Molécula de H_2

Molecular Orbital Coefficients

				1	2
				(SGG)--O	(SGU)--V
	EIGENVALUES --			-0.59022	0.70065
1	1	H	1S	0.54586	1.24624
2	2	H	1S	0.54586	-1.24624

E(1s) = -13.6 eV
E(2p) = 9.5 eV (valor estimado)

Molécula de Li_2

Molecular Orbital Coefficients

				1	2	3	4	5
				(SGU)--O	(SGG)--O	(SGG)--O	(SGU)--V	(PIU)--V
	EIGENVALUES --			-2.33047	-2.33041	-0.14889	0.08228	0.13425
1	1	Li	1S	0.70039	0.70094	-0.19732	-0.17944	0.00000
2			2S	0.03709	0.02026	0.56833	0.70126	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.00000	0.62604
5			2PZ	-0.00805	0.00166	-0.10187	0.30461	0.00000
6	2	Li	1S	-0.70039	0.70094	-0.19732	0.17944	0.00000
7			2S	-0.03709	0.02026	0.56833	-0.70126	0.00000
8			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
9			2PY	0.00000	0.00000	0.00000	0.00000	0.62604
10			2PZ	-0.00805	-0.00166	0.10187	0.30461	0.00000

				6	7	8	9	10
				(PIU)--V	(SGG)--V	(PIG)--V	(PIG)--V	(SGU)--V
	EIGENVALUES --			0.13425	0.15707	0.23933	0.23933	0.46356
1	1	Li	1S	0.00000	-0.03560	0.00000	0.00000	-0.13688
2			2S	0.00000	0.29058	0.00000	0.00000	1.20418
3			2PX	0.62604	0.00000	0.83090	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.83090	0.00000
5			2PZ	0.00000	0.64094	0.00000	0.00000	-1.19039
6	2	Li	1S	0.00000	-0.03560	0.00000	0.00000	0.13688
7			2S	0.00000	0.29058	0.00000	0.00000	-1.20418
8			2PX	0.62604	0.00000	-0.83090	0.00000	0.00000
9			2PY	0.00000	0.00000	0.00000	-0.83090	0.00000
10			2PZ	0.00000	-0.64094	0.00000	0.00000	-1.19039

E(1s) = -67.6 eV
E(2s) = -5.4 eV
E(2p) = 0.7 eV (valor estimado)

Molécula de Be_2

Molecular Orbital Coefficients

				1	2	3	4	5
				(SGU)--O	(SGG)--O	(SGG)--O	(SGU)--O	(SGG)--V
	EIGENVALUES --			-4.48619	-4.48594	-0.27907	-0.22957	0.17624
1	1	Be	1S	0.70181	0.70226	-0.20160	-0.21210	-0.02559
2			2S	0.01972	0.01768	0.70214	0.75371	0.10402
3			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
5			2PZ	-0.00156	0.00090	-0.03619	0.04453	0.66661
6	2	Be	1S	-0.70181	0.70226	-0.20160	0.21210	-0.02559
7			2S	-0.01972	0.01768	0.70214	-0.75371	0.10402
8			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
9			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
10			2PZ	-0.00156	-0.00090	0.03619	0.04453	-0.66661
				6	7	8	9	10
				(PIU)--V	(PIU)--V	(PIG)--V	(PIG)--V	(SGU)--V
	EIGENVALUES --			0.20818	0.20818	0.23318	0.23318	0.28678
1	1	Be	1S	0.00000	0.00000	0.00000	0.00000	0.03218
2			2S	0.00000	0.00000	0.00000	0.00000	-0.13127
3			2PX	0.00000	0.69697	0.71769	0.00000	0.00000
4			2PY	0.69697	0.00000	0.00000	0.71769	0.00000
5			2PZ	0.00000	0.00000	0.00000	0.00000	0.76250
6	2	Be	1S	0.00000	0.00000	0.00000	0.00000	-0.03218
7			2S	0.00000	0.00000	0.00000	0.00000	0.13127
8			2PX	0.00000	0.69697	-0.71769	0.00000	0.00000
9			2PY	0.69697	0.00000	0.00000	-0.71769	0.00000
10			2PZ	0.00000	0.00000	0.00000	0.00000	0.76250

E(1s) = -128.8 eV
E(2s) = -9.3 eV
E(2p) = 0.4 eV (valor estimado)

