040	31.127	31.127	18.872	50.203	1.451	17.784	17.783	10.803
14	O(CC)	0.4954	-12.626	-12.464	1.717	1.717	3.562	9.475	-0.274	1.380	1.380	-1.017
15	M(CC)	-0.2115	-5.389	-5.320	1.254	1.254	-1.520	-4.044	-0.117	0.716	0.716	0.435
16	P(CC)	0.3528	-4.495	-4.438	-1.223	-1.223	1.268	3.374	-0.098	-0.983	-0.983	0.724
17	H(CCC)	0.4189	0.000	0.000	2.417	2.417	46.155	16.272	0.000	1.476	1.475	56.240
18	O(CCC)	-0.0090	-0.000	-0.000	-0.049	-0.049	2.975	1.049	-0.000	-0.036	-0.036	1.813
19	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	F(CH)	0.3845	16.282	28.016	29.590	29.590	7.804	9.351	40.495	33.370	33.370	5.179
22	F(CC)	0.2417	-0.308	-0.304	1.431	1.431	11.262	9.986	-0.007	0.910	0.910	14.013
23	A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25	C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26	D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29	AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	BC	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31	BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32	BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	PEDSUM		100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000

	FREQUENCIES	591.818	
	ASSIGNMENT (PED)	ST11	
	ASSIGNMENT (PED)	ST5	
1	K(CH)	4.6740	0.004
2	K(CD)	4.8082	0.147
3	C(CH)	0.0240	-0.000
4	C(CD)	0.0420	0.0
5	M(CH)	0.0	0.0
6	M(CD)	0.0060	0.0
7	P(CH)	-0.0060	-0.000
8	P(CD)	-0.0080	0.0
9	H(CCH)	0.1701	11.645
10	C(CCH)	0.0015	-0.002
11	M(CCH)	-0.0070	0.009
12	P(CCH)	0.0049	0.007
13	K(CC)	5.2499	10.803
14	O(CC)	0.4954	-1.017
15	M(CC)	-0.2115	0.435
16	P(CC)	0.3528	0.724
17	H(CCC)	0.4189	56.241
18	O(CCC)	-0.0090	1.813
19	M(CCC)	0.0	0.0
20	P(CCC)	0.0	0.0
21	F(CH)	0.3845	5.179
22	F(CC)	0.2417	14.013
23	A	0.3850	0.0
24	B	0.4238	0.0
25	C	0.0377	0.0
26	D	-0.0067	0.0
27	AO	0.0054	0.0
28	AM	-0.0066	0.0
29	AP	0.0076	0.0
30	BC	0.0732	0.0
31	BM	0.0761	0.0
32	BP	0.0365	0.0
	PEDSUM		100.001

BRS SOB 37717

A III 6

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 3 SYM. BLOCK NO. 2

	FREQUENCIES	924.159	924.153	916.854	707.496	707.494	700.303	529.607	369.518	369.515	0.0
	ASSIGNMENT (PED)	ST22	ST27	ST25	ST23	ST29	ST28	ST26	ST30	ST24	
	ASSIGNMENT (PED)	ST24	ST30	ST28	ST22	ST RED3	ST25	ST28		ST22	
1	K(CH)	4.6740	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	K(CD)	4.8082	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	C(CH)	0.0240	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	H(CCH)	0.1701	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	O(CCH)	0.0015	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	M(CCH)	-0.0070	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	P(CCH)	0.0049	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	K(CC)	5.2499	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	O(CC)	0.4954	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	M(CC)	-0.2115	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CC)	0.3528	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	H(CCC)	0.4189	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	O(CCC)	-0.0090	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	F(CH)	0.3845	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
22	F(CC)	0.2417	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
23	A	0.3850	81.906	81.906	100.900	79.472	79.472	35.404	77.892	12.840	12.840	0.0
24	B	0.4238	43.490	43.490	34.217	30.253	30.253	55.267	24.796	103.126	103.126	0.0
25	C	0.0377	-17.697	-17.697	-21.203	-10.090	-10.090	12.572	-1.592	11.051	11.051	0.0
26	D	-0.0067	0.776	0.776	-3.776	2.563	2.563	2.239	-0.284	0.053	0.053	0.0
27	AO	0.0054	-0.682	-0.682	-2.462	0.432	0.432	-0.158	2.147	-0.148	-0.148	0.0
28	AM	-0.0066	1.409	1.409	-3.470	1.367	1.367	-1.218	-2.679	0.221	0.221	0.0
29	AP	0.0076	0.960	0.960	-1.733	0.608	-0.608	-0.112	1.512	0.209	0.209	0.0
30	BC	0.0732	-4.690	-4.690	-11.818	4.088	4.088	-19.088	-8.564	-17.616	-17.616	0.0
31	BM	0.0761	-7.813	-7.813	12.295	-5.435	-5.435	19.858	8.909	-18.527	-18.527	0.0
32	BP	0.0365	2.341	2.341	-2.949	-2.040	-2.040	-4.764	-2.137	8.793	8.792	0.0
	PEDSUM		100.000	100.000	100.000	100.000	100.000	100.000	100.001	100.001	100.001	0.0

A III 7

	FREQUENCIES		0.0	0.0
	ASSIGNMENT (PED)			
	ASSIGNMENT (PED)			
1	K(CH)	4.6740	0.0	0.0
2	K(CD)	4.8082	0.0	0.0
3	O(CH)	0.0240	0.0	0.0
4	C(CD)	0.0420	0.0	0.0
5	M(CH)	0.0	0.0	0.0
6	M(CD)	0.0060	0.0	0.0
7	P(CH)	-0.0060	0.0	0.0
8	P(CD)	-0.0080	0.0	0.0
9	H(CCH)	0.1701	0.0	0.0
10	C(CCH)	0.0015	0.0	0.0
11	M(CCH)	-0.0070	0.0	0.0
12	P(CCH)	0.0049	0.0	0.0
13	K(CC)	5.2499	0.0	0.0
14	C(CC)	0.4954	0.0	0.0
15	M(CC)	-0.2115	0.0	0.0
16	P(CC)	0.3528	0.0	0.0
17	H(CCC)	0.4189	0.0	0.0
18	C(CCC)	-0.0090	0.0	0.0
19	M(CCC)	0.0	0.0	0.0
20	P(CCC)	0.0	0.0	0.0
21	F(CH)	0.3845	0.0	0.0
22	F(CC)	0.2417	0.0	0.0
23	A	0.3850	0.0	0.0
24	B	0.4238	0.0	0.0
25	C	0.0377	0.0	0.0
26	D	-0.0067	0.0	0.0
27	AO	0.0054	0.0	0.0
28	AM	-0.0066	0.0	0.0
29	AP	0.0076	0.0	0.0
30	BC	0.0732	0.0	0.0
31	BM	0.0761	0.0	0.0
32	BP	0.0365	0.0	0.0
	PEDSUM		0.0	0.0

BOS LIBRARY

A IV 1

EIGENVALUES AND EIGENVECTORS OF JWJ-MATRIX

	EIGENVALUE	0.14289E+09	0.10208E+09	0.93710E+08	0.63296E+08	0.58898E+08	0.44049E+08	0.30727E+08
2 K(CD)	4.8082	0.000106	0.000133	0.0	0.0	0.002748	0.001049	-0.002851
9 H(CCH)	0.1701	0.238083	0.055635	0.0	0.0	0.907175	0.156243	0.081322
10 O(CCH)	0.0015	0.402516	0.888887	0.0	0.0	-0.120999	-0.176745	-0.019135
11 M(CCH)	-0.0070	0.868889	-0.443550	0.0	0.0	-0.172069	-0.130391	-0.006445
12 P(CCH)	0.0049	0.150249	0.095573	0.0	0.0	-0.221111	0.955677	0.030041
13 K(CC)	5.2499	0.000671	0.000554	0.0	0.0	0.026745	0.005804	0.003440
14 O(CC)	0.4954	-0.008801	0.016252	0.0	0.0	-0.006629	-0.017665	-0.009305
15 M(CC)	-0.2115	0.014330	-0.014485	0.0	0.0	-0.011094	-0.010864	-0.009010
16 P(CC)	0.3528	-0.006011	-0.002300	0.0	0.0	-0.006753	0.023695	-0.002097
17 H(CCC)	0.4189	-0.002886	0.005061	0.0	0.0	0.056654	0.029566	-0.194569
21 F(CH)	0.3845	0.056808	0.007839	0.0	0.0	0.268407	0.065675	0.015560
23 A	0.3850	0.0	0.0	-0.264383	-0.255129	0.0	0.0	0.0
24 B	0.4238	0.0	0.0	-0.093139	-0.113324	0.0	0.0	0.0
25 C	0.0377	0.0	0.0	0.645529	0.535843	0.0	0.0	0.0
26 D	-0.0067	0.0	0.0	-0.442380	0.507234	0.0	0.0	0.0
27 AO	0.0054	0.0	0.0	0.455686	-0.055502	0.0	0.0	0.0
28 AM	-0.0066	0.0	0.0	-0.254843	0.546767	0.0	0.0	0.0
29 AP	0.0076	0.0	0.0	0.054501	-0.134422	0.0	0.0	0.0
30 BO	0.0732	0.0	0.0	0.162556	-0.049237	0.0	0.0	0.0
31 BM	0.0761	0.0	0.0	-0.082770	0.226041	0.0	0.0	0.0
32 BP	0.0365	0.0	0.0	0.013355	-0.063478	0.0	0.0	0.0
22 F(CC)	0.2417	-0.002073	0.007625	0.0	0.0	0.028340	0.001442	-0.069672
5 M(CH)	0.0	0.000169	-0.000132	0.0	0.0	0.000088	0.000083	-0.011865
6 M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7 P(CH)	-0.0060	-0.000043	-0.000110	0.0	0.0	-0.000113	0.000379	0.003798
8 P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1 K(CH)	4.6740	0.000357	0.000092	0.0	0.0	0.004470	0.001529	-0.000922
3 O(CH)	0.0240	-0.000057	0.000112	0.0	0.0	-0.001052	-0.000962	0.006959
18 O(CCC)	-0.0090	-0.003292	0.010680	0.0	0.0	-0.081047	-0.081553	0.617824
19 M(CCC)	0.0	0.012542	-0.007740	0.0	0.0	0.010412	0.003391	-0.669880
20 P(CCC)	0.0	-0.004921	-0.010532	0.0	0.0	-0.014346	0.033813	0.343911
4 O(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0

A IV2

	EIGENVALUE	0.22391E+08	0.13882E+08	0.12159E+08	0.79423E+07	0.73923E+07	0.32108E+07	0.24201E+07
2 K(CD)	4.8082	0.0	0.0	0.0	-0.007080	0.0	0.0	-0.002313
9 H(CCH)	0.1701	0.0	0.0	0.0	0.062316	0.0	0.0	0.002282
10 O(CCH)	0.0015	0.0	0.0	0.0	-0.029496	0.0	0.0	0.000166
11 M(CCH)	-0.0070	0.0	0.0	0.0	-0.025630	0.0	0.0	-0.000043
12 P(CCH)	0.0049	0.0	0.0	0.0	0.059188	0.0	0.0	-0.000465
13 K(CC)	5.2499	0.0	0.0	0.0	-0.019280	0.0	0.0	0.001045
14 C(CC)	0.4954	0.0	0.0	0.0	0.022156	0.0	0.0	0.001197
15 M(CC)	-0.2115	0.0	0.0	0.0	0.021000	0.0	0.0	0.004834
16 P(CC)	0.3528	0.0	0.0	0.0	-0.028361	0.0	0.0	0.003989
17 H(CCC)	0.4189	0.0	0.0	0.0	-0.376137	0.0	0.0	0.000434
21 F(CH)	0.3845	0.0	0.0	0.0	0.047751	0.0	0.0	-0.008149
23 A	0.3850	0.325952	0.116255	-0.238588	0.0	-0.336185	0.128144	0.0
24 B	0.4238	0.128033	-0.211480	-0.312595	0.0	-0.075108	-0.476345	0.0
25 C	0.0377	-0.063086	-0.297550	-0.149391	0.0	-0.263391	0.039734	0.0
26 D	-0.0067	-0.492301	0.239464	0.039827	0.0	0.184199	-0.285965	0.0
27 AO	0.0054	0.217093	0.667591	-0.184190	0.0	0.301625	-0.391047	0.0
28 AM	-0.0066	0.457393	0.333870	-0.133052	0.0	-0.356880	0.151714	0.0
29 AP	0.0076	-0.440034	0.254201	-0.630031	0.0	0.033092	0.502823	0.0
30 BC	0.0732	-0.067815	0.358864	0.579335	0.0	-0.114505	0.339148	0.0
31 BM	0.0761	0.265389	-0.204966	-0.162406	0.0	0.608381	0.313671	0.0
32 BP	0.0365	-0.325607	0.057584	-0.104332	0.0	-0.418765	-0.176468	0.0
22 F(CC)	0.2417	0.0	0.0	0.0	-0.152068	0.0	0.0	0.008018
5 M(CH)	0.0	0.0	0.0	0.0	0.014992	0.0	0.0	0.999718
6 M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7 P(CH)	-0.0060	0.0	0.0	0.0	-0.008912	0.0	0.0	-0.000438
8 P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1 K(CH)	4.6740	0.0	0.0	0.0	0.001800	0.0	0.0	-0.005218
3 O(CH)	0.0240	0.0	0.0	0.0	0.011041	0.0	0.0	-0.000020
18 C(CCC)	-0.0090	0.0	0.0	0.0	0.612834	0.0	0.0	-0.001324
19 M(CCC)	0.0	0.0	0.0	0.0	0.447312	0.0	0.0	-0.012921
20 P(CCC)	0.0	0.0	0.0	0.0	-0.495937	0.0	0.0	0.013594
4 C(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0

		EIGENVALUE	0.21007E+07	0.16144E+07	0.80856E+06	0.56487E+06	0.50105E+06	0.26500E+06	0.23346E+06
2	K(CD)	4.8082	0.171242	0.006788	0.001094	0.087909	-0.788053	-0.279279	0.0
9	H(CCH)	0.1701	-0.236546	-0.008183	0.000740	0.001026	0.056487	-0.026309	0.0
10	O(CCH)	0.0015	0.012879	0.000264	0.000163	-0.011084	0.002976	-0.009727	0.0
11	M(CCH)	-0.0070	0.009924	0.000643	-0.000571	0.022114	0.000924	-0.001382	0.0
12	P(CCH)	0.0049	-0.012162	-0.000143	-0.000164	-0.000285	-0.000593	0.022087	0.0
13	K(CC)	5.2499	0.004837	0.004311	-0.000127	-0.302826	-0.056023	-0.027416	0.0
14	O(CC)	0.4954	0.048177	0.010055	0.000115	0.648330	0.031816	0.499846	0.0
15	M(CC)	-0.2115	0.014920	0.004218	0.013046	-0.608880	-0.144472	0.537375	0.0
16	P(CC)	0.3528	-0.004382	0.001740	0.003109	0.299154	0.064572	-0.136074	0.0
17	H(CCC)	0.4189	0.012172	0.007486	-0.007216	0.008043	-0.011638	0.014261	0.0
21	F(CH)	0.3845	0.786966	0.025458	0.000193	0.030293	-0.186130	0.099753	0.0
23	A	0.3850	0.0	0.0	0.0	0.0	0.0	0.0	0.702079
24	B	0.4238	0.0	0.0	0.0	0.0	0.0	0.0	0.055516
25	C	0.0377	0.0	0.0	0.0	0.0	0.0	0.0	0.332231
26	D	-0.0067	0.0	0.0	0.0	0.0	0.0	0.0	0.360579
27	AO	0.0054	0.0	0.0	0.0	0.0	0.0	0.0	0.046318
28	AM	-0.0066	0.0	0.0	0.0	0.0	0.0	0.0	-0.361727
29	AP	0.0076	0.0	0.0	0.0	0.0	0.0	0.0	-0.062186
30	BO	0.0732	0.0	0.0	0.0	0.0	0.0	0.0	0.201255
31	BM	0.0761	0.0	0.0	0.0	0.0	0.0	0.0	0.034864
32	BP	0.0365	0.0	0.0	0.0	0.0	0.0	0.0	-0.291606
22	F(CC)	0.2417	0.038785	0.018103	-0.000088	0.061351	-0.059657	0.559411	0.0
5	M(CH)	0.0	0.009397	0.000175	0.000523	0.000779	0.000271	-0.007355	0.0
6	P(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	P(CH)	-0.0060	0.000716	-0.002494	0.999822	0.007064	0.002652	-0.003855	0.0
8	P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	K(CH)	4.6740	0.537239	0.028328	-0.000965	-0.118566	0.554562	-0.171395	0.0
3	O(CH)	0.0240	-0.039779	0.998912	0.002621	-0.002241	-0.003654	-0.012651	0.0
18	O(CCC)	-0.0090	-0.001168	-0.008672	0.001580	0.013207	0.013413	0.073424	0.0
19	M(CCC)	0.0	-0.021007	-0.002430	0.009455	-0.008000	0.012699	-0.036643	0.0
20	P(CCC)	0.0	0.003917	-0.000126	-0.000209	-0.017271	0.018167	-0.058293	0.0
4	C(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0

