Electronic Supplementary Information for:

On the relation between carbonyl stretching frequencies and the donor power of chelating diphosphines in nickel dicarbonyl complexes

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Contents

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1 Experimental: asym. $\nu_{\mathrm{CO}}^{\mathrm{exp}}$ vs pK$_a$ and E^0

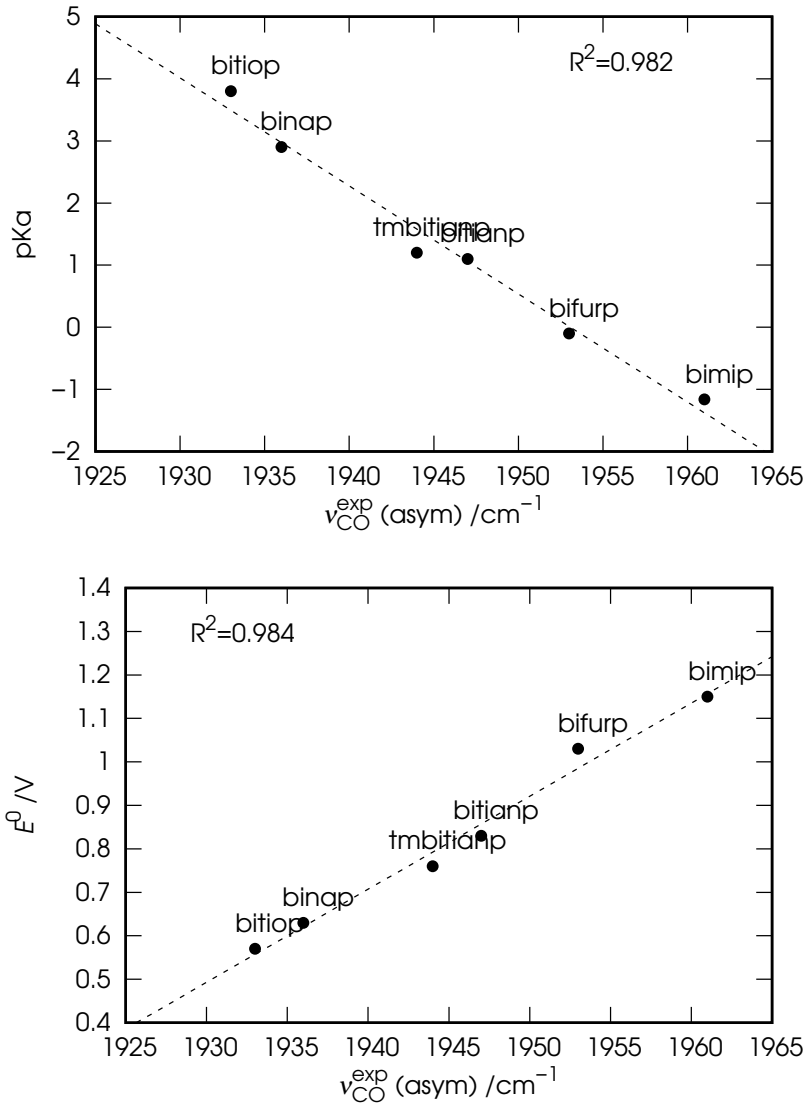


Fig. 1 Correlation between the experimental asymmetric carbonyl stretching frequencies ($\nu_{\mathrm{CO}}^{\mathrm{exp}}$) of the nickel dicarbonyl complexes with the six considered ligands, and the experimental i) basicity (pK$_a$, top panel) and ii) electrochemical oxidative potential (E^0, bottom panel) of the free ligands (see Table 1 in the article).

