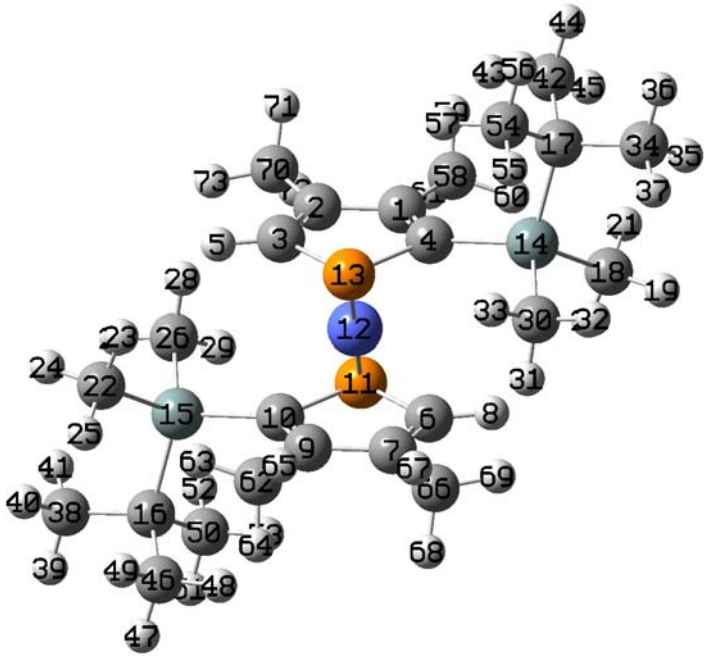
Molecule	2,2'-bisTBS-3,3',4,4'-tetraMe-1,1'-diphosphacobaltocene meso-2.
Software.	Gaussian G03W
Functionnal	B3LYP
Bases	H/C/Si/P 6-311+g** Co LANL2DZ
Calculation	opt (scf=tight) Pop=full, nbo Freq



Optimisation

Item	Value	Threshold	Converged?
Maximum Force	0.000021	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.001796	0.001800	YES
RMS Displacement	0.000334	0.001200	YES

Predicted change in Energy=-5.275710D-08
Optimization completed.
-- Stationary point found.

Géométrie

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.975574	1.794981	-0.741816
2	6	0	-0.980625	1.817916	0.714295
3	6	0	0.310173	1.822137	1.244077
4	6	0	0.321345	1.859537	-1.310294
5	1	0	0.513564	1.790868	2.306222
6	6	0	-0.310173	-1.822137	-1.244077
7	6	0	0.980625	-1.817916	-0.714295
8	1	0	-0.513564	-1.790868	-2.306222
9	6	0	0.975574	-1.794981	0.741816
10	6	0	-0.321345	-1.859537	1.310294
11	15	0	-1.573482	-1.790695	0.015554
12	27	0	0.000000	0.000000	0.000000
13	15	0	1.573482	1.790695	-0.015554
14	14	0	0.838981	2.106377	-3.112648
15	14	0	-0.838981	-2.106377	3.112648
16	6	0	-0.753161	-3.988066	3.561296
17	6	0	0.753161	3.988066	-3.561296
18	6	0	-0.216123	1.119775	-4.342739
19	1	0	0.304551	1.053167	-5.302833
20	1	0	-0.380220	0.099284	-3.986692
21	1	0	-1.193725	1.568584	-4.534318
22	6	0	0.216123	-1.119775	4.342739
23	1	0	0.380220	-0.099284	3.986692
24	1	0	-0.304551	-1.053167	5.302833
25	1	0	1.193725	-1.568584	4.534318
26	6	0	-2.626346	-1.517682	3.311173
27	1	0	-3.000079	-1.754509	4.311957
28	1	0	-2.698081	-0.435202	3.185146
29	1	0	-3.301644	-1.978839	2.586602
30	6	0	2.626346	1.517682	-3.311173
31	1	0	2.698081	0.435202	-3.185146
32	1	0	3.000079	1.754509	-4.311957
33	1	0	3.301644	1.978839	-2.586602
34	6	0	1.082223	4.175461	-5.058212
35	1	0	0.361483	3.665690	-5.704247
36	1	0	1.055578	5.241156	-5.318934
37	1	0	2.080379	3.806453	-5.311717
38	6	0	-1.082223	-4.175461	5.058212
39	1	0	-1.055578	-5.241156	5.318934
40	1	0	-0.361483	-3.665690	5.704247
41	1	0	-2.080379	-3.806453	5.311717
42	6	0	-0.654835	4.555304	-3.292450
43	1	0	-0.918444	4.496158	-2.233263
44	1	0	-0.697332	5.612923	-3.582823
45	1	0	-1.427529	4.032272	-3.864351
46	6	0	0.654835	-4.555304	3.292450
47	1	0	0.697332	-5.612923	3.582823
48	1	0	0.918444	-4.496158	2.233263
49	1	0	1.427529	-4.032272	3.864351
50	6	0	-1.773623	-4.784541	2.722621