AIV3

BDS LILLE

AIV4

	EIGENVALUE	0.11415E+06	0.72089E+05	0.36968E+05	0.68330E+02	0.14952E+02	0.63943E+01	0.28793E+01
2 K(CD)	4.8082	-0.073176	0.392731	0.322483	-0.014299	0.0	0.0	-0.000177
9 H(CCH)	0.1701	-0.037778	0.124361	0.074429	-0.001370	0.0	0.0	-0.000018
10 O(CCH)	0.0015	0.004861	-0.000094	-0.018013	0.000047	0.0	0.0	0.000002
11 M(CCH)	-0.0070	0.011388	-0.013159	0.009529	0.000013	0.0	0.0	-0.000001
12 P(CCH)	0.0049	-0.008620	-0.006436	0.030349	-0.000009	0.0	0.0	-0.000003
13 K(CC)	5.2499	0.678973	-0.107926	0.225368	0.368277	0.0	0.0	-0.493781
14 O(CC)	0.4954	-0.131666	0.145260	0.122183	0.459911	0.0	0.0	-0.243811
15 M(CC)	-0.2115	-0.139541	0.337195	-0.157580	0.309366	0.0	0.0	0.252397
16 P(CC)	0.3528	0.557634	0.371800	-0.350823	0.134886	0.0	0.0	0.499398
17 H(CCC)	0.4189	0.002658	-0.298773	0.338040	0.150559	0.0	0.0	0.372948
21 F(CH)	0.3845	0.053776	-0.357888	-0.348264	0.004976	0.0	0.0	0.000077
23 A	0.3850	0.0	0.0	0.0	0.0	0.050779	-0.251782	0.0
24 B	0.4238	0.0	0.0	0.0	0.0	0.375850	0.665402	0.0
25 C	0.0377	0.0	0.0	0.0	0.0	-0.000005	0.000005	0.0
26 D	-0.0067	0.0	0.0	0.0	0.0	-0.000006	0.000005	0.0
27 AO	0.0054	0.0	0.0	0.0	0.0	0.025395	-0.125895	0.0
28 AM	-0.0066	0.0	0.0	0.0	0.0	-0.025390	0.125890	0.0
29 AP	0.0076	0.0	0.0	0.0	0.0	-0.050791	0.251790	0.0
30 BO	0.0732	0.0	0.0	0.0	0.0	0.432983	0.382129	0.0
31 BM	0.0761	0.0	0.0	0.0	0.0	0.547266	-0.184400	0.0
32 BP	0.0365	0.0	0.0	0.0	0.0	0.604414	-0.467671	0.0
22 F(CC)	0.2417	0.341716	0.088279	0.236455	-0.682855	0.0	0.0	-0.007639
5 M(CH)	0.0	-0.003823	-0.005448	0.002346	0.002349	0.0	0.0	0.000026
6 M(CD)	0.0060	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7 P(CH)	-0.0060	0.001411	-0.009062	0.008477	-0.004689	0.0	0.0	-0.000053
8 P(CD)	-0.0080	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1 K(CH)	4.6740	-0.070415	0.438689	0.402589	-0.007503	0.0	0.0	-0.000107
3 C(CH)	0.0240	-0.006776	-0.007272	-0.011443	0.002443	0.0	0.0	0.000028
18 C(CCC)	-0.0090	0.080797	-0.041345	0.113634	-0.096516	0.0	0.0	0.080496
19 M(CCC)	0.0	-0.002333	0.189534	-0.220183	-0.143169	0.0	0.0	-0.251893
20 P(CCC)	0.0	-0.082398	0.300002	-0.400432	-0.140902	0.0	0.0	-0.417799
4 C(CD)	0.0420	0.0	0.0	0.0	0.0	0.0	0.0	0.0

	EIGENVALUE	0.0	0.0	0.0	-0.57740E+01
2	K(CD)	4.8082	0.0	0.0	0.0	-0.000983
9	H(CCH)	0.1701	0.0	0.0	0.0	-0.000096
10	O(CCH)	0.0015	0.0	0.0	0.0	0.000004
11	M(CCH)	-0.0070	0.0	0.0	0.0	0.000001
12	P(CCH)	0.0049	0.0	0.0	0.0	-0.000002
13	K(CC)	5.2499	0.0	0.0	0.0	0.018478
14	O(CC)	0.4954	0.0	0.0	0.0	0.027949
15	M(CC)	-0.2115	0.0	0.0	0.0	0.024228
16	P(CC)	0.3528	0.0	0.0	0.0	0.015632
17	H(CCC)	0.4189	0.0	0.0	0.0	0.671251
21	F(CH)	0.3845	0.0	0.0	0.0	0.000352
23	A	0.3850	0.0	0.0	0.0	0.0
24	B	0.4238	0.0	0.0	0.0	0.0
25	C	0.0377	0.0	0.0	0.0	0.0
26	D	-0.0067	0.0	0.0	0.0	0.0
27	AO	0.0054	0.0	0.0	0.0	0.0
28	AM	-0.0066	0.0	0.0	0.0	0.0
29	AP	0.0076	0.0	0.0	0.0	0.0
30	BC	0.0732	0.0	0.0	0.0	0.0
31	BM	0.0761	0.0	0.0	0.0	0.0
32	BP	0.0365	0.0	0.0	0.0	0.0
22	F(CC)	0.2417	0.0	0.0	0.0	-0.046353
5	M(CH)	0.0	0.0	0.0	0.0	0.000159
6	M(CD)	0.0060	1.000000	0.0	0.0	0.0
7	P(CH)	-0.0060	0.0	0.0	0.0	-0.000319
8	P(CD)	-0.0080	0.0	1.000000	0.0	0.0
1	K(CH)	4.6740	0.0	0.0	0.0	-0.000525
3	O(CH)	0.0240	0.0	0.0	0.0	0.000166
18	O(CCC)	-0.0090	0.0	0.0	0.0	0.431978
19	M(CCC)	0.0	0.0	0.0	0.0	0.424501
20	P(CCC)	0.0	0.0	0.0	0.0	0.422504
4	O(CD)	0.0420	0.0	0.0	1.000000	0.0

A IV 5

BDS STATE

AV1

EIGENVALUES AND EIGENVECTORS OF JWJ-MATRIX(VARIABLE CONSTANTS)

	EIGENVALUE	0.14287E+09	0.10205E+09	0.93711E+08	0.63296E+08	0.58594E+08	0.43794E+08	0.22391E+08
2	K(CD)	0.000102	0.000146	0.0	0.0	0.002593	0.000906	0.0
9	H(CCH)	0.238131	0.055984	0.0	0.0	0.909430	0.173123	0.0
10	O(CCH)	0.402705	0.888768	0.0	0.0	-0.120197	-0.181327	0.0
11	M(CCH)	0.868885	-0.444008	0.0	0.0	-0.170639	0.133147	0.0
12	P(CCH)	0.150352	0.096124	0.0	0.0	-0.232476	0.055518	0.0
13	K(CC)	0.000682	0.000574	0.0	0.0	0.026700	0.006083	0.0
14	O(CC)	-0.008827	0.016237	0.0	0.0	-0.006634	0.017795	0.0
15	M(CC)	0.014301	-0.014501	0.0	0.0	-0.011159	-0.011037	0.0
16	P(CC)	-0.006007	-0.002261	0.0	0.0	-0.007315	0.023209	0.0
17	H(CCC)	-0.003271	0.005783	0.0	0.0	0.047336	0.019537	0.0
21	F(CH)	0.056790	0.007953	0.0	0.0	0.268598	0.070791	0.0
23	A	0.0	0.0	-0.264384	-0.255130	0.0	0.0	0.325952
24	B	0.0	0.0	-0.093140	-0.113325	0.0	0.0	0.128033
25	C	0.0	0.0	0.645530	0.535844	0.0	0.0	-0.063086
26	D	0.0	0.0	-0.442381	0.507234	0.0	0.0	-0.492302
27	AO	0.0	0.0	0.455687	-0.055502	0.0	0.0	0.217093
28	AM	0.0	0.0	-0.254845	0.546768	0.0	0.0	0.457394
29	AP	0.0	0.0	0.054501	-0.134422	0.0	0.0	-0.440035
30	BO	0.0	0.0	0.162556	-0.049237	0.0	0.0	-0.067815
31	BM	0.0	0.0	-0.082771	0.226041	0.0	0.0	0.265390
32	BP	0.0	0.0	0.013355	-0.063479	0.0	0.0	-0.325608

	EIGENVALUE	0.13882E+08	0.12159E+08	0.73923E+07	0.32108E+07	0.23903E+07	0.15817E+07	0.56126E+06
2	K(CD)	0.0	0.0	0.0	0.0	0.024133	0.286404	0.039371
9	H(CCH)	0.0	0.0	0.0	0.0	-0.049114	-0.268966	-0.016989
10	O(CCH)	0.0	0.0	0.0	0.0	0.036041	0.014058	0.011000
11	M(CCH)	0.0	0.0	0.0	0.0	0.016738	0.009860	-0.021290
12	P(CCH)	0.0	0.0	0.0	0.0	-0.009043	-0.012951	0.001572
13	K(CC)	0.0	0.0	0.0	0.0	0.025646	-0.010877	0.310702
14	O(CC)	0.0	0.0	0.0	0.0	-0.008017	0.078831	-0.633068
15	M(CC)	0.0	0.0	0.0	0.0	-0.013683	0.024659	0.636620
16	P(CC)	0.0	0.0	0.0	0.0	0.041789	-0.011161	-0.307461
17	H(CCC)	0.0	0.0	0.0	0.0	0.996953	0.013078	0.007185
21	F(CH)	0.0	0.0	0.0	0.0	-0.006268	0.015380	0.020187
23	A	0.116256	-0.238588	-0.336184	0.128142	0.0	0.0	0.0
24	B	-0.211479	-0.312595	-0.075107	-0.476344	0.0	0.0	0.0
25	C	-0.297550	-0.149391	-0.263391	0.039733	0.0	0.0	0.0
26	D	0.239464	0.039828	0.184200	-0.285964	0.0	0.0	0.0
27	AO	0.667593	-0.184188	0.301625	-0.391045	0.0	0.0	0.0
28	AM	0.333872	-0.133052	-0.356879	0.151712	0.0	0.0	0.0
29	AP	0.254203	-0.630031	0.033090	0.502823	0.0	0.0	0.0
30	BO	0.358863	0.579335	-0.114506	0.339148	0.0	0.0	0.0
31	BM	-0.204966	-0.162407	0.608378	0.313672	0.0	0.0	0.0
32	BP	0.057584	-0.104331	-0.418764	-0.176470	0.0	0.0	0.0

	EIGENVALUE	0.31237E+06	0.23346E+06	0.18535E+06	0.81522E+05	0.18662E+05	0.14162E+02	0.78918E+01
2	K(CD)	-0.941054	0.0	0.172445	0.019827	0.011062	0.0	0.0
9	H(CCH)	-0.071616	0.0	0.052417	0.003109	-0.013584	0.0	0.0
10	O(CCH)	0.002274	0.0	-0.012338	0.003111	-0.008485	0.0	0.0
11	M(CCH)	0.000172	0.0	-0.010667	0.002216	0.009918	0.0	0.0
12	P(CCH)	0.000423	0.0	0.022726	-0.006755	0.016804	0.0	0.0
13	K(CC)	-0.027695	0.0	-0.319447	0.598697	0.663843	0.0	0.0
14	O(CC)	0.120427	0.0	0.615533	0.316887	0.313757	0.0	0.0
15	M(CC)	0.147942	0.0	0.603865	0.337774	-0.304348	0.0	0.0
16	P(CC)	-0.068500	0.0	-0.327000	0.651566	-0.605642	0.0	0.0
17	H(CCC)	0.027445	0.0	0.033312	-0.036145	0.005595	0.0	0.0
21	F(CH)	0.258231	0.0	-0.114508	-0.027305	-0.025430	0.0	0.0
23	A	0.0	-0.702070	0.0	0.0	0.0	-0.070395	0.247036
24	B	0.0	-0.055533	0.0	0.0	0.0	0.639227	-0.418821
25	C	0.0	-0.332230	0.0	0.0	0.0	-0.000006	0.000001
26	D	0.0	-0.360578	0.0	0.0	0.0	-0.000005	0.000001
27	AO	0.0	-0.046315	0.0	0.0	0.0	-0.035191	0.123516
28	AM	0.0	0.361723	0.0	0.0	0.0	0.035196	-0.123518
29	AP	0.0	0.062180	0.0	0.0	0.0	0.070382	-0.247032
30	BO	0.0	-0.201263	0.0	0.0	0.0	0.560039	-0.140909
31	BM	0.0	-0.034857	0.0	0.0	0.0	0.401680	0.414917
32	BP	0.0	0.291620	0.0	0.0	0.0	0.322508	0.692828

BUS LILLE

AV2

P-MATRIX

		22 F(CC)	5 M(CH)	6 M(CD)	7 P(CH)	8 P(CD)	1 K(CH)	3 O(CH)
		0.2417	0.0	0.0060	-0.0060	-0.0080	4.6740	0.0240
2 K(CD)	4.8082	0.020146	0.0	0.0	-0.023235	0.0	0.858671	0.0
9 H(CCH)	0.1701	0.012850	0.0	0.0	-0.022766	0.0	0.250359	0.0
10 O(CCH)	0.0015	-0.012573	0.0	0.0	-0.011191	0.0	-0.018572	0.0
11 M(CCH)	-0.0070	-0.006805	0.0	0.0	0.012429	0.0	-0.011786	0.0
12 P(CCH)	0.0049	0.025270	0.0	0.0	0.022621	0.0	0.022411	0.0
13 K(CC)	5.2499	-1.670275	0.0	0.0	0.191270	0.0	0.025619	0.0
14 O(CC)	0.4954	-0.844703	0.0	0.0	0.052558	0.0	0.519459	0.0
15 M(CC)	-0.2115	-0.699116	0.0	0.0	-0.240870	0.0	0.468357	0.0
16 P(CC)	0.3528	-1.486621	0.0	0.0	-0.447678	0.0	0.081061	0.0
17 H(CCC)	0.4189	-0.290018	0.0	0.0	0.398628	0.0	-0.014188	0.0
21 F(CH)	0.3845	0.002007	0.0	0.0	-0.011802	0.0	-0.834265	0.0
23 A	0.3850	0.000271	0.0	0.0	0.000769	0.0	-0.000514	0.0
24 B	0.4238	-0.008657	0.0	0.0	-0.006971	0.0	0.004639	0.0
25 C	0.0377	0.000000	0.0	0.0	0.000000	0.0	-0.000000	0.0
26 D	-0.0067	0.000000	0.0	0.0	0.000000	0.0	-0.000000	0.0
27 AO	0.0054	0.000136	0.0	0.0	0.000384	0.0	-0.000257	0.0
28 AM	-0.0066	-0.000136	0.0	0.0	-0.000384	0.0	0.000257	0.0
29 AP	0.0076	-0.000271	0.0	0.0	-0.000769	0.0	0.000514	0.0
30 BO	0.0732	-0.008352	0.0	0.0	-0.006106	0.0	0.004061	0.0
31 BM	0.0761	-0.007742	0.0	0.0	-0.004377	0.0	0.002904	0.0
32 BP	0.0365	-0.007437	0.0	0.0	-0.003512	0.0	0.002326	0.0

		18 O(CCC)	19 M(CCC)	20 P(CCC)	4 O(CD)
		-0.0090	0.0	0.0	0.0420
2 K(CD)	4.8082	0.111086	-0.470513	0.360097	0.0
9 H(CCH)	0.1701	0.177208	-0.667021	0.490482	0.0
10 O(CCH)	0.0015	-0.171565	0.448088	-0.276187	0.0
11 M(CCH)	-0.0070	-0.090001	0.343982	-0.254349	0.0
12 P(CCH)	0.0049	0.344322	-0.898338	0.553338	0.0
13 K(CC)	5.2499	-15.068549	46.283051	-31.234726	0.0
14 O(CC)	0.4954	-2.208709	6.889826	-4.689940	0.0
15 M(CC)	-0.2115	-3.249297	8.312370	-5.048381	0.0
16 P(CC)	0.3528	-17.248032	49.108597	-31.832153	0.0
17 H(CCC)	0.4189	3.451973	-4.203121	2.250375	0.0
21 F(CH)	0.3845	-0.000441	-0.069348	0.070156	0.0
23 A	0.3850	0.019887	-0.055088	0.035177	0.0
24 B	0.4238	-0.112172	0.295032	-0.182652	0.0
25 C	0.0377	0.000000	-0.000000	0.000000	0.0
26 D	-0.0067	0.000000	-0.000000	0.000000	0.0
27 AO	0.0054	0.009943	-0.027543	0.017588	0.0
28 AM	-0.0066	-0.009944	0.027544	-0.017588	0.0
29 AP	0.0076	-0.019887	0.055086	-0.035177	0.0
30 BO	0.0732	-0.089798	0.233058	-0.143077	0.0
31 BM	0.0761	-0.045052	0.109111	-0.063928	0.0
32 BP	0.0365	-0.022680	0.047140	-0.024355	0.0

AV3

CORRELATION MATRIX

FORCE NO.	2	9	10	11	12	13	14	15	16	17	21	23	24	25	26
2	1.00	0.37	-0.09	-0.02	0.07	0.04	0.08	0.01	0.04	-0.04	-0.46	0.0	0.0	0.0	0.0
9	0.37	1.00	-0.05	-0.34	-0.05	-0.32	-0.07	0.36	0.24	-0.09	-0.76	0.0	0.0	0.0	0.0
10	-0.09	-0.05	1.00	-0.30	-0.47	-0.38	-0.49	0.34	0.51	-0.04	0.25	0.0	0.0	0.0	0.0
11	-0.02	-0.34	-0.30	1.00	0.22	0.57	0.44	-0.57	0.44	0.08	-0.03	0.0	0.0	0.0	0.0
12	0.07	-0.05	-0.47	0.22	1.00	0.47	0.53	-0.37	0.63	0.07	-0.22	0.0	0.0	0.0	0.0
13	0.04	-0.32	-0.38	0.57	0.47	1.00	0.74	-0.56	-0.60	-0.03	-0.19	0.0	0.0	0.0	0.0
14	0.08	-0.07	-0.49	0.44	0.53	0.74	1.00	-0.27	0.54	0.03	-0.28	0.0	0.0	0.0	0.0
15	0.01	0.36	0.34	-0.57	-0.37	-0.56	-0.27	1.00	0.73	-0.06	0.03	0.0	0.0	0.0	0.0
16	-0.04	0.24	0.51	-0.44	-0.63	-0.60	-0.54	0.73	1.00	-0.15	0.16	0.0	0.0	0.0	0.0
17	-0.04	-0.09	-0.04	0.08	0.07	-0.03	0.03	-0.06	-0.15	1.00	-0.01	0.0	0.0	0.0	0.0
21	-0.46	-0.76	0.25	-0.03	-0.22	-0.19	-0.28	0.03	0.16	-0.01	1.00	0.0	0.0	0.0	0.0
23	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.00	-0.80	0.02	0.02
24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.80	1.00	-0.00	-0.00
25	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	-0.00	1.00	0.91
26	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	-0.00	0.91	1.00
27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.00	-0.80	0.00	0.00
28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.00	0.80	-0.02	-0.02
29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.00	0.80	-0.00	-0.00
30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.51	0.92	0.00	0.00
31	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.67	-0.09	-0.00	-0.00
32	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.86	-0.38	-0.00	-0.00

FORCE NO.	27	28	29	30	31	32
2	0.0	0.0	0.0	0.0	0.0	0.0
9	0.0	0.0	0.0	0.0	0.0	0.0
10	0.0	0.0	0.0	0.0	0.0	0.0
11	0.0	0.0	0.0	0.0	0.0	0.0
12	0.0	0.0	0.0	0.0	0.0	0.0
13	0.0	0.0	0.0	0.0	0.0	0.0
14	0.0	0.0	0.0	0.0	0.0	0.0
15	0.0	0.0	0.0	0.0	0.0	0.0
16	0.0	0.0	0.0	0.0	0.0	0.0
17	0.0	0.0	0.0	0.0	0.0	0.0
21	0.0	0.0	0.0	0.0	0.0	0.0
23	1.00	-1.00	-1.00	-0.51	0.67	0.86
24	-0.80	0.80	0.80	0.92	-0.09	-0.38
25	0.00	-0.02	-0.00	0.00	-0.00	-0.00
26	0.00	-0.02	-0.00	0.00	-0.00	-0.00
27	1.00	-1.00	-1.00	-0.51	0.67	0.86
28	-1.00	1.00	1.00	0.51	-0.67	-0.86
29	-1.00	1.00	1.00	0.51	-0.67	-0.86
30	-0.51	0.51	0.51	1.00	0.30	0.01
31	0.67	-0.67	-0.67	0.30	1.00	0.96
32	0.86	-0.86	-0.86	0.01	0.96	1.00