2 Calculated bite angles β

Table 1 Calculated bite angles β.

ligand	β (degree)
bitiop	95.4
binap	96.8
tmbitianp	97.9
bitianp	97.2
bifurp1	97.8
bifurp2	99.5
bimip	100.3

3 Correlation between CT_{don} and ν_{CO}^{calc}

Table 2 Donation charge transfers (see Section 3.2 in the article) and calculated carbonyl stretching frequencies.

ligand	CT_{don}	Anharm. + PCM ν_{CO}^{calc} (cm^{-1})		Harm. + PCM ν_{CO}^{calc} (cm^{-1})		Harm. Gas Phase ν_{CO}^{calc} (cm^{-1})	
		sym.	asym.	sym.	asym.	sym.	asym.
bitiop	0.185	2022	1961	2051	1989	2073	2027
binap	0.177	2025	1965	2052	1991	2076	2030
tmbitianp	0.172	2028	1970	2056	1997	2079	2035
bitianp	0.165	2031	1973	2059	2000	2082	2037
bifurp1	0.150	2035	1978	2062	2005	2084	2041
bifurp2	0.139	2039	1980	2066	2006	2087	2043
bimip	0.128	2043	1986	2070	2014	2092	2050

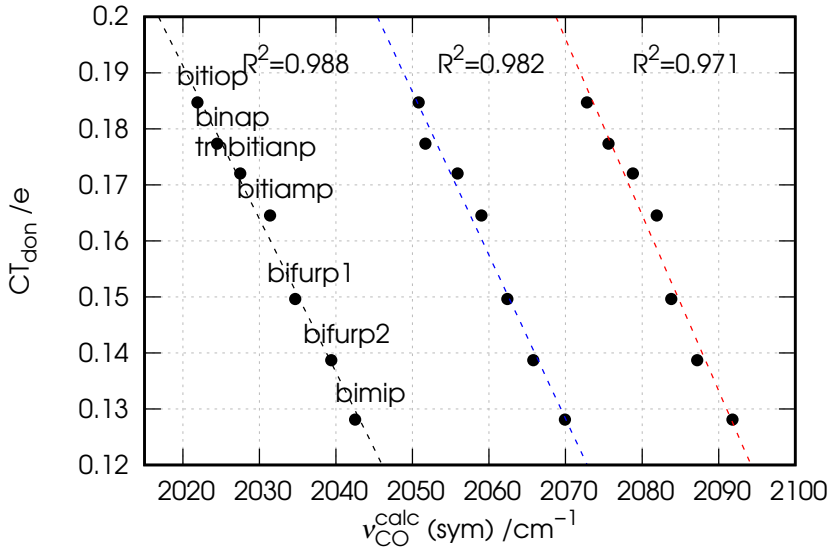
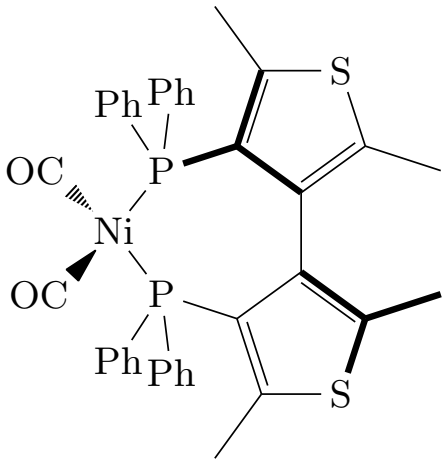


Fig. 2 Correlation between the charge transfer (CT_{don}) associated with the ligand-to-metal donation from the phosphori lone pairs evaluated at $z = 0.7$ bohr and i) the calculated carbonyl stretching frequencies (ν_{CO}^{calc}) in gas phase (red line), ii) including bulk solvent effects (PCM) (blue line), iii) including both PCM and the anharmonic correction (black line).