Molécula de C_2

Molecular Orbital Coefficients

				1	2	3	4	5
				(SGG)--O	(SGU)--O	(SGG)--O	(SGU)--O	(PIU)--O
	EIGENVALUES --			-11.02855	-11.02834	-0.90398	-0.44705	-0.31548
1	1	C	1S	0.70279	0.70228	-0.18744	-0.18844	0.00000
2			2S	0.01434	0.02433	0.56644	0.76631	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.00000	0.64102
5			2PZ	-0.00019	-0.00720	-0.14198	0.21504	0.00000
6	2	C	1S	0.70279	-0.70228	-0.18744	0.18844	0.00000
7			2S	0.01434	-0.02433	0.56644	-0.76631	0.00000
8			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
9			2PY	0.00000	0.00000	0.00000	0.00000	0.64102
10			2PZ	0.00019	-0.00720	0.14198	0.21504	0.00000

				6	7	8	9	10
				(PIU)--O	(SGG)--V	(PIG)--V	(PIG)--V	(SGU)--V
	EIGENVALUES --			-0.31548	0.04799	0.29479	0.29479	0.91941
1	1	C	1S	0.00000	-0.05515	0.00000	0.00000	0.12227
2			2S	0.00000	0.31922	0.00000	0.00000	-0.86889
3			2PX	0.64102	0.00000	0.00000	0.79901	0.00000
4			2PY	0.00000	0.00000	0.79901	0.00000	0.00000
5			2PZ	0.00000	0.62532	0.00000	0.00000	1.06440
6	2	C	1S	0.00000	-0.05515	0.00000	0.00000	-0.12227
7			2S	0.00000	0.31922	0.00000	0.00000	0.86889
8			2PX	0.64102	0.00000	0.00000	-0.79901	0.00000
9			2PY	0.00000	0.00000	-0.79901	0.00000	0.00000
10			2PZ	0.00000	-0.62532	0.00000	0.00000	1.06440

E(2s) = -19.4 eV
E(2p) = -10.6 eV

Molécula de N_2

Molecular Orbital Coefficients

				1	2	3	4	5
				(SGG)--O	(SGU)--O	(SGG)--O	(SGU)--O	(PIU)--O
	EIGENVALUES --			-15.50632	-15.50496	-1.40848	-0.72753	-0.54859
1	1	N	1S	0.70318	0.70282	-0.17370	-0.17255	0.00000
2			2S	0.01286	0.02571	0.50000	0.74661	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.00000	0.62964
5			2PZ	-0.00171	-0.00924	-0.23027	0.25277	0.00000
6	2	N	1S	0.70318	-0.70282	-0.17370	0.17255	0.00000
7			2S	0.01286	-0.02571	0.50000	-0.74661	0.00000
8			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
9			2PY	0.00000	0.00000	0.00000	0.00000	0.62964
10			2PZ	0.00171	-0.00924	0.23027	0.25277	0.00000

				6	7	8	9	10
				(PIU)--O	(SGG)--O	(PIG)--V	(PIG)--V	(SGU)--V
	EIGENVALUES --			-0.54859	-0.53025	0.26532	0.26532	1.04081
1	1	N	1S	0.00000	-0.06956	0.00000	0.00000	0.12483
2			2S	0.00000	0.39958	0.00000	0.00000	-1.09464
3			2PX	0.62964	0.00000	0.00000	0.82266	0.00000
4			2PY	0.00000	0.00000	0.82266	0.00000	0.00000
5			2PZ	0.00000	0.60424	0.00000	0.00000	1.16297
6	2	N	1S	0.00000	-0.06956	0.00000	0.00000	-0.12483
7			2S	0.00000	0.39958	0.00000	0.00000	1.09464
8			2PX	0.62964	0.00000	0.00000	-0.82266	0.00000
9			2PY	0.00000	0.00000	-0.82266	0.00000	0.00000
10			2PZ	0.00000	-0.60424	0.00000	0.00000	1.16297

E(2s) = -25.6 eV
E(2p) = -13.2 eV

Molécula de HF

Molecular Orbital Coefficients

				1	2	3	4	5
				(SG)--O	(SG)--O	(SG)--O	(PI)--O	(PI)--O
	EIGENVALUES --			-25.90350	-1.45989	-0.57369	-0.46312	-0.46312
1	1	H	1S	-0.00534	0.15045	-0.53367	0.00000	0.00000
2	2	F	1S	0.99475	-0.25067	-0.07828	0.00000	0.00000
3			2S	0.02226	0.94668	0.41097	0.00000	0.00000
4			2PX	0.00000	0.00000	0.00000	1.00000	0.00000
5			2PY	0.00000	0.00000	0.00000	0.00000	1.00000
6			2PZ	-0.00267	-0.07828	0.69807	0.00000	0.00000

				6
				(SG)--V
	EIGENVALUES --			0.58993
1	1	H	1S	1.05444
2	2	F	1S	0.08058
3			2S	-0.51597
4			2PX	0.00000
5			2PY	0.00000
6			2PZ	0.81646