AV4

INTRINSIC FORCE CONSTANTS

NO.	F.C.	DISPERSION
1	0.05210	0.00060
2	0.03549	0.00071
3	-0.10330	0.00074
4	-0.12310	0.00090
5	0.45990	0.00093
6	0.11518	0.00108
7	-0.08718	0.00129
8	0.17881	0.00151
9	-0.04160	0.00192
10	-0.20892	0.00205
11	-0.30043	0.00253
12	-0.14553	0.00263
13	-0.10617	0.00399
14	-0.02966	0.00459
15	3.60396	0.00493
16	0.23235	0.00562
17	-0.01128	0.00794
18	-1.13619	0.00950
19	-1.50335	0.01009
20	-2.02758	0.01387
21	0.31281	0.01478
22	3.15567	0.02114
23	3.28400	0.02660
24	4.66170	0.03715
25	1.94028	0.86403
26	0.27419	1.84710
27	0.18233	2.82446
28	-2.43798	4.20912
29	0.00600	
30	-0.00800	
31	0.04200	
32	0.37025	

DISPERSION

NO.		F.C.	DISPERSION
2	K(CD)	4.80815	0.01146
9	H(CCH)	0.17006	0.00211
10	O(CCH)	0.00145	0.00080
11	M(CCH)	-0.00698	0.00080
12	P(CCH)	0.00492	0.00132
13	K(CC)	5.24995	0.03510
14	C(CC)	0.49542	0.01999
15	M(CC)	-0.21147	0.01978
16	P(CC)	0.35278	0.03315
17	H(CCC)	0.41886	0.00435
21	F(CH)	0.38450	0.00607
23	A	0.38496	0.58879
24	B	0.42381	1.47994
25	C	0.03770	0.00463
26	D	-0.00671	0.00511
27	AO	0.00541	0.29436
28	AM	-0.00662	0.29440
29	AP	0.00761	0.58870
30	BO	0.07319	1.02836
31	BM	0.07614	1.19327
32	BP	0.03653	1.70968

POTENTIAL ENERGY DISTRIBUTION
MOLECULE-ISOTOPE NO. 1- 1 SYM. BLOCK NO. 1

	FREQUENCIES	3071.73	3071.167	3067.627	3067.509	3062.226	3062.215	3055.715	3055.701	3054.496	3054.463
S 1	CX ST	54.19	1.71	0.00	0.00	11.57	2.17	46.93	4.17	0.00	0.00
S 2	CCX1 DEF	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.01
S 3	CH ST18	3.61	0.18	0.00	0.00	53.19	1[illegible].95	30.81	2.68	0.00	0.00
S 4	CH ST 7	57.81	2.88	0.00	0.00	19.86	3.76	15.15	1.36	0.00	0.00
S 5	CC ST 8	0.00	0.00	0.00	0.00	0.03	0.01	0.06	0.01	0.00	0.00
S 6	ST+DEF19	0.12	0.01	0.00	0.00	0.22	0.04	0.00	0.00	0.00	0.00
S 7	CCH DEF9	0.00	0.00	0.00	0.00	0.01	0.00	0.02	0.00	0.00	0.00
S 8	CCHDEF20	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
S 9	CCCDEF12	0.01	0.00	0.00	0.00	0.22	0.04	0.55	0.05	0.00	0.00
S10	CC ST 2	0.64	0.03	0.00	0.00	0.04	0.01	0.00	0.00	0.00	0.00
S11	CCC DEF6	0.01	0.00	0.00	0.00	0.11	0.02	0.20	0.02	0.00	0.00
S12	CH ST18	0.00	0.00	57.89	43.[illegible]7	0.00	0.00	0.00	0.00	0.00	0.01
S13	CH ST 7	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	7.65	92.96
S14	CC ST 8	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.01	0.15
S15	ST+DEF19	0.00	0.00	0.34	0.25	0.00	0.00	0.00	0.00	0.00	0.00
S16	CC ST 14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S17	CCHDEF 9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
S18	CCHDEF 9	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
S19	CCC DEF6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.47
S20	CCN DEF	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.02
S21	C-N ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S22	STCHCENT	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.04	0.00
S23	C=N ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S24	BETA 1-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S25	C-N=CDEF	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S26	N=C-CDEF	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S27	CC=CX ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S28	CCCX DEF	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.02	0.00
S29	CH ST18	0.18	3.59	0.00	0.00	1[illegible].04	53.48	2.70	30.51	0.00	0.00
S30	CH ST 7	2.89	57.75	0.00	0.00	3.75	19.75	1.35	15.33	0.00	0.00
S31	CC ST 8	0.00	0.00	0.00	0.00	0.01	0.03	0.01	0.06	0.00	0.00
S32	ST+DEF19	0.01	0.12	0.00	0.00	0.04	0.22	0.00	0.00	0.00	0.00
S33	CCH DEF9	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.02	0.00	0.00
S34	CCHDEF20	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
S35	CCCDEF12	0.00	0.01	0.00	0.00	0.04	0.22	0.05	0.55	0.00	0.00
S36	CC ST 2	0.03	0.64	0.00	0.00	0.01	0.04	0.00	0.00	0.00	0.00
S37	CCC DEF6	0.00	0.01	0.00	0.00	0.02	0.11	0.02	0.20	0.00	0.00
S38	CH ST18	0.00	0.00	43.38	57.88	0.00	0.00	0.00	0.00	0.01	0.00
S39	CH ST 7	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	92.92	7.69
S40	CC ST 8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.15	0.01
S41	ST+DEF19	0.00	0.00	0.25	0.34	0.00	0.00	0.00	0.00	0.00	0.00
S42	CC ST 14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S43	CCHDEF 9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
S44	CCHDEF 9	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
S45	CCC DEF6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.47	0.04
S46	CCY1 DEF	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00
S47	CY1=H ST	1.71	34.25	0.00	0.00	2.26	11.37	4.16	47.06	0.00	0.00
S48	PI CX1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S49	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S50	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S51	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S54	TAU RED3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S55	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S56	PI CH 5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S57	TAU CC 4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S58	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S59	PI CY=CH	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S60	TAU C-N	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S61	TAU C=N	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S62	TAU C-C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S63	PICHCENT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S64	PICX2=CC	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S65	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S66	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S67	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S70	TAU RED3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S71	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S72	PI CH 5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S73	TAU CC 4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S74	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S75	PICH=CY2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

AVI1

37707 BDS

A VI2

	FREQUENCIES	3025.469	1680.650	1631.809	1618.666	1602.366	1588.725	1512.784	1500.971	1466.108	1462.951
S 1	CX ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 2	CCX1 DEF	0.00	0.00	0.02	0.35	7.60	1.02	0.13	0.28	18.95	10.68
S 3	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 4	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 5	CC ST 8	0.00	23.83	6.77	11.77	0.12	18.18	6.28	0.40	0.01	0.09
S 6	ST+DEF19	0.00	4.08	0.23	0.14	0.00	0.25	26.51	5.09	0.20	2.20
S 7	CCH DEF9	0.00	8.37	2.51	4.45	0.05	7.20	2.96	0.20	0.00	0.05
S 8	CCHDEF20	0.00	2.09	0.16	0.11	0.00	0.18	37.16	7.96	0.45	5.16
S 9	CCCDEF12	0.00	1.27	0.05	0.03	0.00	0.04	0.60	0.05	0.00	0.04
S10	CC ST 2	0.00	0.87	0.03	0.01	0.00	0.05	0.42	0.03	0.00	0.04
S11	CCC DEF6	0.00	7.20	1.43	2.24	0.02	2.62	0.37	0.02	0.00	0.00
S12	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S13	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S14	CC ST 8	0.00	0.18	0.34	4.24	64.24	5.93	0.04	0.04	0.27	0.21
S15	ST+DEF19	0.00	0.03	0.01	0.04	0.00	0.09	0.16	0.36	26.23	14.36
S16	CC ST 14	0.00	0.00	0.00	0.01	0.04	0.00	0.00	0.01	0.06	0.04
S17	CCHDEF 9	0.00	0.01	0.03	0.42	7.80	0.88	0.02	0.02	0.37	0.31
S18	CCHDEF 9	0.00	0.01	0.00	0.01	0.01	0.05	0.07	0.16	14.77	8.16
S19	CCC DEF6	0.00	0.03	0.05	0.66	10.01	0.92	0.01	0.01	0.04	0.03
S20	CCN DEF	0.00	0.28	0.13	0.67	3.79	0.01	0.07	0.11	4.13	1.78
S21	C-N ST	0.00	26.11	0.53	0.20	0.00	1.29	5.64	0.39	0.02	0.54
S22	STCHCENT	99.99	0.02	0.06	0.02	0.00	0.00	0.02	0.00	0.01	0.01
S23	C=N ST	0.34	32.93	8.57	9.76	0.19	24.26	3.83	1.30	0.45	2.34
S24	BETA 1-2	0.01	4.77	3.22	2.03	0.20	2.32	1.19	0.01	0.80	0.15
S25	C-N=CDEF	0.10	0.00	0.06	0.46	0.54	0.00	0.20	0.26	0.42	0.40
S26	N=C-CDEF	0.36	0.03	0.95	1.31	0.06	0.14	0.44	0.23	0.20	1.03
S27	CC=CX ST	0.13	1.48	8.03	0.75	0.02	1.89	2.27	3.59	0.00	0.50
S28	CCCX DEF	0.10	1.04	2.73	2.35	0.42	0.12	0.55	0.08	1.65	2.37
S29	CH ST18	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S30	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S31	CC ST 8	0.00	0.04	33.02	30.80	1.23	0.01	1.17	2.50	0.01	0.00
S32	ST+DEF19	0.00	0.00	1.29	0.41	0.00	0.00	5.08	32.45	0.34	0.01
S33	CCH DEF9	0.00	0.01	12.40	11.74	0.48	0.01	0.54	1.21	0.01	0.00
S34	CCHDEF20	0.00	0.00	0.83	0.30	0.00	0.00	7.13	50.95	0.75	0.02
S35	CCCDEF12	0.00	0.00	0.37	0.11	0.00	0.00	0.13	0.36	0.00	0.00
S36	CC ST 2	0.00	0.00	0.21	0.05	0.00	0.00	0.09	0.22	0.00	0.00
S37	CCC DEF6	0.00	0.00	7.31	6.02	0.21	0.01	0.06	0.11	0.00	0.00
S38	CH ST18	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S39	CH ST 7	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S40	CC ST 8	0.00	0.75	17.69	15.40	9.35	29.52	0.93	0.00	0.09	0.27
S41	ST+DEF19	0.00	0.11	0.35	0.17	0.00	0.32	2.34	0.06	14.47	22.79
S42	CC ST 14	0.00	0.01	0.13	0.04	0.01	0.00	0.13	0.00	0.11	0.12
S43	CCHDEF 9	0.00	0.03	1.53	1.52	1.13	4.24	0.35	0.00	0.16	0.46
S44	CCHDEF 9	0.00	0.03	0.05	0.03	0.00	0.17	0.95	0.03	7.93	12.81
S45	CCC DEF6	0.00	0.12	2.69	2.41	1.46	4.62	0.17	0.00	0.01	0.03
S46	CCY1 DEF	0.00	0.02	1.18	1.26	1.11	4.93	2.28	0.03	10.95	17.39
S47	CY1=H ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S48	PI CX1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S49	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S50	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S51	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S54	TAU RED3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S55	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S56	PI CH 5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S57	TAU CC 4	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00
S58	TAU CC16	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00
S59	PI CY=CH	0.00	0.03	0.01	0.02	0.00	0.03	0.01	0.01	0.00	0.00
S60	TAU C-N	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.03	0.01
S61	TAU C=N	0.00	0.00	0.01	0.04	0.35	0.03	0.00	0.00	0.26	0.15
S62	TAU C-C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S63	PICHCENT	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.08	0.00
S64	PICX2=CC	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S65	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S66	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S67	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S70	TAU RED3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S71	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S72	PI CH 5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S73	TAU CC 4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S74	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S75	PICH=CY2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

AVI3

	FREQUENCIES	1353.341	1341.761	1317.949	1312.546	1299.409	1286.333	1237.724	1220.424	1190.865	1185.354
S 1	CX ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
S 2	CCX1 DEF	0.04	6.12	0.22	6.83	0.80	5.49	0.00	0.00	0.00	0.00
S 3	CH ST18	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
S 4	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
S 5	CC ST 8	1.75	0.12	0.43	0.39	0.95	0.00	0.00	0.01	16.46	0.75
S 6	ST+DEF19	0.39	0.01	0.01	0.00	0.00	0.00	0.00	0.09	0.07	0.04
S 7	CCH DEF9	1.79	0.14	0.67	0.65	2.04	0.00	0.00	1.38	66.85	2.14
S 8	CCHDEF20	0.34	0.64	2.40	2.21	5.89	0.01	0.00	0.57	0.20	0.11
S 9	CCCDEF12	3.31	0.28	1.39	1.39	4.31	0.01	0.00	0.94	0.35	0.22
S10	CC ST 2	2.42	0.20	0.97	0.96	2.92	0.01	0.00	0.53	0.35	0.14
S11	CCC DEF6	0.09	0.01	0.06	0.06	0.21	0.00	0.00	0.12	1.84	0.04
S12	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S13	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S14	CC ST 8	0.00	0.39	0.04	0.89	0.23	0.69	0.00	0.00	0.00	0.00
S15	ST+DEF19	0.00	0.83	0.05	0.91	0.22	0.51	0.00	0.00	0.00	0.00
S16	CC ST 14	0.08	3.25	1.03	49.76	23.75	16.48	0.00	0.00	0.00	0.01
S17	CCHDEF 9	0.39	62.60	0.74	11.72	2.26	4.10	0.00	0.00	0.01	0.00
S18	CCHDEF 9	0.01	0.01	0.41	15.71	2.29	0.74	0.00	0.00	0.00	0.00
S19	CCC DEF6	0.00	0.04	0.01	0.16	0.03	0.12	0.00	0.00	0.00	0.00
S20	CCN DEF	0.02	4.20	0.01	0.06	0.55	0.54	0.00	0.00	0.00	0.00
S21	C-N ST	13.83	1.22	4.22	4.31	11.24	0.01	0.00	1.16	0.40	0.20
S22	STCHCENT	0.07	0.01	0.01	0.00	0.00	0.03	0.00	0.03	0.00	0.01
S23	C=N ST	0.22	1.95	0.20	4.48	5.59	3.41	0.00	0.12	0.04	0.00
S24	BETA 1-2	5.25	9.86	6.30	5.83	1.28	27.17	0.00	21.05	0.05	3.01
S25	C-N=CDEF	0.41	3.80	0.06	2.84	0.38	2.73	0.00	0.01	0.06	0.09
S26	N=C-CDEF	2.24	1.19	0.05	1.22	0.03	5.28	0.00	0.03	0.05	0.11
S27	CC=CX ST	1.55	1.89	3.84	0.39	1.27	11.73	0.00	19.17	0.01	4.94
S28	CCCX DEF	2.10	0.00	0.61	0.00	0.44	1.47	0.00	0.02	0.00	0.00
S29	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01
S30	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
S31	CC ST 8	0.24	0.19	0.19	0.02	0.04	0.36	0.00	0.06	0.76	17.49
S32	ST+DEF19	0.06	0.01	0.00	0.00	0.00	0.02	0.00	1.27	0.00	0.78
S33	CCH DEF9	0.25	0.11	0.29	0.03	0.08	0.96	0.00	19.77	3.14	50.43
S34	CCHDEF20	1.27	0.51	1.09	0.89	0.25	2.50	0.00	8.37	0.01	2.39
S35	CCCDEF12	0.41	0.23	0.66	0.06	0.20	2.31	0.00	14.02	0.01	4.74
S36	CC ST 2	0.30	0.16	0.46	0.04	0.14	1.52	0.00	7.90	0.01	3.03
S37	CCC DEF6	0.01	0.01	0.03	0.00	0.01	0.14	0.00	1.73	0.05	0.91
S38	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S39	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S40	CC ST 8	0.00	0.00	1.78	0.17	0.31	0.11	0.00	0.17	0.03	0.06
S41	ST+DEF19	0.03	0.01	2.14	0.19	0.25	0.08	0.00	0.04	0.00	0.00
S42	CC ST 14	9.15	0.83	24.16	0.27	34.15	23.12	0.00	0.68	0.04	0.06
S43	CCHDEF 9	40.71	0.52	35.19	2.71	2.46	0.44	0.00	0.27	0.04	0.07
S44	CCHDEF 9	1.22	0.07	12.76	0.08	3.57	3.28	0.00	0.00	0.00	0.00
S45	CCC DEF6	0.01	0.00	0.32	0.02	0.04	0.04	0.00	0.04	0.01	0.01
S46	CCY1 DEF	3.72	0.00	7.47	0.04	1.31	0.86	0.00	0.08	0.03	0.07
S47	CY1=H ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
S48	PI CX1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S49	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S50	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S51	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S54	TAU RED3	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00
S55	PI CH 17	0.00	0.01	0.00	0.01	0.00	0.02	0.00	0.00	0.00	0.00
S56	PI CH 5	0.00	0.01	0.00	0.02	0.01	0.03	0.00	0.00	0.00	0.00
S57	TAU CC 4	0.00	0.01	0.00	0.02	0.02	0.03	0.00	0.00	0.00	0.00
S58	TAU CC16	0.00	0.01	0.00	0.02	0.01	0.03	0.00	0.00	0.00	0.00
S59	PI CY=CH	0.00	0.08	0.00	0.11	0.05	0.18	0.00	0.00	0.00	0.00
S60	TAU C-N	0.00	0.03	0.00	0.00	0.02	0.03	0.00	0.00	0.00	0.00
S61	TAU C=N	0.00	0.34	0.00	0.02	0.28	0.33	0.01	0.00	0.00	0.00
S62	TAU C-C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S63	PICHCENT	0.00	0.09	0.01	0.01	0.02	0.15	0.04	0.00	0.00	0.00
S64	PICX2=CC	0.00	0.00	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00
S65	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00
S66	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
S67	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S70	TAU RED3	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.00	0.00	0.00
S71	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	2.24	0.00	0.00	0.00
S72	PI CH 5	0.00	0.00	0.00	0.00	0.00	0.00	30.22	0.00	0.00	0.00
S73	TAU CC 4	0.00	0.00	0.00	0.00	0.00	0.00	25.99	0.00	0.00	0.00
S74	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	5.65	0.00	0.00	0.00
S75	PICH=CY2	0.00	0.00	0.00	0.00	0.00	0.00	16.65	0.00	0.00	0.00