4 $^{1}H,^{13}C\{^{1}H\},^{31}P\{^{1}H\}$ NMR spectra of complexes

4.1 bitiop



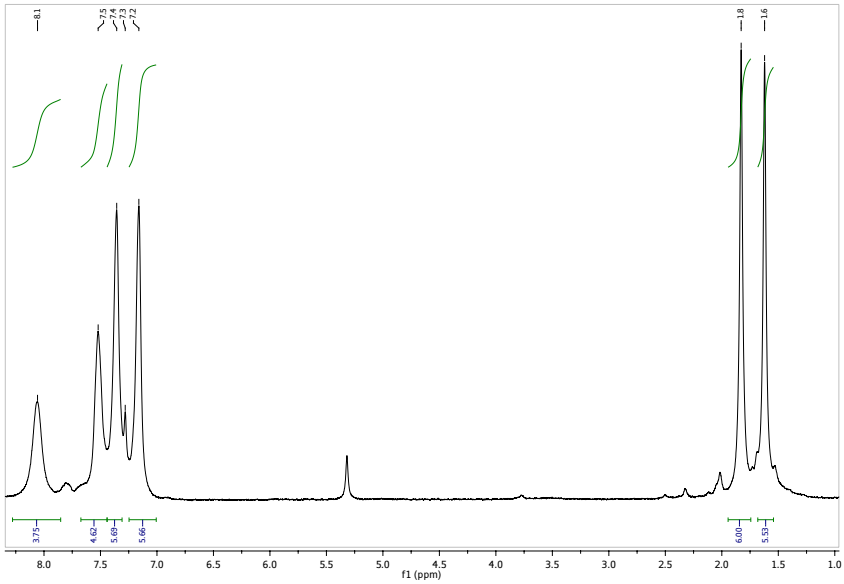


Fig. 3 ^{1}H spectrum of bitiop

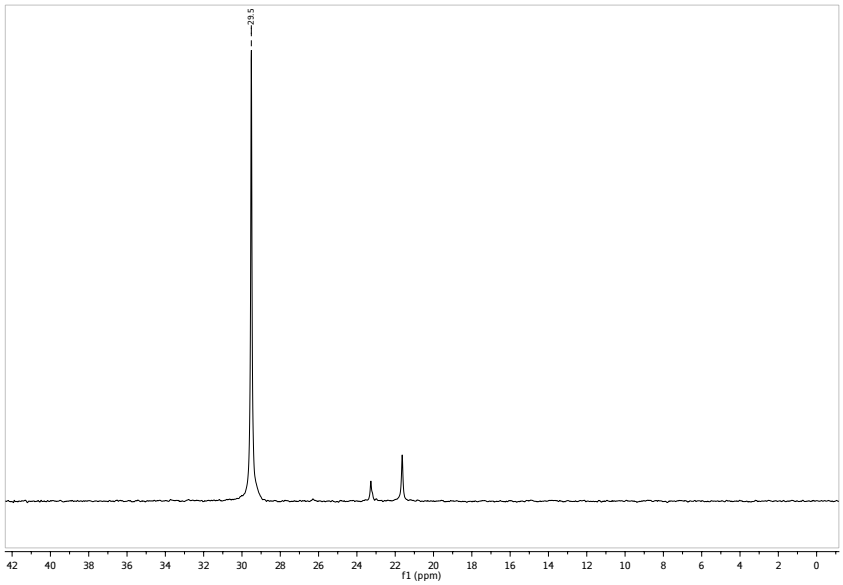


Fig. 4 $^{31}P\{^{1}H\}$ spectrum of bitiop

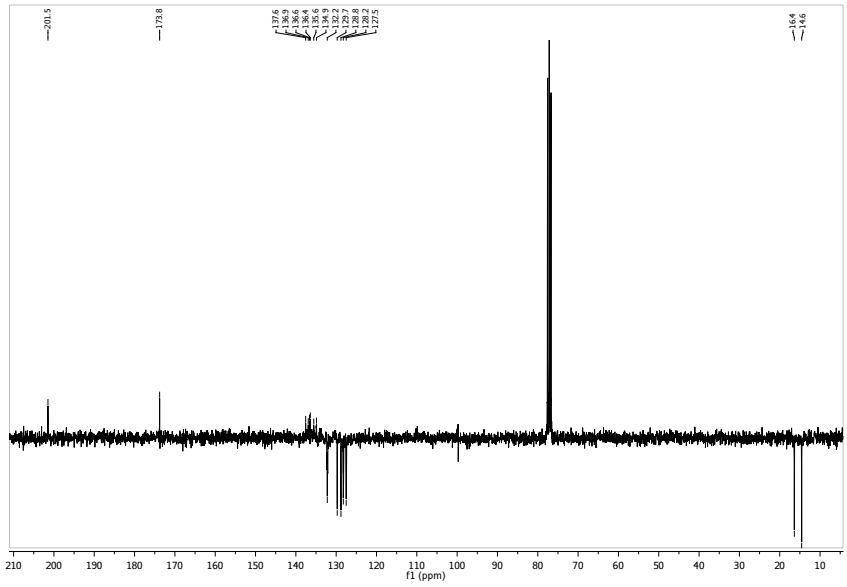
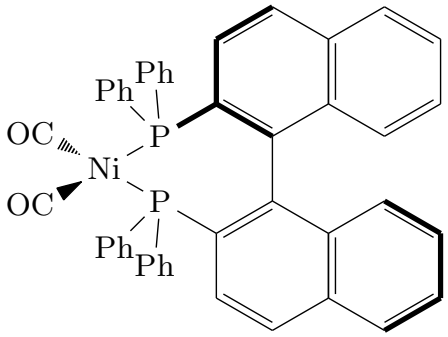