$E(1s_H)$ = -13.6 eV
$E(2s_F)$ = -40.2 eV
$E(2p_F)$ = -18.6 eV

Molécula de BF

Molecular Orbital Coefficients

				1	2	3	4	5
				(SG)--O	(SG)--O	(SG)--O	(SG)--O	(PI)--O
	EIGENVALUES --			-26.04835	-7.34737	-1.59322	-0.68620	-0.58336
1	1	B	1S	0.00051	0.99203	-0.07461	0.14041	0.00000
2			2S	-0.00545	0.02833	0.09912	-0.34532	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	0.24810
4			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
5			2PZ	-0.00603	0.00643	0.08612	-0.17804	0.00000
6	2	F	1S	0.99449	-0.00039	-0.25009	-0.07474	0.00000
7			2S	0.02453	-0.00427	0.93814	0.38743	0.00000
8			2PX	0.00000	0.00000	0.00000	0.00000	0.92479
9			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
10			2PZ	-0.00380	-0.00191	-0.11949	0.81040	0.00000

				6	7	8	9	10
				(PI)--O	(SG)--O	(PI)--V	(PI)--V	(SG)--V
	EIGENVALUES --			-0.58336	-0.27820	0.33351	0.33351	0.80848
1	1	B	1S	0.00000	-0.24330	0.00000	0.00000	-0.12740
2			2S	0.00000	0.90670	0.00000	0.00000	0.67630
3			2PX	0.00000	0.00000	0.00000	0.98613	0.00000
4			2PY	0.24810	0.00000	0.98613	0.00000	0.00000
5			2PZ	0.00000	-0.46141	0.00000	0.00000	1.12119
6	2	F	1S	0.00000	0.01928	0.00000	0.00000	0.10847
7			2S	0.00000	-0.09097	0.00000	0.00000	-0.79384
8			2PX	0.00000	0.00000	0.00000	-0.42281	0.00000
9			2PY	0.92479	0.00000	-0.42281	0.00000	0.00000
10			2PZ	0.00000	0.27394	0.00000	0.00000	0.70299

$E(2s_B) = -14.0$ eV
$E(2p_B) = -8.3$ eV
$E(2s_F) = -40.2$ eV
$E(2p_F) = -18.6$ eV

Molécula de CO

Molecular Orbital Coefficients

				1	2	3	4	5
				(SG)--O	(SG)--O	(SG)--O	(SG)--O	(PI)--O
	EIGENVALUES --			-20.41556	-11.09219	-1.44528	-0.69683	-0.53993
1	1	C	1S	0.00042	0.99363	-0.12384	0.16958	0.00000
2			2S	-0.00831	0.02620	0.24367	-0.55894	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	0.44563
4			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
5			2PZ	-0.00715	0.00685	0.16589	-0.06487	0.00000
6	2	O	1S	0.99418	-0.00013	-0.22254	-0.13170	0.00000
7			2S	0.02734	-0.00685	0.77057	0.64253	0.00000
8			2PX	0.00000	0.00000	0.00000	0.00000	0.79418
9			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
10			2PZ	-0.00655	0.00121	-0.21049	0.61471	0.00000

				6	7	8	9	10
				(PI)--O	(SG)--O	(PI)--V	(PI)--V	(SG)--V
	EIGENVALUES --			-0.53993	-0.44513	0.30615	0.30615	1.00913
1	1	C	1S	0.00000	-0.16508	0.00000	0.00000	-0.12243
2			2S	0.00000	0.74772	0.00000	0.00000	0.93742
3			2PX	0.00000	0.00000	0.00000	0.92906	0.00000
4			2PY	0.44563	0.00000	0.92906	0.00000	0.00000
5			2PZ	0.00000	-0.57471	0.00000	0.00000	1.20587
6	2	O	1S	0.00000	-0.00141	0.00000	0.00000	0.12642
7			2S	0.00000	0.04914	0.00000	0.00000	-1.04109
8			2PX	0.00000	0.00000	0.00000	-0.65651	0.00000
9			2PY	0.79418	0.00000	-0.65651	0.00000	0.00000
10			2PZ	0.00000	0.44458	0.00000	0.00000	0.95848

$E(2s_C)$ = -19.4 eV
$E(2p_C)$ = -10.6 eV
$E(2s_{Ox})$ = -32.3 eV
$E(2p_{Ox})$ = -15.8 eV

Molécula de BeH_2

Molecular Orbital Coefficients

				1	2	3	4	5
				(SGG)--O	(SGG)--O	(SGU)--O	(PIU)--V	(PIU)--V
	EIGENVALUES --			-4.51815	-0.46459	-0.42980	0.21078	0.21078
1	1	Be	1S	0.99175	-0.22784	0.00000	0.00000	0.00000
2			2S	0.03165	0.54705	0.00000	0.00000	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	1.00000
4			2PY	0.00000	0.00000	0.00000	1.00000	0.00000
5			2PZ	0.00000	0.00000	0.50521	0.00000	0.00000
6	2	H	1S	-0.00236	0.39544	0.40092	0.00000	0.00000
7	3	H	1S	-0.00236	0.39544	-0.40092	0.00000	0.00000