BDS 1446

AVI4

	FREQUENCIES	1168.764	1168.691	1132.688	1077.594	1075.462	1022.363	1021.442	1016.501	1008.090	1005.629
S 1	CX ST	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
S 2	CCX1 DEF	28.25	10.42	0.00	8.51	0.98	0.00	0.00	0.23	0.01	0.00
S 3	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00
S 4	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 5	CC ST 8	0.00	0.01	0.00	0.00	0.02	0.01	0.00	0.00	0.00	0.00
S 6	ST+DEF19	0.00	0.00	0.00	0.00	0.18	44.03	0.00	0.04	8.83	0.08
S 7	CCH DEF9	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 8	CCHDEF20	0.00	0.01	0.00	0.00	0.14	20.26	0.00	0.02	3.94	0.03
S 9	CCCDEF12	0.00	0.02	0.00	0.00	0.61	32.88	0.01	0.34	31.37	0.24
S10	CC ST 2	0.00	0.01	0.00	0.00	0.12	0.04	0.00	0.10	49.84	0.63
S11	CCC DEF6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00
S12	CH ST18	0.00	0.00	0.00	0.05	0.01	0.00	0.00	0.00	0.00	0.00
S13	CH ST 7	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
S14	CC ST 8	4.01	1.46	0.00	2.59	0.28	0.00	0.00	0.03	0.00	0.00
S15	ST+DEF19	0.43	0.16	0.00	37.68	4.31	0.00	0.00	2.34	0.10	0.02
S16	CC ST 14	4.79	1.78	0.00	1.32	0.16	0.00	0.00	0.14	0.01	0.00
S17	CCHDEF 9	4.70	1.71	0.00	1.68	0.18	0.00	0.00	0.01	0.00	0.00
S18	CCHDEF 9	23.86	8.93	0.00	24.56	2.69	0.00	0.00	0.37	0.01	0.00
S19	CCC DEF6	0.54	0.20	0.00	0.34	0.04	0.00	0.00	0.04	0.00	0.00
S20	CCN DEF	0.02	0.00	0.00	3.51	0.30	0.00	0.00	0.00	0.00	0.00
S21	C-N ST	0.00	0.01	0.00	0.00	0.01	0.04	0.00	0.01	0.68	0.00
S22	STCHCENT	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00
S23	C=N ST	0.00	0.03	0.00	0.04	0.37	0.00	0.00	0.02	0.01	0.00
S24	BETA 1-2	0.03	0.00	0.00	0.13	0.03	0.00	0.00	0.14	0.20	0.13
S25	C-N=CCEF	0.00	0.00	0.00	0.03	0.17	0.00	0.00	0.30	0.63	0.12
S26	N=C-CCEF	0.01	0.01	0.00	0.06	0.69	0.00	0.00	0.00	0.53	0.10
S27	CC=CX ST	0.00	0.00	0.00	0.01	0.08	0.00	0.06	0.00	0.07	0.84
S28	CCCX DEF	0.01	0.01	0.00	0.47	2.69	0.00	0.00	0.00	0.00	0.00
S29	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05
S30	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S31	CC ST 8	0.00	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
S32	ST+DEF19	0.00	0.00	0.00	0.00	0.04	0.00	42.87	0.06	0.04	7.53
S33	CCH DEF9	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S34	CCHDEF20	0.00	0.01	0.00	0.00	0.03	0.00	19.68	0.03	0.02	3.31
S35	CCCDEF12	0.00	0.02	0.00	0.01	0.09	0.00	34.20	0.08	0.26	23.95
S36	CC ST 2	0.00	0.01	0.00	0.00	0.02	0.00	0.01	0.04	0.36	61.26
S37	CCC DEF6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04
S38	CH ST18	0.00	0.00	0.00	0.01	0.05	0.00	0.00	0.00	0.00	0.00
S39	CH ST 7	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
S40	CC ST 8	1.46	3.91	0.00	0.29	2.59	0.00	0.00	0.00	0.01	0.00
S41	ST+DEF19	0.16	0.42	0.00	4.22	38.51	0.00	0.00	0.25	0.25	0.02
S42	CC ST 14	1.80	4.75	0.00	0.14	1.58	0.00	0.00	0.01	0.04	0.00
S43	CCHDEF 9	1.74	4.63	0.00	0.18	1.57	0.00	0.00	0.00	0.00	0.00
S44	CCHDEF 9	8.80	24.05	0.00	2.80	24.12	0.00	0.00	0.04	0.04	0.00
S45	CCC DEF6	0.20	0.53	0.00	0.03	0.38	0.00	0.00	0.00	0.01	0.00
S46	CCY1 DEF	10.45	28.12	0.00	0.95	8.84	0.00	0.00	0.03	0.02	0.00
S47	CY1=H ST	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00
S48	PI CX1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.02	0.01
S49	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00
S50	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S51	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S54	TAU RED3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
S55	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.02	0.00
S56	PI CH 5	0.00	0.00	0.00	0.01	0.00	0.00	0.00	1.70	0.27	0.06
S57	TAU CC 4	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.54	0.09	0.02
S58	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00
S59	PI CY=CH	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.54	0.06	0.01
S60	TAU C-N	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.71	0.00	0.00
S61	TAU C=N	0.01	0.00	0.00	1.23	0.02	0.00	0.00	12.52	0.00	0.00
S62	TAU C-C	0.00	0.00	0.06	0.07	0.00	0.00	0.00	1.69	0.00	0.00
S63	PICHCENT	0.01	0.00	0.00	1.83	0.00	0.00	0.00	34.96	0.07	0.02
S64	PICX2=CC	0.00	0.00	0.00	0.03	0.00	0.00	0.00	2.63	0.04	0.01
S65	PI CH 17	0.00	0.00	56.54	0.00	0.00	0.00	0.00	0.03	0.00	0.00
S66	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S67	TAU CC16	0.00	0.00	30.91	0.00	0.00	0.00	0.00	0.01	0.00	0.00
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S70	TAU RED3	0.00	0.00	0.01	0.00	0.00	0.00	0.00	1.79	0.06	0.02
S71	PI CH 17	0.00	0.00	0.02	0.04	0.00	0.00	0.00	11.52	0.28	0.07
S72	PI CH 5	0.00	0.00	0.11	0.01	0.00	0.00	0.00	7.05	0.19	0.05
S73	TAU CC 4	0.00	0.00	0.05	0.00	0.00	0.00	0.00	1.07	0.02	0.01
S74	TAU CC16	0.00	0.00	0.01	0.04	0.00	0.00	0.00	9.43	0.21	0.05
S75	PICH=CY2	0.00	0.00	0.00	0.02	0.00	0.00	0.00	6.83	0.17	0.05

AVI 5

	FREQUENCIES	988.348	981.577	979.557	944.147	913.684	849.360	818.832	812.401	749.214	739.195
S 1	CX ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 2	CCX1 DEF	0.02	0.04	0.02	0.03	0.01	0.00	0.00	0.00	0.00	0.00
S 3	CH ST18	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00
S 4	CH ST 7	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
S 5	CC ST 8	0.00	0.00	0.00	0.04	0.25	0.00	0.00	1.64	0.12	0.01
S 6	ST+DEF19	0.00	0.00	0.00	0.89	2.60	0.00	0.00	2.95	0.08	0.00
S 7	CCH DEF9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00
S 8	CCHDEF20	0.00	0.00	0.00	0.26	0.63	0.00	0.00	0.40	0.01	0.00
S 9	CCCDEF12	0.00	0.00	0.00	2.50	6.70	0.00	0.00	6.64	0.18	0.01
S10	CC ST 2	1.78	0.07	0.06	9.13	15.10	0.00	0.00	8.32	0.18	0.01
S11	CCC DEF6	0.00	0.00	0.00	0.11	0.63	0.00	0.00	5.05	0.47	0.02
S12	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S13	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S14	CC ST 8	0.01	0.03	0.01	0.08	0.06	0.00	0.00	0.01	0.00	0.01
S15	ST+DEF19	0.18	0.65	0.23	0.77	0.44	0.00	0.00	0.07	0.00	0.07
S16	CC ST 14	0.01	0.08	0.03	0.21	0.12	0.00	0.00	0.03	0.00	0.02
S17	CCHDEF 9	0.00	0.01	0.00	0.03	0.02	0.00	0.00	0.01	0.00	0.00
S18	CCHDEF 9	0.02	0.06	0.02	0.04	0.01	0.00	0.00	0.00	0.00	0.00
S19	CCC DEF6	0.00	0.03	0.01	0.09	0.07	0.00	0.00	0.04	0.00	0.04
S20	CCN DEF	0.01	0.01	0.01	0.03	0.02	0.00	0.00	0.01	0.02	0.06
S21	C-N ST	0.00	0.00	0.00	0.86	3.02	0.00	0.00	5.73	0.18	0.01
S22	STCHCENT	0.01	0.00	0.00	0.06	0.09	0.00	0.00	0.01	0.00	0.00
S23	C=N ST	0.13	0.00	0.00	0.14	0.03	0.00	0.00	0.35	0.16	0.00
S24	BETA 1-2	0.23	0.01	0.01	2.06	1.96	0.00	0.00	1.03	0.00	0.01
S25	C-N=CDEF	0.75	0.06	0.05	8.65	10.28	0.00	0.00	2.47	0.46	0.07
S26	N=C-CDEF	0.17	0.02	0.01	5.13	12.30	0.00	0.00	1.39	0.85	0.19
S27	CC=CX ST	0.02	0.00	0.00	1.07	2.34	0.00	0.00	17.75	1.93	0.01
S28	CCCX DEF	0.00	0.01	0.00	0.00	0.13	0.00	0.00	0.00	0.19	0.01
S29	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00
S30	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S31	CC ST 8	0.00	0.00	0.00	0.01	0.02	0.00	0.00	2.95	0.55	0.00
S32	ST+DEF19	0.00	0.00	0.00	0.14	0.21	0.00	0.00	5.45	0.37	0.00
S33	CCH DEF9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.01	0.00
S34	CCHDEF20	0.00	0.00	0.00	0.04	0.05	0.00	0.00	0.71	0.04	0.00
S35	CCCDEF12	0.00	0.00	0.00	0.44	0.64	0.00	0.00	11.58	0.81	0.00
S36	CC ST 2	0.58	0.02	0.02	1.58	1.40	0.00	0.00	14.72	0.81	0.00
S37	CCC DEF6	0.00	0.00	0.00	0.02	0.07	0.00	0.00	8.45	2.11	0.00
S38	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S39	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S40	CC ST 8	0.01	0.00	0.00	0.11	0.30	0.00	0.00	0.00	0.02	0.00
S41	ST+DEF19	0.12	0.08	0.04	0.86	2.22	0.00	0.00	0.02	0.11	0.01
S42	CC ST 14	0.03	0.01	0.00	0.31	0.64	0.00	0.00	0.01	0.02	0.00
S43	CCHDEF 9	0.00	0.00	0.00	0.04	0.10	0.00	0.00	0.00	0.01	0.00
S44	CCHDEF 9	0.01	0.01	0.00	0.05	0.07	0.00	0.00	0.00	0.00	0.00
S45	CCC DEF6	0.01	0.00	0.00	0.14	0.35	0.00	0.00	0.01	0.02	0.01
S46	CCY1 DEF	0.01	0.01	0.00	0.03	0.07	0.00	0.00	0.00	0.00	0.00
S47	CY1=F ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S48	PI CX1	14.77	11.26	2.65	14.61	8.44	0.00	0.00	0.54	24.82	1.26
S49	PI CH 17	0.27	18.23	58.69	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S50	PI+TAU10	0.00	0.00	0.00	0.00	0.00	68.75	0.00	0.00	0.00	0.00
S51	TAU CC16	0.13	9.09	29.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	28.63	0.00	0.00	0.00	0.00
S54	TAU RED3	0.21	0.00	0.00	3.65	5.33	0.00	0.00	0.44	10.03	0.43
S55	PI CH 17	0.80	3.04	0.91	17.83	6.56	0.00	0.00	0.17	37.25	2.23
S56	PI CH 5	38.01	11.40	1.95	10.25	13.63	0.00	0.00	0.20	1.07	0.04
S57	TAU CC 4	21.38	9.42	1.88	0.10	2.25	0.00	0.00	0.33	3.15	0.07
S58	TAU CC16	3.24	4.38	1.15	12.24	5.70	0.00	0.00	0.01	0.68	0.05
S59	PI CY=CH	1.32	0.01	0.03	3.52	0.15	0.00	0.00	0.37	6.51	0.20
S60	TAU C-N	0.14	0.41	0.00	0.01	0.00	0.09	0.00	0.00	0.03	0.00
S61	TAU C=N	2.85	5.92	2.63	0.62	0.05	0.00	0.01	0.00	0.23	1.20
S62	TAU C-C	0.27	0.77	0.35	0.23	0.01	0.00	0.08	0.00	0.02	0.10
S63	PICHCENT	4.54	13.40	5.94	3.93	0.05	0.01	0.03	0.03	0.45	0.09
S64	PICX2=CC	0.15	0.01	0.00	0.11	0.03	0.00	0.01	0.01	0.43	5.55
S65	PI CH 17	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S66	PI+TAU10	0.00	0.01	0.00	0.00	0.00	0.00	73.79	0.01	0.01	0.04
S67	TAU CC16	0.02	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	28.53	0.00	0.00	0.02
S70	TAU RED3	2.20	2.50	0.86	0.28	0.02	0.00	0.00	0.01	0.53	10.83
S71	PI CH 17	6.01	5.42	1.77	0.16	0.00	0.00	0.07	0.00	1.62	43.18
S72	PI CH 5	4.99	4.90	1.64	0.25	0.00	0.00	0.09	0.00	0.04	1.29
S73	TAU CC 4	0.66	0.66	0.22	0.06	0.01	0.00	0.00	0.00	0.05	0.52
S74	TAU CC16	4.35	3.89	1.26	0.15	0.01	0.00	0.01	0.00	0.01	0.28
S75	PICH=CY2	4.81	4.89	1.64	0.38	0.03	0.00	0.00	0.01	1.30	30.51

BIBLIOTHEQUE

AVI 6

	FREQUENCIES	686.844	671.004	615.755	605.661	602.127	534.012	517.044	476.580	414.495	398.707
S 1	CX ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 2	CCX1 DEF	0.00	0.00	0.00	0.07	0.09	0.02	0.04	0.10	0.01	0.00
S 3	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 4	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S 5	CC ST 8	2.76	3.02	0.03	0.00	0.22	3.51	1.12	0.01	0.00	0.00
S 6	ST+DEF19	0.51	0.35	0.00	0.00	0.00	0.27	0.11	0.00	0.00	0.00
S 7	CCH DEF9	0.06	0.07	0.00	0.00	0.01	0.08	0.03	0.00	0.00	0.00
S 8	CCHDEF20	0.03	0.02	0.00	0.00	0.00	0.02	0.01	0.00	0.00	0.00
S 9	CCCDEF12	1.19	0.87	0.00	0.00	0.00	0.29	0.15	0.00	0.00	0.00
S10	CC ST 2	0.82	0.50	0.00	0.00	0.00	0.88	0.37	0.00	0.00	0.00
S11	CCC DEF6	13.20	15.23	0.16	0.03	1.35	26.80	8.71	0.07	0.00	0.02
S12	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.00	0.00
S13	CH ST 7	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00
S14	CC ST 8	0.00	0.00	0.67	5.87	7.10	0.30	0.49	0.70	0.00	0.00
S15	ST+DEF19	0.07	0.02	0.19	0.06	0.22	0.73	1.86	4.69	0.30	0.05
S16	CC ST 14	0.03	0.01	0.05	0.00	0.01	0.07	0.14	0.21	0.00	0.00
S17	CCHDEF 9	0.01	0.00	0.04	0.03	0.01	0.04	0.10	0.25	0.02	0.00
S18	CCHDEF 9	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.05	0.01	0.00
S19	CCC DEF6	0.24	0.21	8.42	36.25	38.74	0.01	0.07	0.89	0.21	0.02
S20	CCN DEF	0.02	0.00	0.35	0.27	0.64	2.96	9.04	30.07	3.36	0.49
S21	C-N ST	1.20	0.83	0.00	0.00	0.02	2.69	2.02	0.01	0.00	0.02
S22	STCHCENT	0.02	0.03	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
S23	C=N ST	0.26	0.28	0.01	0.02	0.06	0.18	0.00	0.05	0.00	0.00
S24	BETA 1-2	0.09	0.11	0.04	0.03	0.07	0.37	0.09	0.01	0.00	0.00
S25	C-N=CDEF	4.30	1.78	0.59	0.72	0.47	5.84	9.23	0.46	0.03	0.01
S26	N=C-CDEF	2.66	6.30	0.17	0.55	0.00	3.10	14.71	0.09	0.04	0.01
S27	CC=CX ST	0.67	0.02	0.01	0.04	0.01	2.34	7.38	0.25	0.01	0.01
S28	CCCX DEF	0.07	0.26	0.01	0.06	0.20	4.72	14.39	0.03	0.85	0.29
S29	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S30	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S31	CC ST 8	2.70	2.29	0.04	0.03	0.15	3.03	1.26	0.04	0.00	0.00
S32	ST+DEF19	0.53	0.31	0.00	0.00	0.00	0.34	0.13	0.01	0.00	0.00
S33	CCH DEF9	0.06	0.05	0.00	0.00	0.00	0.07	0.03	0.00	0.00	0.00
S34	CCHDEF20	0.03	0.01	0.00	0.00	0.00	0.02	0.01	0.00	0.00	0.00
S35	CCCDEF12	1.16	0.66	0.00	0.00	0.00	0.30	0.16	0.01	0.00	0.00
S36	CC ST 2	0.82	0.40	0.00	0.00	0.00	0.90	0.41	0.02	0.00	0.00
S37	CCC DEF6	12.43	10.98	0.26	0.19	0.94	24.79	9.66	0.34	0.00	0.03
S38	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
S39	CH ST 7	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00
S40	CC ST 8	0.00	0.00	0.00	6.39	6.51	0.65	1.56	0.03	0.01	0.01
S41	ST+DEF19	0.22	0.47	0.00	0.01	0.07	1.20	3.39	0.02	0.09	0.04
S42	CC ST 14	0.10	0.20	0.00	0.00	0.01	0.17	0.45	0.01	0.00	0.00
S43	CCHDEF 9	0.02	0.05	0.00	0.05	0.03	0.05	0.15	0.00	0.00	0.00
S44	CCHDEF 9	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
S45	CCC DEF6	0.82	2.16	0.06	42.54	38.50	0.05	0.02	0.02	0.03	0.00
S46	CCY1 DEF	0.00	0.00	0.00	0.06	0.07	0.03	0.07	0.00	0.00	0.00
S47	CY1=H ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S48	PI CX1	0.38	1.03	0.00	0.12	0.05	1.19	2.09	3.18	0.36	0.16
S49	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.72	22.96
S50	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
S51	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.23	2.12	59.77
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S54	TAU RED3	0.12	0.01	0.00	0.00	0.00	0.29	0.67	1.56	0.20	0.06
S55	PI CH 17	12.88	2.09	0.00	0.09	0.02	0.76	1.25	1.36	0.02	0.00
S56	PI CH 5	4.75	6.18	0.00	0.07	0.03	0.48	0.77	0.89	0.04	0.01
S57	TAU CC 4	27.67	33.21	0.00	0.14	0.07	0.35	0.42	0.20	0.00	0.00
S58	TAU CC16	0.01	0.48	0.00	0.06	0.03	0.98	1.89	3.72	0.84	0.57
S59	PI CY=CH	3.47	2.95	0.00	0.06	0.01	3.41	7.68	17.58	2.55	0.89
S60	TAU C-N	0.00	0.00	0.05	0.00	0.00	0.03	0.16	4.23	1.98	1.11
S61	TAU C=N	0.04	0.01	3.31	0.09	0.00	0.06	0.06	7.58	2.31	0.00
S62	TAU C-C	0.00	0.00	0.02	0.00	0.00	0.05	0.23	2.88	2.70	0.02
S63	PICHCENT	0.04	0.02	0.54	0.00	0.02	0.00	0.05	7.10	0.05	0.00
S64	PICX2=CC	0.08	0.09	27.32	1.63	0.94	0.01	0.00	0.62	26.12	0.78
S65	PI CH 17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.40	0.02
S66	PI+TAU10	0.00	0.00	0.13	0.01	0.00	0.00	0.00	0.03	0.02	0.00
S67	TAU CC16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.48	0.02
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.01	0.01	0.00
S70	TAU RED3	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.16	1.76	0.04
S71	PI CH 17	0.31	0.14	5.31	0.22	0.12	0.00	0.00	0.00	1.11	0.09
S72	PI CH 5	0.10	0.09	24.67	1.68	1.00	0.10	0.31	3.40	8.79	0.17
S73	TAU CC 4	0.07	0.08	32.92	2.33	1.40	0.16	0.55	6.62	21.75	0.45
S74	TAU CC16	0.01	0.01	0.28	0.01	0.00	0.00	0.01	0.69	17.78	0.77
S75	PICH=CY2	0.12	0.04	0.01	0.02	0.02	0.03	0.12	2.41	20.19	0.61