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51	1	0	-1.715864	-5.852015	2.971044
52	1	0	-2.801504	-4.462306	2.911925
53	1	0	-1.584950	-4.686870	1.649769
54	6	0	1.773623	4.784541	-2.722621
55	1	0	2.801504	4.462306	-2.911925
56	1	0	1.715864	5.852015	-2.971044
57	1	0	1.584950	4.686870	-1.649769
58	6	0	-2.273851	1.815719	-1.510049
59	1	0	-2.666985	2.836364	-1.574533
60	1	0	-2.150778	1.441275	-2.524218
61	1	0	-3.031721	1.202140	-1.021049
62	6	0	2.273851	-1.815719	1.510049
63	1	0	2.150778	-1.441275	2.524218
64	1	0	2.666985	-2.836364	1.574533
65	1	0	3.031721	-1.202140	1.021049
66	6	0	2.235115	-1.920206	-1.539175
67	1	0	2.978090	-1.170609	-1.261717
68	1	0	2.696544	-2.905560	-1.408570
69	1	0	2.010006	-1.800430	-2.599845
70	6	0	-2.235115	1.920206	1.539175
71	1	0	-2.696544	2.905560	1.408570
72	1	0	-2.978090	1.170609	1.261717
73	1	0	-2.010006	1.800430	2.599845

Fréquences

	1	2	3
	AG	AU	AU
Frequencies --	-35.6536	-9.2172	22.9441
Red. masses --	1.5586	3.9337	2.1931
Frc consts --	0.0012	0.0002	0.0007
IR Inten --	0.0000	0.2675	0.0170

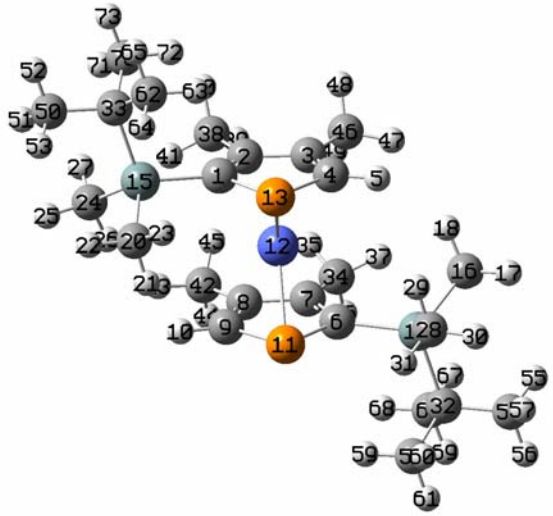
	4	5	6
	AG	AU	AU
Frequencies --	32.5452	32.5655	38.1700
Red. masses --	2.6293	2.2849	3.2392
Frc consts --	0.0016	0.0014	0.0028
IR Inten --	0.0000	0.0091	0.0569

NB: les fréquences imaginaires sont des rotations 1) des méthyles en béta et 2) des cycles phospholyles

Energie libre

Zero-point correction=	0.617723 (Hartree/Particle)
Thermal correction to Energy=	0.657906
Thermal correction to Enthalpy=	0.658851
Thermal correction to Gibbs Free Energy=	0.548169
Sum of electronic and zero-point Energies=	-2347.668017
Sum of electronic and thermal Energies=	-2347.627834
Sum of electronic and thermal Enthalpies=	-2347.626890
Sum of electronic and thermal Free Energies=	-2347.737571

Molecule	2,2'-bisTBS-3,3',4,4'-tetraMe-1,1'-diphosphacobaltocene rac-2.
Software.	Gaussian G03W
Functionnal	B3LYP
Bases	H/C/Si/P 6-311+g** Co LANL2DZ
Calculation	opt (scf=tight) Pop=full, nbo Freq



Optimisation

Item	Value	Threshold	Converged?
Maximum Force	0.000348	0.000450	YES
RMS Force	0.000092	0.000300	YES
Maximum Displacement	0.001092	0.001800	YES
RMS Displacement	0.000251	0.001200	YES

Predicted change in Energy=-3.467842D-04
Optimization completed.
-- Stationary point found.