				6	7
				(SGG)--V	(SGU)--V
	EIGENVALUES --			0.48046	0.99792
1	1	Be	1S	-0.21348	0.00000
2			2S	1.27104	0.00000
3			2PX	0.00000	0.00000
4			2PY	0.00000	0.00000
5			2PZ	0.00000	1.51417
6	2	H	1S	-0.84297	-1.08155
7	3	H	1S	-0.84297	1.08155

$E(1s_H) = -13.6$ eV
$E(2s_{Be}) = -9.3$ eV
$E(2p_{Be}) = 0.4$ eV (valor estimado)

Molécula de H_2O

Molecular Orbital Coefficients

				1	2	3	4	5
				(A1)--O	(A1)--O	(B2)--O	(A1)--O	(B1)--O
	EIGENVALUES --			-20.25151	-1.25759	-0.59391	-0.45974	-0.39260
1	1	O	1S	0.99422	-0.23376	0.00000	-0.10404	0.00000
2			2S	0.02585	0.84439	0.00000	0.53816	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	1.00000
4			2PY	0.00000	0.00000	0.61264	0.00000	0.00000
5			2PZ	-0.00417	-0.12289	0.00000	0.75599	0.00000
6	2	H	1S	-0.00559	0.15561	0.44925	-0.29498	0.00000
7	3	H	1S	-0.00559	0.15561	-0.44925	-0.29498	0.00000

				6	7
				(A1)--V	(B2)--V
	EIGENVALUES --			0.58190	0.69288
1	1	O	1S	-0.12585	0.00000
2			2S	0.82044	0.00000
3			2PX	0.00000	0.00000
4			2PY	0.00000	0.95993
5			2PZ	-0.76347	0.00000
6	2	H	1S	-0.76929	-0.81474
7	3	H	1S	-0.76929	0.81474

$E(1s_H) = -13.6$ eV
$E(2s_{Ox}) = -32.3$ eV
$E(2p_{Ox}) = -15.8$ eV

Molécula de CO_2

Molecular Orbital Coefficients

				1	2	3	4	5
				(SGU)--O	(SGG)--O	(SGG)--O	(SGG)--O	(SGU)--O
	EIGENVALUES --			-20.35690	-20.35665	-11.26305	-1.43279	-1.36824
1	1	C	1S	0.00000	0.00057	0.99334	-0.16217	0.00000
2			2S	0.00000	-0.00971	0.02740	0.35010	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
5			2PZ	-0.01122	0.00000	0.00000	0.00000	0.30660
6	2	O	1S	0.70295	0.70308	-0.00009	-0.14879	-0.16148
7			2S	0.02002	0.01796	-0.00449	0.52051	0.54356
8			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
9			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
10			2PZ	-0.00516	-0.00386	0.00050	-0.14142	-0.11321
11	3	O	1S	-0.70295	0.70308	-0.00009	-0.14879	0.16148
12			2S	-0.02002	0.01796	-0.00449	0.52051	-0.54356
13			2PX	0.00000	0.00000	0.00000	0.00000	0.00000
14			2PY	0.00000	0.00000	0.00000	0.00000	0.00000
15			2PZ	-0.00516	0.00386	-0.00050	0.14142	-0.11321

				6	7	8	9	10
				(SGG)--O	(PIU)--O	(PIU)--O	(SGU)--O	(PIG)--O
	EIGENVALUES --			-0.68101	-0.62077	-0.62077	-0.58315	-0.38766
1	1	C	1S	-0.16348	0.00000	0.00000	0.00000	0.00000
2			2S	0.55739	0.00000	0.00000	0.00000	0.00000
3			2PX	0.00000	0.55708	0.00000	0.00000	0.00000
4			2PY	0.00000	0.00000	0.55708	0.00000	0.00000
5			2PZ	0.00000	0.00000	0.00000	-0.44907	0.00000
6	2	O	1S	0.10903	0.00000	0.00000	-0.08212	0.00000
7			2S	-0.52306	0.00000	0.00000	0.45067	0.00000
8			2PX	0.00000	0.47591	0.00000	0.00000	0.00000
9			2PY	0.00000	0.00000	0.47591	0.00000	0.70865
10			2PZ	-0.40496	0.00000	0.00000	0.49723	0.00000
11	3	O	1S	0.10903	0.00000	0.00000	0.08212	0.00000
12			2S	-0.52306	0.00000	0.00000	-0.45067	0.00000
13			2PX	0.00000	0.47591	0.00000	0.00000	0.00000
14			2PY	0.00000	0.00000	0.47591	0.00000	-0.70865
15			2PZ	0.40496	0.00000	0.00000	0.49723	0.00000