AVI7

	FREQUENCIES	369.480	349.337	266.277	254.443	178.560	143.489	74.175	55.352	46.904	0.0
S 1	CX ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S 2	CCX1 DEF	0.02	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.0
S 3	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S 4	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S 5	CC ST 8	0.26	0.01	0.06	0.41	0.21	0.00	0.00	0.00	0.00	0.0
S 6	ST+DEF19	0.17	0.00	0.08	0.52	0.32	0.00	0.00	0.00	0.00	0.0
S 7	CCH DEF9	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.0
S 8	CCHDEF20	0.01	0.00	0.00	0.02	0.01	0.00	0.00	0.00	0.00	0.0
S 9	CCCDEF12	0.25	0.01	0.11	0.74	0.47	0.00	0.00	0.00	0.00	0.0
S10	CC ST 2	0.39	0.01	0.17	1.05	0.65	0.00	0.00	0.00	0.00	0.0
S11	CCC DEF6	2.82	0.07	0.88	5.49	3.00	0.01	0.00	0.00	0.00	0.0
S12	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S13	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S14	CC ST 8	0.12	0.01	0.11	0.03	0.00	0.00	0.04	0.04	0.00	0.0
S15	ST+DEF19	0.92	0.10	0.10	0.08	0.24	0.49	0.09	0.10	0.00	0.0
S16	CC ST 14	0.03	0.00	0.04	0.01	0.01	0.00	0.04	0.05	0.00	0.0
S17	CCHDEF 9	0.05	0.01	0.01	0.00	0.01	0.02	0.00	0.00	0.00	0.0
S18	CCHDEF 9	0.01	0.00	0.00	0.00	0.01	0.02	0.01	0.01	0.00	0.0
S19	CCC DEF6	0.21	0.03	0.02	0.00	0.23	0.31	0.25	0.28	0.00	0.0
S20	CCN DEF	8.03	0.97	0.11	0.52	5.40	9.21	4.31	5.01	0.06	0.0
S21	C-N ST	2.22	0.05	0.76	5.74	4.04	0.02	0.07	0.00	0.00	0.0
S22	STCHCENT	0.02	0.00	0.01	0.03	0.00	0.00	0.01	0.00	0.00	0.0
S23	C=N ST	1.63	0.05	0.63	1.59	0.31	0.01	0.34	0.00	0.00	0.0
S24	BETA 1-2	0.11	0.00	0.01	0.01	0.05	0.00	0.01	0.00	0.00	0.0
S25	C-N=CDEF	1.27	0.01	3.34	6.07	3.61	0.66	25.28	0.03	0.00	0.0
S26	N=C--CDEF	1.06	0.01	0.82	1.07	15.81	1.24	28.18	0.02	0.00	0.0
S27	CC=CX ST	1.50	0.05	1.93	6.65	1.87	0.05	2.51	0.00	0.00	0.0
S28	CCCX DEF	19.71	0.31	2.33	0.76	23.09	1.26	12.46	0.18	0.00	0.0
S29	CH ST18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S30	CH ST 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S31	CC ST 8	0.24	0.01	0.07	0.38	0.16	0.00	0.00	0.00	0.00	0.0
S32	ST+DEF19	0.25	0.01	0.09	0.65	0.43	0.00	0.00	0.00	0.00	0.0
S33	CCH DEF9	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.0
S34	CCHDEF20	0.01	0.00	0.00	0.02	0.01	0.00	0.00	0.00	0.00	0.0
S35	CCCDEF12	0.30	0.01	0.13	0.83	0.52	0.00	0.00	0.00	0.00	0.0
S36	CC ST 2	0.47	0.01	0.19	1.19	0.74	0.00	0.00	0.00	0.00	0.0
S37	CCC DEF6	3.19	0.08	0.97	5.93	3.19	0.01	0.00	0.00	0.00	0.0
S38	CH ST18	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.0
S39	CH ST 7	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S40	CC ST 8	0.79	0.01	0.04	0.18	0.00	0.00	0.06	0.00	0.00	0.0
S41	ST+DEF19	2.83	0.04	0.22	0.24	0.93	0.05	0.29	0.01	0.00	0.0
S42	CC ST 14	0.25	0.00	0.01	0.07	0.02	0.00	0.07	0.00	0.00	0.0
S43	CCHDEF 9	0.13	0.00	0.01	0.01	0.04	0.00	0.01	0.00	0.00	0.0
S44	CCHDEF 9	0.03	0.00	0.00	0.00	0.04	0.00	0.02	0.00	0.00	0.0
S45	CCC DEF6	0.22	0.00	0.05	0.01	1.05	0.05	0.67	0.01	0.00	0.0
S46	CCY1 DEF	0.05	0.00	0.00	0.00	0.03	0.00	0.01	0.00	0.00	0.0
S47	CY1=H ST	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
S48	PI CX1	3.80	0.02	0.43	1.10	0.08	0.04	0.01	0.00	0.00	0.0
S49	PI CH 17	0.23	0.00	0.28	0.01	0.00	0.28	0.00	0.01	0.33	0.0
S50	PI+TAU10	0.00	0.00	0.01	0.00	0.00	0.02	0.00	0.00	0.03	0.0
S51	TAU CC16	0.49	0.00	0.36	0.01	0.00	0.26	0.00	0.01	0.27	0.0
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.0
S54	TAU RED3	0.48	0.00	0.14	0.10	1.41	0.62	2.74	0.63	0.01	0.0
S55	PI CH 17	1.15	0.02	1.77	3.39	2.92	1.34	2.43	0.54	0.01	0.0
S56	PI CH 5	0.01	0.00	0.16	0.32	0.39	0.19	0.35	0.08	0.00	0.0
S57	TAU CC 4	0.54	0.01	0.78	1.89	1.04	0.55	0.62	0.14	0.00	0.0
S58	TAU CC16	21.85	0.14	8.10	17.63	8.17	3.90	4.88	1.07	0.01	0.0
S59	PI CY=CH	13.71	0.03	0.00	0.59	5.30	2.24	15.59	3.64	0.04	0.0
S60	TAU C-N	0.95	0.00	14.57	0.61	0.42	30.05	0.03	1.08	43.08	0.0
S61	TAU C=N	1.02	0.00	5.30	5.40	2.44	2.53	0.02	34.45	6.25	0.0
S62	TAU C-C	1.12	1.41	15.95	1.25	0.13	21.52	0.01	1.26	47.78	0.0
S63	PICHCENT	0.37	0.26	2.04	2.15	0.93	0.06	0.00	19.77	0.78	0.0
S64	PICX2=CC	0.25	0.43	1.22	0.20	0.72	3.98	1.10	16.69	0.15	0.0
S65	PI CH 17	0.71	42.70	0.61	0.02	0.00	0.40	0.00	0.02	0.58	0.0
S66	PI+TAU10	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.01	0.03	0.0
S67	TAU CC16	1.15	68.10	0.43	0.00	0.02	0.55	0.00	0.06	0.51	0.0
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.01	0.0
S70	TAU RED3	0.00	0.02	1.63	0.64	0.30	1.69	0.23	3.50	0.03	0.0
S71	PI CH 17	0.12	0.05	8.38	4.07	0.72	4.09	0.22	3.35	0.03	0.0
S72	PI CH 5	0.01	0.06	1.31	0.67	0.20	1.20	0.07	1.12	0.01	0.0
S73	TAU CC 4	0.05	0.18	2.74	1.31	0.52	3.16	0.27	4.07	0.03	0.0
S74	TAU CC16	0.51	0.88	22.72	11.46	1.87	10.85	0.54	8.17	0.05	0.0
S75	PICH=CY2	0.23	0.28	1.53	0.85	0.04	0.21	0.00	0.00	0.00	0.0

BUS LILLE

	FREQUENCIES	0.0	0.0	0.0	0.0	0.0
S 1	CX ST	0.0	0.0	0.0	0.0	0.0
S 2	CCX1 DEF	0.0	0.0	0.0	0.0	0.0
S 3	CH ST18	0.0	0.0	0.0	0.0	0.0
S 4	CH ST 7	0.0	0.0	0.0	0.0	0.0
S 5	CC ST 8	0.0	0.0	0.0	0.0	0.0
S 6	ST+DEF19	0.0	0.0	0.0	0.0	0.0
S 7	CCH DEF9	0.0	0.0	0.0	0.0	0.0
S 8	CCHDEF20	0.0	0.0	0.0	0.0	0.0
S 9	CCCDEF12	0.0	0.0	0.0	0.0	0.0
S10	CC ST 2	0.0	0.0	0.0	0.0	0.0
S11	CCC DEF6	0.0	0.0	0.0	0.0	0.0
S12	CH ST18	0.0	0.0	0.0	0.0	0.0
S13	CH ST 7	0.0	0.0	0.0	0.0	0.0
S14	CC ST 8	0.0	0.0	0.0	0.0	0.0
S15	ST+DEF19	0.0	0.0	0.0	0.0	0.0
S16	CC ST 14	0.0	0.0	0.0	0.0	0.0
S17	CCHDEF 9	0.0	0.0	0.0	0.0	0.0
S18	CCHDEF 9	0.0	0.0	0.0	0.0	0.0
S19	CCC DEF6	0.0	0.0	0.0	0.0	0.0
S20	CCN DEF	0.0	0.0	0.0	0.0	0.0
S21	C-N ST	0.0	0.0	0.0	0.0	0.0
S22	STCHCENT	0.0	0.0	0.0	0.0	0.0
S23	C=N ST	0.0	0.0	0.0	0.0	0.0
S24	BETA 1-2	0.0	0.0	0.0	0.0	0.0
S25	C-N=CDEF	0.0	0.0	0.0	0.0	0.0
S26	N=C-CDEF	0.0	0.0	0.0	0.0	0.0
S27	CC=CX ST	0.0	0.0	0.0	0.0	0.0
S28	CCCX DEF	0.0	0.0	0.0	0.0	0.0
S29	CH ST18	0.0	0.0	0.0	0.0	0.0
S30	CH ST 7	0.0	0.0	0.0	0.0	0.0
S31	CC ST 8	0.0	0.0	0.0	0.0	0.0
S32	ST+DEF19	0.0	0.0	0.0	0.0	0.0
S33	CCH DEF9	0.0	0.0	0.0	0.0	0.0
S34	CCHDEF20	0.0	0.0	0.0	0.0	0.0
S35	CCCDEF12	0.0	0.0	0.0	0.0	0.0
S36	CC ST 2	0.0	0.0	0.0	0.0	0.0
S37	CCC DEF6	0.0	0.0	0.0	0.0	0.0
S38	CH ST18	0.0	0.0	0.0	0.0	0.0
S39	CH ST 7	0.0	0.0	0.0	0.0	0.0
S40	CC ST 8	0.0	0.0	0.0	0.0	0.0
S41	ST+DEF19	0.0	0.0	0.0	0.0	0.0
S42	CC ST 14	0.0	0.0	0.0	0.0	0.0
S43	CCHDEF 9	0.0	0.0	0.0	0.0	0.0
S44	CCHDEF 9	0.0	0.0	0.0	0.0	0.0
S45	CCC DEF6	0.0	0.0	0.0	0.0	0.0
S46	CCY1 DEF	0.0	0.0	0.0	0.0	0.0
S47	CY1=H ST	0.0	0.0	0.0	0.0	0.0
S48	PI CX1	0.0	0.0	0.0	0.0	0.0
S49	PI CH 17	0.0	0.0	0.0	0.0	0.0
S50	PI+TAU10	0.0	0.0	0.0	0.0	0.0
S51	TAU CC16	0.0	0.0	0.0	0.0	0.0
S52	TAU RED1	0.0	0.0	0.0	0.0	0.0
S53	TAU RED2	0.0	0.0	0.0	0.0	0.0
S54	TAU RED3	0.0	0.0	0.0	0.0	0.0
S55	PI CH 17	0.0	0.0	0.0	0.0	0.0
S56	PI CH 5	0.0	0.0	0.0	0.0	0.0
S57	TAU CC 4	0.0	0.0	0.0	0.0	0.0
S58	TAU CC16	0.0	0.0	0.0	0.0	0.0
S59	PI CY=CH	0.0	0.0	0.0	0.0	0.0
S60	TAU C-N	0.0	0.0	0.0	0.0	0.0
S61	TAU C=N	0.0	0.0	0.0	0.0	0.0
S62	TAU C-C	0.0	0.0	0.0	0.0	0.0
S63	PICHCENT	0.0	0.0	0.0	0.0	0.0
S64	PICX2=CC	0.0	0.0	0.0	0.0	0.0
S65	PI CH 17	0.0	0.0	0.0	0.0	0.0
S66	PI+TAU10	0.0	0.0	0.0	0.0	0.0
S67	TAU CC16	0.0	0.0	0.0	0.0	0.0
S68	TAU RED1	0.0	0.0	0.0	0.0	0.0
S69	TAU RED2	0.0	0.0	0.0	0.0	0.0
S70	TAU RED3	0.0	0.0	0.0	0.0	0.0
S71	PI CH 17	0.0	0.0	0.0	0.0	0.0
S72	PI CH 5	0.0	0.0	0.0	0.0	0.0
S73	TAU CC 4	0.0	0.0	0.0	0.0	0.0
S74	TAU CC16	0.0	0.0	0.0	0.0	0.0
S75	PICH=CY2	0.0	0.0	0.0	0.0	0.0

PED FOR FORCE CONSTANTS
MOLECULE-ISOTOPE NO. 1- 1 SYM. BLOCK NO. 1

	FREQUENCIES	3071.173	3071.167	3067.627	3067.609	3062.226	3062.205	3055.716	3055.701	3054.496	3054.463
	ASSIGNMENT (PED)	CH ST 7	CH ST 7	CH ST18	CH ST18	CH ST18	CH ST18	CX ST	CY1=H ST	CH ST 7	CH ST 7
	ASSIGNMENT (PED)	CX ST	CY1=H ST	CH ST18	CH ST18	CH ST 7	CH ST 7	CH ST18	CH ST18		
1 K(CH)	4.6740	90.441	90.441	90.629	90.629	90.958	90.958	91.344	91.345	91.382	91.416
2 O(CH)	0.0240	0.803	0.803	0.465	0.465	-0.079	-0.080	-0.733	-0.731	-0.469	-0.469
3 M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4 P(CH)	-0.0060	-0.066	-0.066	0.116	0.116	0.046	0.047	0.020	0.020	-0.117	0.117
5 H(CCH)	0.1700	0.056	0.056	0.023	0.023	0.056	0.056	0.113	0.113	0.085	0.085
6 O(CCH)	0.0015	0.000	0.000	0.000	0.000	0.000	0.000	-0.000	-0.000	-0.000	-0.000
7 M(CCH)	-0.0170	0.000	0.000	0.001	0.001	0.001	0.001	0.000	0.000	0.001	0.001
8 P(CCH)	0.0050	-0.000	-0.000	-0.001	-0.001	-0.000	-0.000	0.000	0.000	0.001	0.001
9 K(CC)	5.2490	0.558	0.558	0.422	0.422	0.260	0.259	0.060	0.060	0.140	0.139
10 O(CC)	0.4950	0.097	0.097	0.040	0.040	0.021	0.022	-0.005	-0.005	-0.013	0.013
11 M(CC)	-0.2110	-0.034	-0.034	0.017	0.017	0.006	0.006	0.002	0.002	0.006	0.006
12 P(CC)	0.3530	0.026	0.026	-0.028	-0.028	-0.008	-0.008	0.004	0.004	0.009	0.009
13 H(CCC)	0.4190	0.015	0.015	0.034	0.034	0.252	0.253	0.505	0.504	0.328	0.328
14 O(CCC)	-0.0090	0.000	0.000	-0.001	-0.001	0.012	0.012	0.028	0.028	0.011	0.011
15 M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16 P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17 F(CH)	0.3850	8.077	8.077	8.234	8.234	8.383	8.382	8.572	8.572	8.535	8.539
18 F(CC)	0.2420	0.071	0.071	0.023	0.023	0.055	0.055	0.086	0.085	0.039	0.039
19 A	0.3730	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
20 B	0.3130	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
21 C	0.0300	0.000	-0.000	-0.000	-0.000	-0.000	-0.000	0.000	-0.000	-0.000	-0.000
22 D	-0.0200	0.000	0.000	0.000	-0.000	0.000	0.000	-0.000	0.000	-0.000	-0.000
23 AO	0.0030	-0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
24 AM	0.0020	-0.000	-0.000	0.000	-0.000	0.000	0.000	0.000	0.000	0.000	0.000
25 AP	0.0090	0.000	0.000	0.000	-0.000	-0.000	0.000	0.000	0.000	0.000	-0.000
26 BC	-0.0420	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
27 BM	-0.0250	-0.000	-0.000	-0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
28 BP	-0.0490	0.000	0.000	0.000	-0.000	-0.000	0.000	0.000	0.000	0.000	-0.000
29 K(CC)	3.1000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
30 H(CC=C)	0.4190	0.000	0.006	0.008	0.010	0.005	0.027	0.000	0.001	0.018	0.002
31 F(CC=C)	0.3000	0.000	0.001	0.001	0.001	0.000	0.002	0.000	0.000	0.002	0.000
32 PI(CCC)	0.3700	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
33 K(C-N)	6.5000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
34 H(NC=C)	0.4000	0.005	0.000	0.009	0.007	0.026	0.005	0.001	0.000	0.001	0.016
35 F(NC=C)	0.4500	0.001	0.000	0.001	0.001	0.004	0.001	0.000	0.000	0.000	0.002
36 PI(NCC)	0.3700	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
37 K(N=C)	8.0000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
38 K(C-H)	4.5000	0.000	0.000	0.036	0.009	0.001	0.008	0.000	0.000	0.036	0.004
39 H(N=CH)	0.2700	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
40 F(N=CH)	0.5200	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.003	0.000
41 H(H-C-C)	0.3600	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
42 F(H-C-C)	0.2700	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000
43 H(N=C-C)	0.4600	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
44 F(N=C-C)	1.5000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
45 PI(CH)	0.3700	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
46 H(C-N=C)	0.6000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
47 F(C-N=C)	0.3500	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
48 TAU(C-N)	0.1300	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
49 TAU(C=N)	0.4100	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
50 TAU(C-CE	0.1200	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PEDSUM		100.001	100.001	100.001	100.001	99.999	99.999	99.997	99.998	99.998	99.997