Géométrie

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.277467	-0.052841
2	6	0	-0.475752	1.856831	1.213767
3	6	0	-1.670037	1.021414	1.145537
4	6	0	-2.078077	0.792038	-0.172814
5	1	0	-2.923097	0.159720	-0.424441
6	6	0	0.000000	-2.277467	-0.052841
7	6	0	0.475752	-1.856831	1.213767
8	6	0	1.670037	-1.021414	1.145537
9	6	0	2.078077	-0.792038	-0.172814
10	1	0	2.923097	-0.159720	-0.424441
11	15	0	0.993800	-1.542413	-1.376441
12	27	0	0.000000	0.000000	0.118098
13	15	0	-0.993800	1.542413	-1.376441
14	14	0	-1.429858	-3.428023	-0.507621
15	14	0	1.429858	3.428023	-0.507621
16	6	0	-2.922023	-3.294522	0.666414
17	1	0	-3.792436	-3.776406	0.204306
18	1	0	-3.188436	-2.247637	0.850581
19	1	0	-2.762481	-3.776526	1.637292
20	6	0	2.043604	2.937623	-2.234408
21	1	0	2.432841	1.912879	-2.224744
22	1	0	2.854765	3.598242	-2.564264
23	1	0	1.252797	2.976757	-2.991119
24	6	0	2.922023	3.294522	0.666414
25	1	0	3.792436	3.776406	0.204306
26	1	0	3.188436	2.247637	0.850581
27	1	0	2.762481	3.776526	1.637292
28	6	0	-2.043604	-2.937623	-2.234408
29	1	0	-2.432841	-1.912879	-2.224744
30	1	0	-2.854765	-3.598242	-2.564264
31	1	0	-1.252797	-2.976757	-2.991119
32	6	0	-0.810021	-5.260984	-0.533241
33	6	0	0.810021	5.260984	-0.533241
34	6	0	-0.086723	-2.294852	2.544830
35	1	0	0.107507	-1.557701	3.330092
36	1	0	0.377307	-3.236407	2.868247
37	1	0	-1.164443	-2.458826	2.497682
38	6	0	0.086723	2.294852	2.544830
39	1	0	-0.107507	1.557701	3.330092
40	1	0	-0.377307	3.236407	2.868247
41	1	0	1.164443	2.458826	2.497682
42	6	0	2.429486	-0.544245	2.357370
43	1	0	3.209922	0.166835	2.071637
44	1	0	2.919087	-1.386119	2.865154
45	1	0	1.784474	-0.053530	3.093252
46	6	0	-2.429486	0.544245	2.357370
47	1	0	-3.209922	-0.166835	2.071637
48	1	0	-2.919087	1.386119	2.865154
49	1	0	-1.784474	0.053530	3.093252
50	6	0	1.996805	6.206184	-0.824714

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51	1	0	2.774258	6.142692	-0.053695
52	1	0	1.653743	7.251011	-0.855028
53	1	0	2.466806	5.992343	-1.792664
54	6	0	-1.996805	-6.206184	-0.824714
55	1	0	-2.774258	-6.142692	-0.053695
56	1	0	-1.653743	-7.251011	-0.855028
57	1	0	-2.466806	-5.992343	-1.792664
58	6	0	0.259077	-5.452003	-1.629932
59	1	0	1.129242	-4.803967	-1.471140
60	1	0	-0.135814	-5.239580	-2.630644
61	1	0	0.619445	-6.491469	-1.635502
62	6	0	-0.259077	5.452003	-1.629932
63	1	0	-1.129242	4.803967	-1.471140
64	1	0	0.135814	5.239580	-2.630644
65	1	0	-0.619445	6.491469	-1.635502
66	6	0	-0.192927	-5.643515	0.828408
67	1	0	-0.908476	-5.535812	1.653492
68	1	0	0.684896	-5.028743	1.060551
69	1	0	0.135201	-6.693540	0.819699
70	6	0	0.192927	5.643515	0.828408
71	1	0	0.908476	5.535812	1.653492
72	1	0	-0.684896	5.028743	1.060551
73	1	0	-0.135201	6.693540	0.819699

Fréquences

	1	2	3
	A	A	B
Frequencies --	10.9965	18.9619	22.9851
Red. masses --	4.4987	2.7492	2.8636
Frc consts --	0.0003	0.0006	0.0009
IR Inten --	0.0002	0.0043	0.0942

	4	5	6
	B	A	B
Frequencies --	30.3266	35.1023	38.5179
Red. masses --	3.8576	3.2403	4.0725
Frc consts --	0.0021	0.0024	0.0036
IR Inten --	0.0324	0.0025	0.1462

Energie libre

Zero-point correction=	0.617398 (Hartree/Particle)
Thermal correction to Energy=	0.658658
Thermal correction to Enthalpy=	0.659602
Thermal correction to Gibbs Free Energy=	0.546238
Sum of electronic and zero-point Energies=	-2347.668721
Sum of electronic and thermal Energies=	-2347.627461
Sum of electronic and thermal Enthalpies=	-2347.626517
Sum of electronic and thermal Free Energies=	-2347.739881