				11	12	13	14	15
				(PIG)--O	(PIU)--V	(PIU)--V	(SGG)--V	(SGU)--V
	EIGENVALUES --			-0.38766	0.31058	0.31058	0.53743	1.30801
1	1	C	1S	0.00000	0.00000	0.00000	-0.19718	0.00000
2			2S	0.00000	0.00000	0.00000	1.28138	0.00000
3			2PX	0.00000	0.00000	0.89317	0.00000	0.00000
4			2PY	0.00000	0.89317	0.00000	0.00000	0.00000
5			2PZ	0.00000	0.00000	0.00000	0.00000	1.56967
6	2	O	1S	0.00000	0.00000	0.00000	0.07797	0.09613
7			2S	0.00000	0.00000	0.00000	-0.51580	-0.81737
8			2PX	0.70865	0.00000	-0.57022	0.00000	0.00000
9			2PY	0.00000	-0.57022	0.00000	0.00000	0.00000
10			2PZ	0.00000	0.00000	0.00000	0.70063	0.75221
11	3	O	1S	0.00000	0.00000	0.00000	0.07797	-0.09613
12			2S	0.00000	0.00000	0.00000	-0.51580	0.81737
13			2PX	-0.70865	0.00000	-0.57022	0.00000	0.00000
14			2PY	0.00000	-0.57022	0.00000	0.00000	0.00000
15			2PZ	0.00000	0.00000	0.00000	-0.70063	0.75221

Molécula de BH_3

Molecular Orbital Coefficients

				1	2	3	4	5
				(A1')--O	(A1')--O	(E')--O	(E')--O	(A2")--V
	EIGENVALUES --			-7.41430	-0.67580	-0.47121	-0.47121	0.23784
1	1	B	1S	0.99085	-0.22966	0.00000	0.00000	0.00000
2			2S	0.03771	0.54750	0.00000	0.00000	0.00000
3			2PX	0.00000	0.00000	0.50938	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.50938	0.00000
5			2PZ	0.00000	0.00000	0.00000	0.00000	1.00000
6	2	H	1S	-0.00653	0.28006	0.00000	0.51377	0.00000
7	3	H	1S	-0.00653	0.28006	0.44494	-0.25689	0.00000
8	4	H	1S	-0.00653	0.28006	-0.44494	-0.25689	0.00000

				6	7	8
				(A1')--V	(E')--V	(E')--V
	EIGENVALUES --			0.72576	0.77780	0.77780
1	1	B	1S	-0.26431	0.00000	0.00000
2			2S	1.52930	0.00000	0.00000
3			2PX	0.00000	0.00000	1.21236
4			2PY	0.00000	1.21236	0.00000
5			2PZ	0.00000	0.00000	0.00000
6	2	H	1S	-0.76856	-1.02094	0.00000
7	3	H	1S	-0.76856	0.51047	-0.88416
8	4	H	1S	-0.76856	0.51047	0.88416

Molécula de NH_3

Molecular Orbital Coefficients

				1	2	3	4	5
				(A)--O	(A)--O	(E)--O	(E)--O	(A)--O
	EIGENVALUES --			-15.31277	-1.08685	-0.56167	-0.56167	-0.35847
1	1	N	1S	0.99345	-0.21894	0.00000	0.00000	-0.09586
2			2S	0.03134	0.73977	0.00000	0.00000	0.48184
3			2PX	0.00000	0.00000	-0.22425	0.54940	0.00000
4			2PY	0.00000	0.00000	0.54940	0.22425	0.00000
5			2PZ	-0.00519	-0.14123	0.00000	0.00000	0.87075
6	2	H	1S	-0.00647	0.15902	0.46382	0.18932	-0.13815
7	3	H	1S	-0.00647	0.15902	-0.06795	-0.49634	-0.13815
8	4	H	1S	-0.00647	0.15902	-0.39587	0.30702	-0.13815

				6	7	8
				(A)--V	(E)--V	(E)--V
	EIGENVALUES --			0.62523	0.70051	0.70051
1	1	N	1S	-0.18000	0.00000	0.00000
2			2S	1.21198	0.00000	0.00000
3			2PX	0.00000	0.66680	-0.78983
4			2PY	0.00000	0.78983	0.66680
5			2PZ	-0.61272	0.00000	0.00000
6	2	H	1S	-0.70134	-0.74559	-0.62944
7	3	H	1S	-0.70134	0.91791	-0.33098
8	4	H	1S	-0.70134	-0.17232	0.96042