AVI 10

	FREQUENCIES	3025.469	1680.650	1631.809	1618.666	1602.366	1588.725	1512.784	1500.971	1466.108	1462.951
	ASSIGNMENT (PED)	STCHCENT	C=N ST	CC ST 8	CC ST 8	CC ST 8	CC ST 8	CCHDEF20	CCHDEF20	ST+DEF19	ST+DEF19
	ASSIGNMENT (PED)		C-N ST	CC ST 8	CC ST 8	CCC DEF6	C=N ST	ST+DEF19	ST+DEF19	CCY1 DEF	CCY1 DEF
1	K(CH)	4.6740	0.069	0.004	0.002	0.001	0.002	0.004	0.004	0.004	0.004
2	D(CH)	0.0240	-0.001	0.001	0.000	0.000	-0.000	-0.000	0.001	0.000	-0.000
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	-0.000	-0.000	-0.000	-0.000	-0.000	0.000	0.000	0.000	-0.000
5	H(CCH)	0.1700	0.000	6.971	12.536	13.514	13.187	12.791	33.382	36.814	36.095	36.401
6	D(CCH)	0.0015	0.000	-0.035	-0.099	-0.114	-0.098	-0.068	0.242	0.324	0.301	0.304
7	M(CCH)	-0.0070	0.000	0.282	0.514	0.552	0.478	0.423	1.352	1.586	1.087	1.023
8	P(CCH)	0.0050	-0.000	0.118	0.330	0.381	0.336	0.243	-0.806	-1.079	-0.809	-0.783
9	K(CC)	5.2490	0.002	24.998	51.714	54.425	64.641	46.938	32.167	30.110	30.286	29.111
10	D(CC)	0.4950	-0.000	-1.616	-4.588	-5.023	-6.102	-4.325	1.650	2.373	2.733	2.596
11	M(CC)	-0.2110	0.000	0.930	2.038	2.175	2.591	1.882	1.229	1.187	1.191	1.142
12	P(CC)	0.3530	-0.000	1.274	3.271	3.577	4.339	3.091	-1.139	-1.659	-1.993	1.887
13	H(CCC)	0.4190	0.000	5.486	7.482	7.157	7.605	5.255	2.770	2.521	2.408	2.332
14	D(CCC)	-0.0090	-0.000	0.186	0.242	0.231	0.245	0.168	-0.022	-0.051	-0.075	-0.070
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	0.009	2.031	4.741	5.198	6.887	5.486	15.545	18.220	19.708	19.722
18	F(CC)	0.2420	0.000	0.660	0.645	0.574	0.618	0.483	1.575	1.624	1.648	1.584
19	A	0.3730	0.000	0.001	0.001	0.001	0.000	0.001	0.001	0.001	0.001	0.000
20	B	0.3100	0.000	0.028	0.027	0.013	0.001	0.027	0.006	0.004	0.002	0.003
21	C	0.0300	-0.000	0.006	0.001	0.003	0.000	0.006	0.001	0.001	0.000	0.000
22	D	-0.0200	0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	0.000
23	AO	0.0030	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
24	AM	0.0020	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
25	AP	0.0090	0.000	0.000	0.000	0.000	0.000	-0.000	0.000	0.000	0.000	-0.000
26	BO	-0.0420	0.000	0.004	0.001	0.002	0.000	0.004	0.001	0.001	0.000	0.001
27	BM	-0.0250	0.000	-0.000	-0.000	-0.000	0.000	-0.001	-0.000	0.000	-0.000	-0.000
28	BP	-0.0490	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
29	K(CC)	3.1000	0.082	0.930	5.053	0.472	0.014	1.186	1.426	2.257	0.001	0.314
30	H(CC=C)	0.4190	0.081	0.833	3.422	2.727	0.359	0.097	0.496	0.415	1.354	1.896
31	F(CC=C)	0.3000	0.031	0.277	0.273	0.621	0.077	0.466	0.108	0.070	0.144	0.218
32	PI(CCC)	0.3700	0.000	0.002	0.002	0.002	0.000	0.002	0.001	0.000	0.000	0.000
33	K(C-N)	5.5000	0.000	22.329	0.455	0.173	0.001	1.101	4.821	0.332	0.015	0.458
34	H(NC=C)	0.4000	0.000	1.825	0.314	0.777	2.747	0.176	0.277	0.125	2.991	1.301
35	F(NC=C)	0.4500	0.000	0.072	0.144	0.360	0.649	0.899	-0.013	0.060	0.514	0.463
36	PI(NCC)	0.3700	0.000	0.035	0.009	0.022	0.002	0.032	0.009	0.009	0.005	0.001
37	K(N=C)	8.0000	0.284	27.318	7.111	8.096	0.157	20.127	3.174	1.079	0.376	1.945
38	K(C-H)	4.5000	89.567	0.014	0.056	0.021	0.001	0.001	0.018	0.000	0.009	0.010
39	H(N=CH)	0.2700	0.002	1.309	0.883	0.557	0.054	0.637	0.326	0.002	0.219	0.042
40	F(N=CH)	0.5200	6.547	0.491	0.250	0.173	0.078	0.350	0.092	0.040	0.267	0.027
41	H(H-C-C)	0.3600	0.002	1.745	1.178	0.743	0.072	0.850	0.435	0.003	0.292	0.057
42	F(H-C-C)	0.2700	2.896	0.392	0.131	0.505	0.039	0.132	0.050	0.192	0.123	0.010
43	H(N=C-C)	0.4600	0.158	0.015	0.421	0.579	0.028	0.063	0.195	0.103	0.086	0.452
44	F(N=C-C)	1.5000	0.077	1.196	1.106	0.899	0.057	1.179	0.299	1.087	0.252	0.732
45	PI(CH)	0.3700	0.000	0.000	0.003	0.000	0.044	0.000	0.000	0.000	0.075	0.003
46	H(C-N=C)	0.6000	0.085	0.000	0.054	0.398	0.467	0.001	0.168	0.222	0.369	0.349
47	F(C-N=C)	0.3500	0.005	-0.112	0.299	0.177	0.048	0.277	0.467	0.041	0.035	0.090
48	TAU(C-N)	0.1300	0.000	0.000	0.000	0.002	0.033	0.001	0.000	0.000	0.029	0.012
49	TAU(C=N)	0.4100	0.000	0.003	0.005	0.037	0.349	0.026	0.001	0.002	0.263	0.150
50	TAU(C-CE	0.1200	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000
	PEDSUM		99.999	100.005	100.006	100.008	100.008	100.006	100.010	100.011	100.012	100.010

AVI11

	FREQUENCIES	1352.341	1341.761	1317.549	1312.546	1299.409	1286.333	1237.724	1220.424	1190.869	1185.354
	ASSIGNMENT (PED)	CCHDEF 9	CCHDEF 9	CCHDEF 9	CC ST 14	CC ST 14	BETA 1-2	PI CH 5	BETA 1-2	CCH DEF9	CCH DEF9
	ASSIGNMENT (PED)	C-N ST	BETA 1-2	CC ST 14	CCHDEF 9	CC ST 14	CC ST 14	TAU CC 4	CCH DEF9	CC ST 8	CC ST 8
1	K(CH)	4.6740	0.005	0.002	0.004	0.003	0.007	0.003	0.000	0.027	0.022	0.024
2	O(CH)	0.0240	0.002	0.000	0.001	0.001	0.002	0.001	0.000	0.004	0.001	0.004
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.001	0.000	0.001
5	H(CCH)	0.1700	37.980	45.431	39.948	25.856	13.958	8.913	0.002	20.213	43.556	34.799
6	O(CCH)	0.0015	0.501	0.709	0.272	-0.032	-0.064	-0.044	-0.000	-0.065	-0.380	-0.273
7	M(CCH)	-0.0070	-1.746	-3.264	-2.691	-1.743	-0.269	-0.352	0.000	0.766	1.782	1.400
8	P(CCH)	0.0050	0.667	1.305	0.428	-0.088	-0.141	-0.067	0.000	0.221	1.266	0.908
9	K(CC)	5.2490	15.948	6.670	37.430	57.201	78.781	53.795	0.003	8.017	15.230	18.723
10	O(CC)	0.4950	-2.034	-0.938	-6.034	-12.067	-13.831	-9.522	-0.000	1.026	-1.359	-1.032
11	M(CC)	-0.2110	-1.035	-0.399	-2.562	-5.155	-6.134	-4.151	-0.000	-0.498	0.575	0.474
12	P(CC)	0.3530	-0.586	-0.344	-2.098	-4.256	-4.834	-3.339	-0.000	0.285	1.009	1.169
13	H(CCC)	0.4190	2.383	0.401	1.657	1.112	2.986	1.650	0.001	10.460	1.396	3.696
14	O(CCC)	-0.0090	0.149	0.020	0.086	0.061	0.184	0.097	0.000	0.629	0.052	0.215
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	21.931	27.345	18.940	9.908	7.498	5.119	0.001	12.294	35.599	30.347
18	F(CC)	0.2420	0.761	0.121	0.375	0.053	0.590	0.258	0.000	2.785	0.231	1.130
19	A	0.3730	0.002	0.022	0.002	0.028	0.012	0.055	49.912	0.003	0.001	0.001
20	B	0.3100	0.001	0.026	0.001	0.040	0.029	0.063	26.555	0.003	0.001	0.000
21	C	0.0300	-0.000	0.007	0.000	0.010	0.006	0.016	12.328	0.001	0.000	0.000
22	D	-0.0200	0.000	-0.003	-0.000	-0.003	-0.002	-0.006	6.521	0.000	-0.000	-0.000
23	AC	0.0030	0.000	0.001	0.000	0.001	0.001	0.002	-0.674	-0.000	0.000	0.000
24	AM	0.0020	0.000	0.000	0.000	0.000	0.000	0.000	0.334	0.000	0.000	0.000
25	AP	0.0090	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.635	-0.000	-0.000	-0.000
26	BC	-0.0420	0.000	0.004	0.000	0.006	0.005	0.009	6.448	0.001	0.000	0.000
27	BM	-0.0250	0.000	-0.000	0.000	-0.000	-0.001	-0.001	-3.033	-0.000	-0.000	0.000
28	BP	-0.0490	0.000	-0.000	0.000	0.000	0.000	-0.000	2.089	0.000	-0.000	-0.000
29	K(CC)	3.1000	0.976	1.189	2.413	0.244	0.798	7.381	0.001	12.055	0.006	3.109
30	H(CC=C)	0.4190	1.704	0.018	0.542	0.006	0.372	1.404	0.000	1.921	0.005	0.076
31	F(CC=C)	0.3000	0.275	0.151	0.687	0.042	0.517	0.740	0.000	0.204	0.016	0.377
32	PI(CCC)	0.3700	0.003	0.001	0.001	0.001	0.000	0.000	0.097	0.001	0.000	0.000
33	K(C-N)	5.5000	11.821	1.041	3.609	3.688	9.610	0.008	0.000	0.989	0.340	0.173
34	H(NC=C)	0.4000	0.206	3.059	0.112	0.158	0.769	0.394	0.000	0.123	0.070	0.004
35	F(NC=C)	0.4500	1.048	0.655	0.238	0.860	0.864	0.351	0.000	0.011	0.380	0.016
36	PI(NCC)	0.3700	0.002	0.082	0.003	0.106	0.054	0.183	0.000	0.001	0.002	0.002
37	K(N=C)	8.0000	0.182	1.620	0.164	3.719	4.636	2.829	0.002	0.103	0.035	0.000
38	K(C-H)	4.5000	0.064	0.007	0.010	0.003	0.003	0.025	0.000	0.029	0.001	0.006
39	H(N=CH)	0.2700	1.438	2.703	1.727	1.599	0.352	7.449	0.000	5.771	0.014	0.824
40	F(N=CH)	0.5200	0.912	2.963	1.194	2.249	0.912	7.519	0.001	4.794	0.005	0.649
41	H(H-C-C)	0.3600	1.918	3.604	2.302	2.133	0.469	9.932	0.001	7.694	0.019	1.099
42	F(H-C-C)	0.2700	0.455	0.894	0.408	0.632	0.408	1.974	0.001	6.476	0.005	1.160
43	H(N=C-C)	0.4600	0.989	0.524	0.021	0.539	0.012	2.326	0.000	0.013	0.021	0.047
44	F(N=C-C)	1.5000	2.293	0.494	0.442	0.394	-0.033	1.920	-0.000	2.606	0.022	0.779
45	PI(CH)	0.3700	0.005	0.091	0.005	0.006	0.019	0.154	0.035	0.001	0.000	0.000
46	H(C-N=C)	0.6000	0.356	3.276	0.052	2.449	0.332	2.353	0.000	0.012	0.048	0.080
47	F(C-N=C)	0.3500	0.437	0.212	0.325	0.224	0.814	0.189	0.000	0.015	0.011	0.004
48	TAU(C-N)	0.1300	0.000	0.032	0.000	0.001	0.018	0.029	0.001	0.000	0.000	0.000
49	TAU(C=N)	0.4100	0.002	0.337	0.001	0.021	0.282	0.330	0.007	0.000	0.001	0.001
50	TAU(C-CE	0.1200	0.000	0.002	0.000	0.000	0.002	0.005	0.001	0.000	0.000	0.000
	PEDSUM		100.012	100.013	100.014	100.009	99.995	99.996	99.999	99.992	99.993	99.991