Fig. 5 $^{13}C\{^{1}H\}$ spectrum of bitiop

4.2 binap



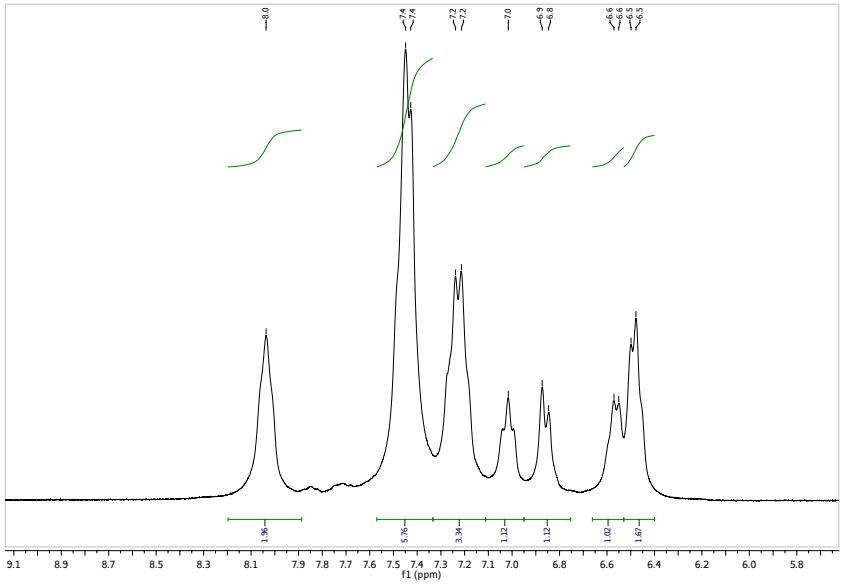


Fig. 6 ^{1}H spectrum of binap

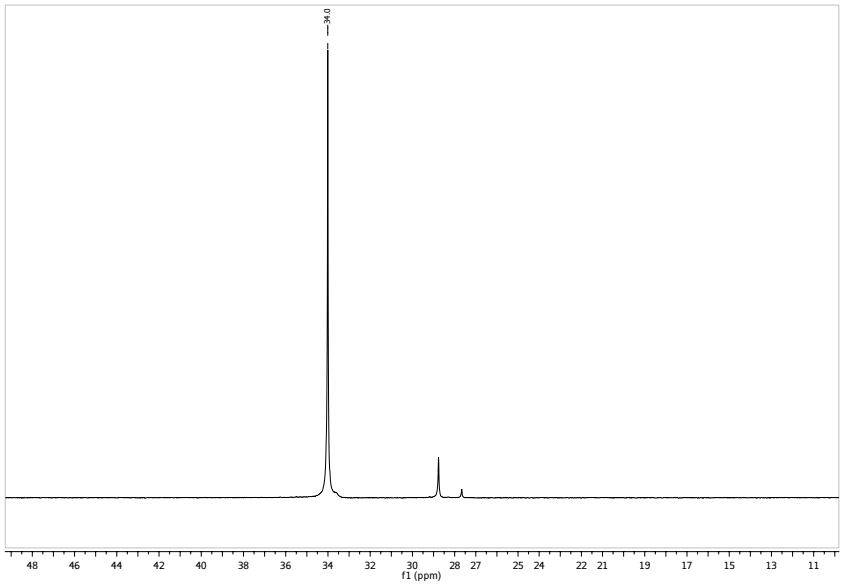


Fig. 7 $^{31}P\{^{1}H\}$ spectrum of binap