Molécula de CH_4

Molecular Orbital Coefficients

				1	2	3	4	5
				(A1)--O	(A1)--O	(T2)--O	(T2)--O	(T2)--O
	EIGENVALUES --			-11.02968	-0.91209	-0.52049	-0.52049	-0.52049
1	1	C	1S	0.99193	-0.22143	0.00000	0.00000	0.00000
2			2S	0.03836	0.62759	0.00000	0.00000	0.00000
3			2PX	0.00000	0.00000	0.57197	0.00000	0.00000
4			2PY	0.00000	0.00000	0.00000	0.57197	0.00000
5			2PZ	0.00000	0.00000	0.00000	0.00000	0.57197
6	2	H	1S	-0.00701	0.18057	0.30082	0.30082	0.30082
7	3	H	1S	-0.00701	0.18057	-0.30082	-0.30082	0.30082
8	4	H	1S	-0.00701	0.18057	-0.30082	0.30082	-0.30082
9	5	H	1S	-0.00701	0.18057	0.30082	-0.30082	-0.30082

				6	7	8	9
				(T2)--V	(T2)--V	(T2)--V	(A1)--V
	EIGENVALUES --			0.71922	0.71922	0.71922	0.76106
1	1	C	1S	0.00000	0.00000	0.00000	-0.25232
2			2S	0.00000	0.00000	0.00000	1.63282
3			2PX	0.00000	0.00000	1.10636	0.00000
4			2PY	0.00000	1.10636	0.00000	0.00000
5			2PZ	1.10636	0.00000	0.00000	0.00000
6	2	H	1S	-0.61483	-0.61483	-0.61483	-0.66772
7	3	H	1S	-0.61483	0.61483	0.61483	-0.66772
8	4	H	1S	0.61483	-0.61483	0.61483	-0.66772
9	5	H	1S	0.61483	0.61483	-0.61483	-0.66772

Molécula de Butadieno

Molecular Orbital Coefficients

				1	2	3	4	5
				(A')--O	(A')--O	(A')--O	(A')--O	(A')--O
	EIGENVALUES --			-11.03179	-11.03158	-11.01818	-11.01817	-1.03520
1	1	C	1S	0.02584	0.02443	0.73519	0.66540	-0.10624
2			2S	-0.00493	-0.00474	0.02730	0.02454	0.27272
3			2PX	0.00263	0.00272	-0.00117	-0.00100	-0.06846
4			2PY	-0.00190	-0.00175	0.00082	0.00065	0.05384
5			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	2	H	1S	-0.00005	-0.00016	-0.00508	-0.00459	0.06142
7	3	H	1S	-0.00006	-0.00010	-0.00508	-0.00460	0.05634
8	4	C	1S	0.70179	0.70053	-0.02661	-0.02280	-0.14889
9			2S	0.02977	0.02125	-0.00734	-0.00592	0.38593
10			2PX	0.00078	0.00097	-0.00295	-0.00251	0.04894
11			2PY	0.00247	-0.00353	0.00179	0.00188	0.02158
12			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
13	5	H	1S	-0.00491	-0.00482	0.00033	0.00016	0.08673
14	6	C	1S	-0.69980	0.70252	0.02421	-0.02533	-0.14889
15			2S	-0.02971	0.02133	0.00672	-0.00663	0.38592
16			2PX	0.00077	-0.00097	-0.00269	0.00279	-0.04893
17			2PY	0.00248	0.00353	0.00160	-0.00204	-0.02158
18			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	7	H	1S	0.00490	-0.00484	-0.00031	0.00019	0.08673
20	8	C	1S	-0.02577	0.02450	-0.66534	0.73524	-0.10624
21			2S	0.00492	-0.00476	-0.02473	0.02713	0.27271
22			2PX	0.00263	-0.00272	-0.00107	0.00111	0.06846
23			2PY	-0.00190	0.00176	0.00076	-0.00072	-0.05384
24			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	9	H	1S	0.00005	-0.00016	0.00459	-0.00507	0.06142
26	10	H	1S	0.00006	-0.00010	0.00460	-0.00508	0.05634