AVI 12

	FREQUENCIES	1168.764	1168.691	1132.688	1077.594	1075.462	1022.063	1021.442	1016.501	1006.090	1005.629
	ASSIGNMENT (PED)	CCX1 DEF	CCY1 DEF	PI CH 17	ST+DEF19	ST+DEF19	ST+DEF19	ST+DEF19	PICKCENT	CC ST 2	CC ST 2
	ASSIGNMENT (PED)	CCHDEF 9	CCHDEF 9	TAL CC16	CCHDEF 9	CCHDEF 9	CCCDEF12	CCCDEF12	TAL C=N	CCCDEF12	CCCDEF12
1	K(CH)	4.6740	0.013	0.013	0.000	0.054	0.058	0.046	0.046	0.003	0.053	0.042
2	O(CH)	0.0240	-0.000	-0.000	0.000	0.000	0.000	-0.000	-0.000	-0.000	-0.002	-0.002
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	-0.000	-0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5	H(CCH)	0.1700	51.072	51.158	0.000	26.253	26.247	17.248	17.043	0.565	5.722	4.538
6	O(CCH)	0.0015	-0.745	-0.749	-0.000	-0.119	-0.099	0.113	0.110	0.002	0.022	0.019
7	M(CCH)	-0.0070	-2.122	-2.157	-0.000	-0.010	0.053	0.528	0.512	0.005	0.103	0.087
8	P(CCH)	0.0050	-0.502	-0.518	-0.000	-0.348	-0.357	-0.377	-0.366	-0.009	-0.074	-0.062
9	K(CC)	5.2490	13.555	13.578	0.000	34.127	35.939	31.448	30.997	2.303	41.761	48.995
10	O(CC)	0.4950	-2.009	-1.995	-0.000	2.218	2.288	2.966	2.920	0.164	7.226	8.717
11	M(CC)	-0.2110	-0.477	-0.477	-0.000	1.145	1.161	1.261	1.245	0.056	-2.560	-3.272
12	P(CC)	0.3530	-0.284	-0.283	-0.000	-1.962	-2.067	-2.109	-2.081	-0.137	1.912	2.551
13	H(CCC)	0.4190	0.513	0.533	0.000	2.625	3.183	22.733	23.587	0.440	20.022	15.397
14	O(CCC)	-0.0090	0.014	0.016	0.000	-0.068	-0.043	1.223	1.281	0.012	1.238	0.949
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	40.743	40.753	0.000	26.900	27.355	18.514	18.255	0.714	9.575	9.521
18	F(CC)	0.2420	0.030	0.037	0.000	1.663	1.828	5.539	5.678	0.173	8.875	9.125
19	A	0.3730	0.000	0.000	56.076	0.080	0.002	0.003	0.003	27.313	0.959	0.240
20	B	0.3100	0.000	0.000	28.566	0.046	0.002	0.001	0.001	11.338	0.329	0.084
21	C	0.0300	0.000	0.000	12.229	0.003	0.000	0.000	0.000	3.039	0.046	0.013
22	D	-0.0200	-0.000	-0.000	0.007	-0.002	0.000	-0.000	-0.000	-1.224	-0.050	-0.013
23	AC	0.0030	0.000	0.000	-0.450	0.001	0.000	0.000	0.000	0.165	0.003	0.001
24	AM	0.0020	0.000	0.000	-0.299	0.000	0.000	0.000	-0.000	-0.052	-0.000	-0.000
25	AP	0.0190	-0.000	-0.000	1.347	-0.001	-0.000	-0.000	-0.000	-0.138	-0.007	-0.002
26	BC	-0.0420	0.000	0.000	3.873	0.007	0.000	0.000	0.000	1.258	0.042	0.010
27	BM	-0.0250	0.000	0.000	2.294	0.002	-0.000	-0.000	0.000	0.558	0.004	0.001
28	BP	-0.0490	-0.000	0.000	-3.711	-0.002	0.000	0.000	-0.000	-0.214	0.007	0.002
29	K(CC)	3.1000	0.000	0.001	0.000	0.005	0.053	0.006	0.036	0.000	0.043	0.529
30	H(CC=C)	0.4190	0.006	0.006	0.000	0.375	2.161	0.000	0.466	0.010	0.017	1.726
31	F(CC=C)	0.3000	0.001	0.002	0.000	0.083	0.501	0.000	0.237	0.010	0.014	0.284
32	PI(CCC)	0.3700	0.000	0.000	0.002	0.034	0.001	0.000	0.000	2.627	0.045	0.009
33	K(C=N)	5.5000	0.001	0.011	0.000	0.000	0.013	0.032	0.000	0.008	0.578	0.002
34	H(NC=C)	0.4000	0.012	0.004	0.000	2.537	0.265	0.418	0.000	0.021	2.116	0.017
35	F(NC=C)	0.4500	0.003	0.001	0.000	0.857	0.103	0.393	0.000	0.063	0.617	0.003
36	PI(NCC)	0.3700	0.000	0.000	0.000	0.015	0.000	0.001	0.000	0.542	0.062	0.013
37	K(N=C)	8.0000	0.001	0.024	0.000	0.034	0.306	0.000	0.001	0.015	0.009	0.001
38	K(C-H)	4.5000	0.000	0.000	0.000	0.000	0.011	0.000	0.000	0.001	0.005	0.001
39	H(N=CH)	0.2700	0.008	0.000	0.000	0.037	0.008	0.000	0.000	0.039	0.056	0.035
40	F(N=CH)	0.5200	0.007	0.000	0.000	0.043	0.028	0.000	0.000	0.037	0.033	0.028
41	H(H-C-C)	0.3600	0.010	0.001	0.000	0.049	0.011	0.000	0.000	0.051	0.074	0.046
42	F(H-C-C)	0.2700	0.003	0.000	0.000	0.014	0.019	0.000	0.001	0.022	0.051	0.101
43	H(N=C-C)	0.4600	0.004	0.004	0.000	0.027	0.365	0.000	0.000	0.000	0.233	0.043
44	F(N=C-C)	1.5000	0.004	0.019	0.000	0.014	0.433	0.000	0.013	0.001	0.181	0.075
45	PI(CH)	0.3700	0.014	0.001	0.002	1.831	0.001	0.005	0.003	34.959	0.066	0.016
46	H(C-N=C)	0.6000	0.000	0.000	0.000	0.023	0.148	0.002	0.000	0.262	0.547	0.102
47	F(C-N=C)	0.3500	0.000	0.003	0.000	0.007	0.067	0.003	0.000	0.042	0.033	0.020
48	TAU(C-N)	0.1300	0.001	0.000	0.000	0.098	0.001	0.000	0.000	0.709	0.000	0.000
49	TAU(C=N)	0.4100	0.015	0.003	0.002	1.228	0.017	0.002	0.001	12.515	0.002	0.001
50	TAU(C-CE	0.1200	0.000	0.000	0.062	0.068	0.000	0.000	0.000	1.690	0.002	0.001
	PEDSUM		99.994	99.994	99.999	99.994	99.992	99.994	99.994	99.996	99.993	99.993

AVI 13

	FREQUENCIES		988.948	981.577	979.557	944.147	913.684	849.369	818.832	812.401	749.214	739.195
	ASSIGNMENT (PED)		PI CH 5	PI CH 17	PI CH 17	PI CH 17	CC ST 2	PI+TAU10	PI+TAU10	CC=CX ST	PI CH 17	PI CH 17
	ASSIGNMENT (PED)		TAU CC 4	PICHCENT	TAU CC16	PI CX1	PI CH 5	TAU RED2	TAU RED2	CC ST 2	PI CX1	PICH=CY2
1	K(CH)	4.6740	0.000	0.001	0.000	0.007	0.017	0.000	0.000	0.035	0.002	0.000
2	O(CH)	0.0240	-0.000	0.000	0.000	-0.001	-0.003	-0.000	-0.000	-0.039	-0.001	0.000
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5	H(CCH)	0.1700	0.043	0.096	0.035	0.724	1.640	0.000	0.001	4.802	0.474	0.015
6	O(CCH)	0.0015	0.000	0.001	0.000	0.003	0.006	0.000	0.000	0.006	-0.000	-0.000
7	M(CCH)	-0.0070	0.000	0.001	0.001	0.004	0.021	0.000	0.000	0.031	0.002	0.001
8	P(CCH)	0.0150	-0.001	-0.002	-0.001	-0.006	-0.015	-0.000	-0.000	-0.019	-0.001	0.000
9	K(CC)	5.2490	1.935	0.743	0.309	10.278	16.987	0.000	0.004	26.277	1.725	0.102
10	C(CC)	0.4950	0.322	0.039	0.020	1.448	2.307	0.000	0.000	3.238	0.108	0.001
11	M(CC)	-0.2110	-0.128	0.008	0.000	-0.571	-0.827	0.000	-0.000	-0.897	-0.017	0.001
12	P(CC)	0.3530	0.094	-0.037	-0.011	0.344	0.482	0.000	0.000	0.939	0.058	-0.004
13	H(CCC)	0.4190	0.026	0.063	0.024	2.190	5.520	0.000	0.002	19.959	2.231	0.054
14	O(CCC)	-0.0090	-0.000	-0.001	-0.000	0.119	0.303	0.000	0.000	0.973	0.089	0.002
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	0.226	0.155	0.060	1.239	2.262	0.000	0.001	4.333	0.356	0.021
18	F(CC)	0.2420	0.241	0.040	0.020	1.514	2.805	0.000	0.001	7.072	0.670	0.013
19	A	0.3730	70.635	59.231	68.651	42.821	28.804	70.257	75.573	0.936	64.731	76.950
20	B	0.3100	26.664	26.468	32.509	15.406	12.031	25.952	27.867	0.680	12.739	11.253
21	C	0.0300	-8.642	7.265	12.747	5.169	-4.434	-7.534	8.089	-0.110	-0.733	1.146
22	D	-0.0200	-6.531	-3.490	-0.805	2.152	1.562	10.045	-10.787	0.017	1.403	-1.835
23	AC	0.0030	-0.622	-0.488	-0.538	0.216	0.034	0.065	0.036	0.010	1.096	1.258
24	AM	0.0020	0.295	-0.004	-0.301	-0.140	-0.091	-0.377	-0.404	0.007	0.688	0.772
25	AP	0.0090	-0.723	0.202	1.369	-0.186	-0.238	-1.695	-1.620	0.021	1.529	1.677
26	BO	-0.0420	5.364	4.026	4.412	1.137	0.556	-3.516	-3.773	0.016	-0.516	1.246
27	BM	-0.0250	-2.060	0.206	2.220	1.212	0.539	2.093	2.247	-0.008	0.412	0.790
28	BP	-0.0490	2.269	-0.687	-4.281	-1.258	0.196	4.102	2.263	0.103	1.810	1.542
29	K(CC)	3.1000	0.015	0.001	0.001	0.673	1.473	0.000	0.001	11.163	1.216	0.009
30	H(CC=C)	0.4190	0.001	0.005	0.002	0.021	0.122	0.000	0.000	0.008	0.194	0.010
31	F(CC=C)	0.3000	0.016	0.006	0.003	0.331	0.677	0.000	0.000	4.478	0.385	0.005
32	PI(CCC)	0.3700	0.148	0.014	0.001	0.113	0.028	0.000	0.006	0.014	0.430	5.554
33	K(C-N)	5.5000	0.004	0.001	0.001	0.737	2.580	0.000	0.001	4.897	0.154	0.012
34	H(NC=C)	0.4000	0.009	0.009	0.004	0.117	0.243	0.000	0.001	0.006	0.023	0.041
35	F(NC=C)	0.4500	0.044	0.040	0.017	1.352	2.519	0.000	0.001	2.348	0.057	0.032
36	PI(NCC)	0.3700	1.315	0.010	0.027	3.519	0.145	0.000	0.001	0.374	6.515	0.201
37	K(N=C)	8.0000	0.079	0.001	0.002	0.114	0.026	0.000	0.000	0.288	0.136	0.000
38	K(C-H)	4.5000	0.005	0.000	0.000	0.352	0.077	0.000	0.000	0.010	0.000	0.000
39	H(N=CH)	0.2700	0.063	0.003	0.003	0.565	0.538	0.000	0.000	0.283	0.000	0.003
40	F(N=CH)	0.5200	0.070	0.002	0.003	0.476	0.332	0.000	0.000	0.311	0.006	0.003
41	H(H-C-C)	0.3600	0.084	0.003	0.004	0.754	0.717	0.000	0.000	0.378	0.000	0.004
42	F(H-C-C)	0.2700	0.047	0.002	0.002	0.579	0.732	0.000	0.000	1.534	0.091	0.000
43	H(N=C-C)	0.4600	0.076	0.007	0.006	2.250	5.423	0.000	0.000	0.614	0.376	0.093
44	F(N=C-C)	1.5000	0.106	0.008	0.006	1.929	4.101	0.000	0.000	1.474	0.234	0.075
45	PI(CH)	0.3700	4.543	13.399	5.942	3.926	0.055	0.011	0.029	0.033	0.447	0.086
46	H(C-N=C)	0.6000	0.644	0.051	0.044	7.464	8.866	0.000	0.000	2.131	0.400	0.063
47	F(C-N=C)	0.3500	0.121	0.008	0.007	0.967	0.819	0.000	0.000	1.235	0.148	0.007
48	TAU(C-N)	0.1300	0.141	0.413	0.005	0.014	0.000	0.093	0.001	0.000	0.025	0.003
49	TAU(C=N)	0.4100	2.851	5.925	2.633	0.623	0.047	0.003	0.014	0.004	0.225	1.203
50	TAU(C-CE	0.1200	0.267	0.771	0.349	0.228	0.008	0.001	0.075	0.001	0.023	0.096
	PEDSUM		99.998	99.998	99.999	99.996	99.993	100.001	100.000	99.994	99.998	100.001

BIBS 1726

AVI 14

	FREQUENCIES	686.944	671.004	615.755	605.661	602.127	584.002	517.044	476.580	414.495	398.707
	ASSIGNMENT (PED)	TAU CC 4	TAU CC 4	TAU CC 4	CCC DEF6	CCC DEF6	CCC DEF6	N=C-CDEF	CCN DEF	PICX2=CC	TAU CC16
	ASSIGNMENT (PED)	CCC DEF6	CCC DEF6	PICX2=CC	CCC DEF6	CCC DEF6	CCC DEF6	CCCX DEF	PI CY=CH	TAU CC 4	PI CH 17
1	K(CH)	4.6740	0.005	0.004	0.001	0.010	0.012	0.018	0.027	0.021	0.002	0.001
2	O(CH)	0.0240	-0.000	-0.000	0.000	-0.000	-0.000	-0.003	-0.007	0.000	-0.000	-0.000
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	0.000	0.000	0.000	0.000	-0.000	-0.000	-0.000	0.000	0.000	0.000
5	H(CCH)	0.1700	3.194	3.223	1.188	10.558	11.529	4.175	1.713	0.462	0.061	0.013
6	O(CCH)	0.0015	-0.001	-0.001	-0.001	0.000	0.000	-0.008	-0.024	-0.029	-0.004	0.001
7	M(CCH)	-0.0070	0.006	0.007	0.004	-0.008	-0.005	0.019	0.041	0.036	0.002	0.001
8	P(CCH)	0.0050	0.001	0.002	0.002	-0.004	-0.008	-0.012	-0.038	-0.040	-0.005	-0.001
9	K(CC)	5.2490	6.992	6.315	0.839	10.668	12.316	9.847	9.097	4.368	0.301	0.092
10	O(CC)	0.4950	-0.170	-0.286	-0.059	0.998	-1.123	-0.261	-0.029	0.209	0.025	0.005
11	M(CC)	-0.2110	0.121	0.145	0.026	0.429	0.492	0.208	0.208	0.139	0.011	0.003
12	P(CC)	0.3530	0.319	0.277	0.029	0.711	0.797	0.375	-0.023	-0.202	-0.018	0.004
13	H(CCC)	0.4190	17.791	18.475	5.785	51.412	51.679	31.903	11.729	1.123	0.184	0.055
14	O(CCC)	-0.0090	0.615	0.621	0.186	1.656	1.664	1.031	0.364	0.019	0.004	0.001
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	1.880	1.828	0.554	4.365	4.326	1.863	1.415	0.836	0.075	0.017
18	F(CC)	0.2420	4.771	4.823	1.354	12.954	13.262	8.148	3.162	0.310	0.042	0.014
19	A	0.3730	18.191	9.656	30.613	2.243	1.259	2.548	4.527	11.399	31.850	23.774
20	B	0.3100	22.027	26.739	27.397	2.095	1.245	1.608	3.297	11.567	38.603	58.186
21	C	0.0300	1.880	3.720	-3.100	-0.223	-0.149	0.135	0.045	-2.252	-10.532	10.623
22	D	-0.0200	1.062	2.083	-2.327	-0.154	-0.100	0.039	-0.117	-1.851	-5.329	-0.162
23	AC	0.0030	0.283	-0.066	0.063	-0.007	-0.000	-0.043	-0.086	-0.232	-0.537	-0.196
24	AM	0.0020	-0.013	-0.017	-0.246	-0.010	-0.006	0.023	0.039	0.109	0.369	-0.111
25	AP	0.0090	0.126	-0.022	-0.472	0.032	-0.018	-0.093	-0.191	-0.496	-1.326	0.494
26	BC	-0.0420	5.913	7.178	7.366	0.556	0.331	0.202	0.374	1.899	7.161	7.911
27	BM	-0.0250	-3.517	-4.198	-4.345	-0.321	-0.192	0.029	0.069	-0.423	-1.217	4.681
28	BP	-0.0490	3.470	4.075	2.735	0.204	0.122	-0.048	-0.094	0.078	0.171	-9.018
29	K(CC)	3.1000	0.422	0.012	0.009	0.022	0.007	1.475	4.642	0.160	0.006	0.007
30	H(CC=C)	0.4190	0.714	0.374	0.333	0.065	0.250	6.909	12.771	0.071	0.682	0.237
31	F(CC=C)	0.3000	0.155	0.161	0.004	0.183	0.314	3.082	5.812	0.081	0.201	0.077
32	PI(CCC)	0.3700	0.077	0.094	27.325	1.623	0.936	0.008	0.003	0.625	26.117	0.778
33	K(C-N)	5.5000	1.028	0.710	0.003	0.004	0.016	2.303	1.726	0.710	0.000	0.013
34	H(NC=C)	0.4000	0.635	0.901	0.266	0.198	0.589	5.296	7.609	21.768	2.431	0.358
35	F(NC=C)	0.4500	0.223	0.162	0.075	0.425	0.795	3.612	4.449	10.294	1.026	0.163
36	PI(NCC)	0.3700	3.475	2.954	0.002	0.062	0.014	3.405	7.677	17.581	2.553	0.893
37	K(N=C)	8.0000	0.212	0.230	0.008	0.013	0.051	0.149	0.000	0.038	0.000	0.004
38	K(C-H)	4.5000	0.022	0.025	0.000	0.001	0.002	0.001	0.014	0.000	0.000	0.000
39	H(N=CH)	0.2700	0.025	0.030	0.010	0.007	0.020	0.102	0.226	0.001	0.000	0.001
40	F(N=CH)	0.5200	0.039	0.044	0.011	0.009	0.025	0.136	0.030	0.006	0.000	0.000
41	H(H-C-C)	0.3600	0.034	0.040	0.013	0.009	0.026	0.136	0.034	0.002	0.000	0.001
42	F(H-C-C)	0.2700	0.005	0.015	0.003	0.001	0.016	0.269	0.259	0.017	0.001	0.001
43	H(N=C-C)	0.4600	1.170	2.778	0.376	0.241	0.000	1.367	6.485	0.041	0.018	0.005
44	F(N=C-C)	1.5000	2.914	4.292	0.061	0.205	0.000	3.411	3.768	0.014	0.012	0.022
45	PI(CH)	0.3700	0.038	0.020	0.537	0.000	0.023	0.001	0.048	7.105	0.048	0.003
46	H(C-N=C)	0.6000	3.706	1.523	0.511	0.619	0.409	5.039	7.964	0.393	0.030	0.006
47	F(C-N=C)	0.3500	1.062	0.524	0.283	0.101	0.069	1.553	0.819	0.059	0.005	0.000
48	TAU(C-N)	0.1300	0.000	0.000	0.046	0.002	0.000	0.026	0.156	4.225	1.978	1.114
49	TAU(C=N)	0.4100	0.041	0.007	3.313	0.086	0.000	0.059	0.055	7.590	2.309	0.000
50	TAU(C-CE	0.1200	0.000	0.000	0.021	0.001	0.001	0.052	0.234	2.877	2.696	0.025
	PEDSUM		99.997	99.998	100.002	99.998	99.996	100.000	99.999	99.998	100.009	100.006