				6	7	8	9	10
				(A')--O	(A')--O	(A')--O	(A')--O	(A')--O
	EIGENVALUES --			-0.95242	-0.76872	-0.70916	-0.59655	-0.59150
1	1	C	1S	0.14537	-0.11941	0.05523	0.01912	-0.00684
2			2S	-0.38509	0.35315	-0.17310	-0.08173	0.03135
3			2PX	0.06640	0.08379	-0.18172	-0.15595	0.25209
4			2PY	-0.03842	-0.09266	-0.00030	0.32334	0.20213
5			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	2	H	1S	-0.09835	0.15437	-0.18144	-0.04100	0.25469
7	3	H	1S	-0.10311	0.18576	-0.06637	-0.28306	-0.15279
8	4	C	1S	0.09926	0.08558	-0.09463	-0.04101	0.00713
9			2S	-0.26027	-0.25907	0.29054	0.11768	-0.01920
10			2PX	-0.09833	0.10458	-0.17941	0.26328	0.08188
11			2PY	0.11828	-0.16211	-0.12012	-0.03500	0.27572
12			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
13	5	H	1S	-0.06190	-0.10704	0.25827	-0.11545	-0.15261
14	6	C	1S	-0.09926	0.08558	0.09463	0.04101	0.00713
15			2S	0.26027	-0.25907	-0.29054	-0.11769	-0.01919
16			2PX	-0.09833	-0.10457	-0.17941	0.26326	-0.08192
17			2PY	0.11828	0.16211	-0.12011	-0.03504	-0.27572
18			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	7	H	1S	0.06190	-0.10704	-0.25826	0.11543	-0.15263
20	8	C	1S	-0.14537	-0.11940	-0.05523	-0.01912	-0.00684
21			2S	0.38510	0.35315	0.17311	0.08174	0.03135
22			2PX	0.06640	-0.08379	-0.18172	-0.15598	-0.25208
23			2PY	-0.03842	0.09266	-0.00029	0.32332	-0.20216

24			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	9	H	1S	0.09835	0.15437	0.18144	0.04103	0.25469
26	10	H	1S	0.10311	0.18576	0.06638	0.28304	-0.15283
				11	12	13	14	15
				(A')--O	(A')--O	(A')--O	(A")--O	(A")--O
	EIGENVALUES --			-0.50452	-0.49791	-0.43245	-0.39901	-0.27608
1	1	C	1S	-0.02659	-0.00623	0.00053	0.00000	0.00000
2			2S	0.06941	0.01192	0.00587	0.00000	0.00000
3			2PX	-0.26723	-0.29497	-0.10138	0.00000	0.00000
4			2PY	0.24770	-0.20877	-0.21573	0.00000	0.00000
5			2PZ	0.00000	0.00000	0.00000	0.37128	-0.52094
6	2	H	1S	-0.10353	-0.32272	-0.21728	0.00000	0.00000
7	3	H	1S	-0.18259	0.21919	0.24506	0.00000	0.00000
8	4	C	1S	-0.00175	0.02104	-0.02081	0.00000	0.00000
9			2S	-0.01669	-0.08555	0.08407	0.00000	0.00000
10			2PX	0.33774	0.20632	0.15019	0.00000	0.00000
11			2PY	-0.17460	-0.01737	0.37183	0.00000	0.00000
12			2PZ	0.00000	0.00000	0.00000	0.47504	-0.40382
13	5	H	1S	-0.22180	-0.20217	-0.29267	0.00000	0.00000
14	6	C	1S	-0.00176	-0.02104	-0.02081	0.00000	0.00000
15			2S	-0.01665	0.08556	0.08407	0.00000	0.00000
16			2PX	-0.33764	0.20648	-0.15020	0.00000	0.00000
17			2PY	0.17460	-0.01747	-0.37183	0.00000	0.00000
18			2PZ	0.00000	0.00000	0.00000	0.47504	0.40382
19	7	H	1S	-0.22171	0.20227	-0.29267	0.00000	0.00000
20	8	C	1S	-0.02658	0.00624	0.00053	0.00000	0.00000
21			2S	0.06940	-0.01195	0.00587	0.00000	0.00000
22			2PX	0.26708	-0.29510	0.10139	0.00000	0.00000
23			2PY	-0.24781	-0.20863	0.21573	0.00000	0.00000
24			2PZ	0.00000	0.00000	0.00000	0.37127	0.52095
25	9	H	1S	-0.10338	0.32276	-0.21728	0.00000	0.00000
26	10	H	1S	-0.18270	-0.21909	0.24507	0.00000	0.00000
				16	17	18	19	20
				(A")--V	(A")--V	(A')--V	(A')--V	(A')--V
	EIGENVALUES --			0.25592	0.42039	0.57843	0.66975	0.68198
1	1	C	1S	0.00000	0.00000	0.01823	-0.00691	-0.05577
2			2S	0.00000	0.00000	-0.11501	0.03507	0.32596
3			2PX	0.00000	0.00000	0.33527	0.10967	-0.04019
4			2PY	0.00000	0.00000	0.32616	0.52654	-0.07831
5			2PZ	0.62835	-0.51232	0.00000	0.00000	0.00000
6	2	H	1S	0.00000	0.00000	-0.40906	-0.37142	-0.08392
7	3	H	1S	0.00000	0.00000	0.44682	0.49198	-0.27139
8	4	C	1S	0.00000	0.00000	-0.02693	0.08057	0.16843
9			2S	0.00000	0.00000	0.15943	-0.53289	-1.03417
10			2PX	0.00000	0.00000	0.33981	0.31398	0.32538
11			2PY	0.00000	0.00000	0.49172	0.22294	-0.32985
12			2PZ	-0.47518	0.69865	0.00000	0.00000	0.00000
13	5	H	1S	0.00000	0.00000	0.47293	0.62567	0.67935
14	6	C	1S	0.00000	0.00000	0.02693	0.08056	-0.16844
15			2S	0.00000	0.00000	-0.15943	-0.53283	1.03419
16			2PX	0.00000	0.00000	0.33982	-0.31395	0.32538
17			2PY	0.00000	0.00000	0.49171	-0.22297	-0.32984
18			2PZ	-0.47518	-0.69865	0.00000	0.00000	0.00000
19	7	H	1S	0.00000	0.00000	-0.47294	0.62563	-0.67937
20	8	C	1S	0.00000	0.00000	-0.01823	-0.00692	0.05576
21			2S	0.00000	0.00000	0.11503	0.03515	-0.32592
22			2PX	0.00000	0.00000	0.33528	-0.10972	-0.04022
23			2PY	0.00000	0.00000	0.32614	-0.52652	-0.07828

24			2PZ	0.62835	0.51232	0.00000	0.00000	0.00000
25	9	H	1S	0.00000	0.00000	0.40905	-0.37148	0.08390
26	10	H	1S	0.00000	0.00000	-0.44682	0.49193	0.27134

				21	22	23	24	25
				(A')--V	(A')--V	(A')--V	(A')--V	(A')--V
	EIGENVALUES --			0.69633	0.70843	0.88560	0.93629	1.01911
1	1	C	1S	0.14166	-0.14067	0.03428	-0.05838	-0.04782
2			2S	-0.92485	0.91041	-0.23812	0.44130	0.38419
3			2PX	-0.30516	0.37556	0.56703	-0.27083	-0.72447
4			2PY	0.13529	-0.16971	0.41417	0.78713	-0.09603
5			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	2	H	1S	0.65848	-0.69713	-0.41759	-0.22487	0.37746
7	3	H	1S	0.55485	-0.58147	0.44977	0.41884	-0.22172
8	4	C	1S	0.01624	0.02240	-0.08320	0.09707	0.02586
9			2S	-0.11918	-0.11646	0.59521	-0.71365	-0.24614
10			2PX	0.22728	-0.08375	-0.26027	-0.60544	-0.14923
11			2PY	-0.20824	0.07595	-0.42533	-0.10789	0.89430
12			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
13	5	H	1S	0.17841	0.07832	-0.54220	-0.17275	0.26975
14	6	C	1S	-0.01625	0.02241	-0.08320	-0.09707	-0.02586
15			2S	0.11924	-0.11652	0.59519	0.71368	0.24613
16			2PX	0.22731	0.08373	0.26029	-0.60545	-0.14918
17			2PY	-0.20822	-0.07592	0.42531	-0.10785	0.89431
18			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	7	H	1S	-0.17848	0.07836	-0.54219	0.17274	-0.26978
20	8	C	1S	-0.14167	-0.14067	0.03428	0.05839	0.04782
21			2S	0.92487	0.91040	-0.23811	-0.44131	-0.38419
22			2PX	-0.30516	-0.37555	-0.56702	-0.27084	-0.72446
23			2PY	0.13536	0.16971	-0.41418	0.78715	-0.09603
24			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	9	H	1S	-0.65846	-0.69713	-0.41758	0.22485	-0.37746
26	10	H	1S	-0.55491	-0.58147	0.44979	-0.41884	0.22174

				26
				(A')--V
	EIGENVALUES --			1.10674
1	1	C	1S	0.07976
2			2S	-0.65898
3			2PX	0.57276
4			2PY	-0.50985
5			2PZ	0.00000
6	2	H	1S	0.00789
7	3	H	1S	-0.11043
8	4	C	1S	-0.06514
9			2S	0.53652
10			2PX	0.90141
11			2PY	-0.29340
12			2PZ	0.00000
13	5	H	1S	0.28300
14	6	C	1S	-0.06514
15			2S	0.53648
16			2PX	-0.90138
17			2PY	0.29347
18			2PZ	0.00000
19	7	H	1S	0.28298
20	8	C	1S	0.07976
21			2S	-0.65897
22			2PX	-0.57275
23			2PY	0.50984

24			2PZ	0.00000
25	9	H	1S	0.00788
26	10	H	1S	-0.11042