AVI 15

	FREQUENCIES		369.480	349.337	266.277	254.443	176.560	143.489	74.175	59.352	46.904	0.0
	ASSIGNMENT (PED)		TAU CC16	TAU CC16	TAU CC16	TAU CC16	CCCX DEF	TAU C-N	N=C-CDEF	TAU C=N	TAU C-C	
	ASSIGNMENT (PED)		CCCX DEF	PI CH 17	TAU C-C	TAU CC16	N=C-CDEF	TAU C-C	C-N=CDEF	PICKCENT	TAU C-N	
1	K(CH)	4.6740	0.022	0.001	0.003	0.009	0.017	0.005	0.006	0.002	0.000	0.0
2	O(CH)	0.0240	-0.001	-0.000	-0.001	-0.004	-0.002	0.000	-0.000	0.000	0.000	0.0
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	-0.000	-0.000	-0.000	0.000	-0.000	0.000	-0.000	0.000	0.000	0.0
5	F(CCH)	0.1700	0.726	0.024	0.155	0.820	0.889	0.095	0.164	0.053	0.001	0.0
6	O(CCH)	0.0015	-0.026	-0.001	-0.002	-0.001	-0.019	-0.008	-0.010	-0.003	-0.000	0.0
7	M(CCH)	-0.0070	0.027	0.001	0.002	0.004	-0.007	-0.001	-0.011	-0.003	-0.000	0.0
8	P(CCH)	0.0050	-0.034	-0.001	-0.003	-0.002	-0.026	-0.010	-0.014	-0.004	-0.000	0.0
9	K(CC)	5.2490	5.193	0.171	0.904	3.538	2.720	0.402	0.503	0.177	0.002	0.0
10	O(CC)	0.4950	0.214	0.009	0.046	0.299	0.276	0.036	-0.008	-0.008	-0.000	0.0
11	M(CC)	-0.2110	0.093	0.004	-0.001	-0.057	-0.012	0.015	0.003	-0.000	0.000	0.0
12	P(CC)	0.3530	-0.104	-0.005	0.004	0.085	-0.009	-0.026	-0.022	-0.007	-0.000	0.0
13	F(CCC)	0.4190	4.507	0.122	1.345	7.997	5.319	0.277	0.624	0.197	0.002	0.0
14	O(CCC)	-0.0090	0.141	0.004	0.046	0.283	0.184	0.007	0.019	0.006	0.000	0.0
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	0.795	0.029	0.105	0.342	0.386	0.098	0.100	0.030	0.000	0.0
18	F(CC)	0.2420	1.192	0.032	0.354	2.066	1.345	0.065	0.159	0.052	0.001	0.0
19	A	0.3730	6.214	42.667	14.133	10.189	4.244	7.641	2.994	5.031	1.000	0.0
20	B	0.3100	23.532	63.875	32.891	30.013	12.189	19.164	8.491	15.546	0.861	0.0
21	C	0.0300	-0.896	-15.857	-3.552	-0.635	2.101	-2.176	2.805	4.288	-0.101	0.0
22	D	-0.0200	-0.886	-0.048	-0.469	-0.236	-0.012	-0.463	-0.407	-0.449	-0.003	0.0
23	AC	0.0030	0.020	-0.344	-0.054	0.021	-0.086	-0.121	-0.130	-0.199	-0.009	0.0
24	AM	0.0020	0.030	-0.222	-0.029	-0.006	-0.017	-0.017	-0.024	-0.013	-0.005	0.0
25	AP	0.0090	-0.310	1.001	0.285	0.131	0.110	0.165	0.037	0.050	0.021	0.0
26	BC	-0.0420	3.132	8.669	4.399	4.229	1.399	2.424	0.517	1.538	0.105	0.0
27	BM	-0.0250	1.735	5.114	1.958	1.798	0.681	0.811	0.513	0.418	0.063	0.0
28	BP	-0.0490	-3.309	-8.976	-2.212	-3.050	-0.983	-1.191	-0.264	-0.180	-0.082	0.0
29	K(CC)	3.1000	0.945	0.031	1.214	4.185	1.176	0.029	1.577	0.001	0.000	0.0
30	H(CC=C)	0.4190	16.231	0.263	2.050	1.735	19.128	1.008	9.977	0.148	0.001	0.0
31	F(CC=C)	0.3000	5.593	0.096	0.986	2.207	5.550	0.263	2.623	0.037	0.000	0.0
32	PI(CCC)	0.3700	0.248	0.431	1.219	0.200	0.713	3.985	1.096	16.686	0.149	0.0
33	K(C-N)	5.5000	1.895	0.047	0.649	4.904	3.452	0.019	0.063	0.001	0.000	0.0
34	H(NC=C)	0.4000	6.261	0.712	0.234	1.350	4.461	6.664	3.123	3.629	0.047	0.0
35	F(NC=C)	0.4500	3.510	0.336	0.391	2.377	2.946	2.701	1.127	1.308	0.017	0.0
36	PI(NCC)	0.3700	13.709	0.028	0.001	0.587	5.305	2.236	15.586	3.643	0.037	0.0
37	K(N=C)	8.0000	1.351	0.044	0.523	1.319	0.257	0.008	0.280	0.000	0.000	0.0
38	K(C-H)	4.5000	0.018	0.000	0.005	0.027	0.004	0.000	0.006	0.000	0.000	0.0
39	H(N=CH)	0.2700	0.030	0.000	0.001	0.003	0.014	0.000	0.003	0.000	0.000	0.0
40	F(N=CH)	0.5200	0.015	0.001	0.028	0.061	0.006	0.000	0.019	0.000	0.000	0.0
41	H(H-C-C)	0.3600	0.041	0.000	0.002	0.003	0.018	0.000	0.004	0.000	0.000	0.0
42	F(H-C-C)	0.2700	0.116	0.003	0.066	0.231	0.045	0.002	0.083	0.000	0.000	0.0
43	H(N=C-C)	0.4600	0.467	0.003	0.360	0.472	6.971	0.545	12.419	0.009	0.000	0.0
44	F(N=C-C)	1.5000	2.889	0.057	0.331	5.505	11.466	0.526	10.529	0.011	0.000	0.0
45	PI(CH)	0.3700	0.366	0.262	2.041	2.145	0.929	0.067	0.004	19.769	0.781	0.0
46	F(C-N=C)	0.6000	1.093	0.008	2.878	5.232	3.114	0.572	21.802	0.022	0.001	0.0
47	F(C-N=C)	0.3500	0.099	0.004	0.883	2.335	0.973	0.084	3.572	0.003	0.000	0.0
48	TAU(C-N)	0.1300	0.948	0.004	14.570	0.611	0.420	30.045	0.028	1.076	43.075	0.0
49	TAU(C=N)	0.4100	1.023	0.000	5.302	5.399	2.435	2.532	0.019	34.455	6.248	0.0
50	TAU(C-CE	0.1200	1.115	1.410	15.949	1.255	0.125	21.523	0.013	1.260	47.785	0.0
	PEDSUM		100.005	100.010	99.994	99.993	100.001	99.995	100.000	100.000	100.001	0.0

BIBS LILLE

	FREQUENCIES	0.0	0.0	0.0	0.0	0.0
	ASSIGNMENT					
	(PED)					
	ASSIGNMENT					
	(PED)					
1	K(CH)	4.6740	0.0	0.0	0.0	0.0	0.0
2	C(CH)	0.0240	0.0	0.0	0.0	0.0	0.0
3	M(CH)	0.0	0.0	0.0	0.0	0.0	0.0
4	P(CH)	-0.0060	0.0	0.0	0.0	0.0	0.0
5	F(CCH)	0.1700	0.0	0.0	0.0	0.0	0.0
6	C(CCH)	0.0015	0.0	0.0	0.0	0.0	0.0
7	M(CCH)	-0.0170	0.0	0.0	0.0	0.0	0.0
8	P(CCH)	0.0050	0.0	0.0	0.0	0.0	0.0
9	K(CC)	5.2490	0.0	0.0	0.0	0.0	0.0
10	C(CC)	0.4950	0.0	0.0	0.0	0.0	0.0
11	M(CC)	-0.2110	0.0	0.0	0.0	0.0	0.0
12	P(CC)	0.3530	0.0	0.0	0.0	0.0	0.0
13	F(CCC)	0.4190	0.0	0.0	0.0	0.0	0.0
14	C(CCC)	-0.0590	0.0	0.0	0.0	0.0	0.0
15	M(CCC)	0.0	0.0	0.0	0.0	0.0	0.0
16	P(CCC)	0.0	0.0	0.0	0.0	0.0	0.0
17	F(CH)	0.3850	0.0	0.0	0.0	0.0	0.0
18	F(CC)	0.2420	0.0	0.0	0.0	0.0	0.0
19	A	0.3730	0.0	0.0	0.0	0.0	0.0
20	B	0.3100	0.0	0.0	0.0	0.0	0.0
21	C	0.0300	0.0	0.0	0.0	0.0	0.0
22	D	-0.0200	0.0	0.0	0.0	0.0	0.0
23	AD	0.0030	0.0	0.0	0.0	0.0	0.0
24	AM	0.0020	0.0	0.0	0.0	0.0	0.0
25	AP	0.0090	0.0	0.0	0.0	0.0	0.0
26	BD	-0.0420	0.0	0.0	0.0	0.0	0.0
27	BM	-0.0250	0.0	0.0	0.0	0.0	0.0
28	BP	-0.0490	0.0	0.0	0.0	0.0	0.0
29	K(CC)	3.1000	0.0	0.0	0.0	0.0	0.0
30	H(CC=C)	0.4190	0.0	0.0	0.0	0.0	0.0
31	F(CC=C)	0.3000	0.0	0.0	0.0	0.0	0.0
32	PI(CCC)	0.3700	0.0	0.0	0.0	0.0	0.0
33	K(C-N)	5.5000	0.0	0.0	0.0	0.0	0.0
34	H(NC=C)	0.4000	0.0	0.0	0.0	0.0	0.0
35	F(NC=C)	0.4500	0.0	0.0	0.0	0.0	0.0
36	PI(NCC)	0.3700	0.0	0.0	0.0	0.0	0.0
37	K(N=C)	8.0000	0.0	0.0	0.0	0.0	0.0
38	K(C-H)	4.5000	0.0	0.0	0.0	0.0	0.0
39	H(N=CH)	0.2700	0.0	0.0	0.0	0.0	0.0
40	F(N=CH)	0.5200	0.0	0.0	0.0	0.0	0.0
41	H(H-C-C)	0.3800	0.0	0.0	0.0	0.0	0.0
42	F(H-C-C)	0.2700	0.0	0.0	0.0	0.0	0.0
43	H(N=C-C)	0.4500	0.0	0.0	0.0	0.0	0.0
44	F(N=C-C)	1.5000	0.0	0.0	0.0	0.0	0.0
45	PI(CH)	0.3700	0.0	0.0	0.0	0.0	0.0
46	H(C-N=C)	0.5000	0.0	0.0	0.0	0.0	0.0
47	F(C-N=C)	0.3500	0.0	0.0	0.0	0.0	0.0
48	TAU(C-N)	0.1300	0.0	0.0	0.0	0.0	0.0
49	TAU(C=N)	0.4100	0.0	0.0	0.0	0.0	0.0
50	TAU(C-CE	0.1200	0.0	0.0	0.0	0.0	0.0
	PEDSUM		0.0	0.0	0.0	0.0	0.0

BENZYLIDENE-ANILINE GEOMETRIE SIMPLIFIEE SEPTEMBRE 1972

A VII 1

MOLECULE A 27 ATOMES

M	X(M)	Y(M)	Z(M)	KONF	J	K	L	D1	D2	D3	A1	A2	A3	IS	KAL	AMAS
6	0.0	0.0	0.0													
7	1.460000	0.0	0.0													
8	2.078500	1.071273	0.0													
9	3.574500	1.071273	0.000000	7	6	7	8	1.460	1.237	1.496	120.000	120.000	180.000	0	0	12.0112
20	1.548500	1.989260	0.0	7	6	7	8	1.460	1.237	1.060	120.000	120.000	0.0	0	0	1.0080
1	-0.698500	-0.690471	0.993457	3	6	7	8	1.460	1.237	1.397	120.000	120.000	124.800	0	0	12.0112
5	-0.698500	0.690471	-0.993457	3	6	7	8	1.460	1.237	1.397	120.000	120.000	304.800	0	0	12.0112
15	-0.156500	-1.226240	1.764329	3	1	6	5	1.397	1.397	1.084	120.000	120.000	180.000	0	1	1.0080
2	-2.095500	-0.690471	0.993457	3	1	6	5	1.397	1.397	1.397	120.000	120.000	360.000	0	0	12.0112
19	-0.156500	1.226240	-1.764329	7	1	6	5	1.397	1.397	1.084	120.000	120.000	180.000	0	0	1.0080
4	-2.095500	0.690471	-0.993457	7	1	6	5	1.397	1.397	1.397	120.000	120.000	360.000	0	0	12.0112
18	-2.637500	1.226240	-1.764329	7	6	5	4	1.397	1.397	1.084	120.000	120.000	180.000	0	1	1.0080
3	-2.794000	-0.000000	-0.000000	7	6	5	4	1.397	1.397	1.397	120.000	120.000	360.000	0	0	12.0112
16	-2.637500	-1.226240	1.764329	7	4	3	2	1.397	1.397	1.084	120.000	120.000	180.000	0	1	1.0080
17	-3.878000	0.000000	0.000000	5	4	3	2	1.397	1.397	1.084	120.000	120.000	120.000	1	0	1.0080
10	4.273000	2.261614	0.216322	7	7	8	9	1.237	1.496	1.397	120.000	120.000	190.300	0	1	12.0112
14	4.273000	-0.119068	-0.216322	7	7	8	9	1.237	1.496	1.397	120.000	120.000	10.300	0	0	12.0112
21	3.731000	3.185258	0.384176	3	10	9	14	1.397	1.397	1.084	120.000	120.000	180.000	0	1	1.0080
11	5.670000	2.261614	0.216322	3	10	9	14	1.397	1.397	1.397	120.000	120.000	360.000	0	0	12.0112
25	3.731000	-1.042711	-0.384176	7	10	9	14	1.397	1.397	1.084	120.000	120.000	180.000	0	0	1.0080
13	5.670000	-0.119068	-0.216322	7	10	9	14	1.397	1.397	1.397	120.000	120.000	360.000	0	0	12.0112
22	6.212000	3.185258	0.384176	7	9	10	11	1.397	1.397	1.084	120.000	120.000	180.000	0	1	1.0080
12	6.368500	1.071273	0.000000	7	9	10	11	1.397	1.397	1.397	120.000	120.000	360.000	0	0	12.0112
23	7.452500	1.071273	-0.000000	5	11	12	13	1.397	1.397	1.084	120.000	120.000	120.000	1	1	1.0080
24	6.212000	-1.042711	-0.384176	7	11	12	13	1.397	1.397	1.084	120.000	120.000	180.000	0	0	1.0080
26	1.460000	0.000000	0.000000	7	14	9	8	1.397	1.496	1.237	120.000	120.000	10.300	0	1	0.0
27	-0.156500	-1.226240	1.764329	7	7	6	1	1.460	1.397	1.084	120.000	120.000	360.000	0	1	0.0

BUS LILLE

BIBLIOTHEQUE

A VII 2

ESPECE ISOTOPIQUE 1

BENZYLIDENE-ANILINE GEOMETRIE SIMPLIFIEE SEPTEMBRE 1972

XG= 1.779933 YG= 0.537824 ZG= -0.000000 MG= 181.240300

I	COORDONNEES PAR RAPPORT AU CENTRE DE GRAVITE			AM(I)
1	-2.478433	-1.223294	0.993457	12.011200
2	-3.875433	-1.223294	0.993457	12.011200
3	-4.573933	-0.537824	0.000000	12.011200
4	-3.875433	0.152647	-0.993457	12.011200
5	-2.478433	0.152647	-0.993457	12.011200
6	-1.779933	-0.537824	0.000000	12.011200
7	-0.319933	-0.537824	0.000000	14.006700
8	0.298567	0.533450	0.000000	12.011200
9	1.794567	0.533450	0.000000	12.011200
10	2.493067	1.723791	0.216322	12.011200
11	3.890067	1.723791	0.216322	12.011200
12	4.588567	0.533450	0.000000	12.011200
13	3.890067	-0.656891	-0.216322	12.011200
14	2.493067	-0.656891	-0.216322	12.011200
15	-1.936433	-1.764064	1.764329	1.008000
16	-4.417433	-1.764064	1.764329	1.008000
17	-5.657933	-0.537824	0.000000	1.008000
18	-4.417433	0.688417	-1.764329	1.008000
19	-1.936433	0.688417	-1.764329	1.008000
20	-0.231433	1.451437	0.000000	1.008000
21	1.951067	2.647434	0.384176	1.008000
22	4.432067	2.647434	0.384176	1.008000
23	5.672567	0.533450	-0.000000	1.008000
24	4.432067	-1.580535	-0.384176	1.008000
25	1.951067	-1.580535	-0.384176	1.008000
26	-0.319933	-0.537824	0.000000	0.0
27	-1.936433	-1.764064	1.764329	0.0

TENSEUR D INERTIE

I	TT(I,1)	TT(I,2)	TT(I,3)
1	231.713531	-269.689420	0.000000
2	-269.689420	1826.346780	26.033745
3	0.000000	26.033745	1932.435248

TENSEUR PRINCIPAL D INERTIE

1	187.327463	-0.000000	-0.000000
2	-0.000000	1861.430418	-0.000000
3	-0.000000	-0.000000	1941.737678

COORDONNEES PAR RAPPORT AUX AXES PRINCIPAUX

1	-2.647404	-1.096979	0.652829
2	-4.026855	-0.882502	0.726860
3	-4.600544	0.203253	0.061670
4	-3.796781	1.074532	-0.677551
5	-2.418330	0.860056	-0.751582
6	-1.843641	-0.225700	-0.086392
7	-0.403026	-0.449848	-0.163762
8	0.381233	0.449071	0.163424
9	1.857370	0.219395	0.084147
10	2.739379	1.142014	0.650523
11	4.117831	0.928437	0.576492
12	4.614273	-0.209558	-0.063916
13	3.732263	-1.133077	-0.630292
14	2.353812	-0.918600	-0.556260
15	-2.201475	-1.939469	1.168982
16	-4.649534	-1.558570	1.300457
17	-5.670151	0.369676	0.119115
18	-4.242710	1.917022	-1.193704
19	-1.794651	1.536123	-1.325179
20	0.007348	1.382103	0.499966
21	2.354166	2.025939	1.147446
22	4.802225	1.645040	1.015970
23	5.683880	-0.375981	-0.121360
24	4.117477	-2.016102	-1.127215
25	1.669418	-1.635203	-0.995739
26	-0.403026	-0.449848	-0.163762
27	-2.201475	-1.939469	1.168982

MATRICE DE TRANSFORMATION

1	0.986723	0.162397	-0.002423
2	-0.153526	0.927751	-0.340158
3	-0.052993	0.336013	0.940365

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MOMENTS PRINCIPAUX D INERTIE

IA	XX	IB	YY	IC	ZZ
187.3275	A.M.U*(A)^2	1861.4304	A.M.U*(A)^2	1941.7377	A.M.U*(A)^2
311.0450	G*CM^2 *10^{-40}	3090.7833	G*CM^2 *10^{-40}	3224.1282	G*CM^2 *10^{-40}

CONSTANTES ROTATIONNELLES

A	B	C
0.0900 CM^{-1}	0.0091 CM^{-1}	0.0087 CM^{-1}
1.787465 *10^{-17} ERG	0.179884 *10^{-17} ERG	0.172444 *10^{-17} ERG
2697.82 MHZ	271.50 MHZ	260.27 MHZ

* PARAMETRES D ASYMETRIE *
****

RO(A)	RO(C)	RO	BETA(PRO)	BETA(OBL)	BETA	KAPA	BE	DELTA	PI
9.93677E+00	0.958642	8.97813E+00	8.93677E+00	-0.041358	8.89541E+00	-0.990787	-0.002309	0.004607	8.93687E+00

CARACTERISTIQUE GLOBALE DU ROTATEUR
********** ROTATEUR NONPLAN A TOUPIE ASYMETRIQUE ALLONGEE