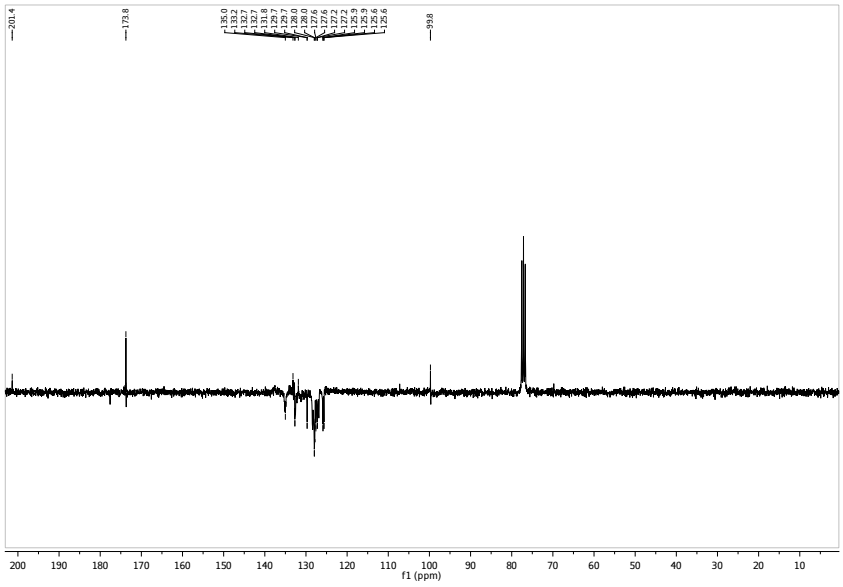
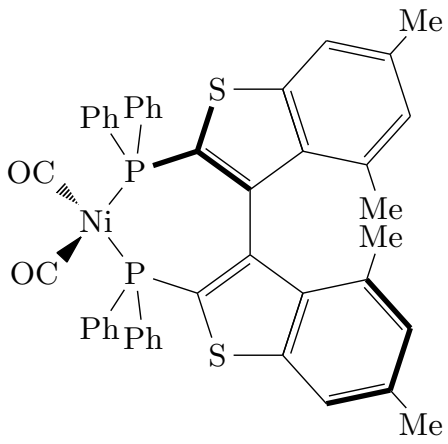


Fig. 8 $^{13}C\{^{1}H\}$ spectrum of binap

4.3 tmbitianp



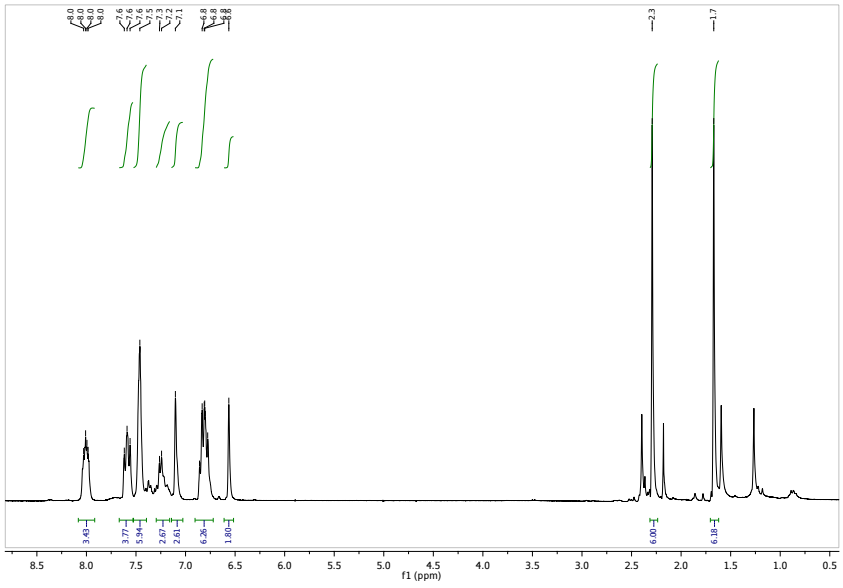


Fig. 9 ^{1}H spectrum of tmbitianp

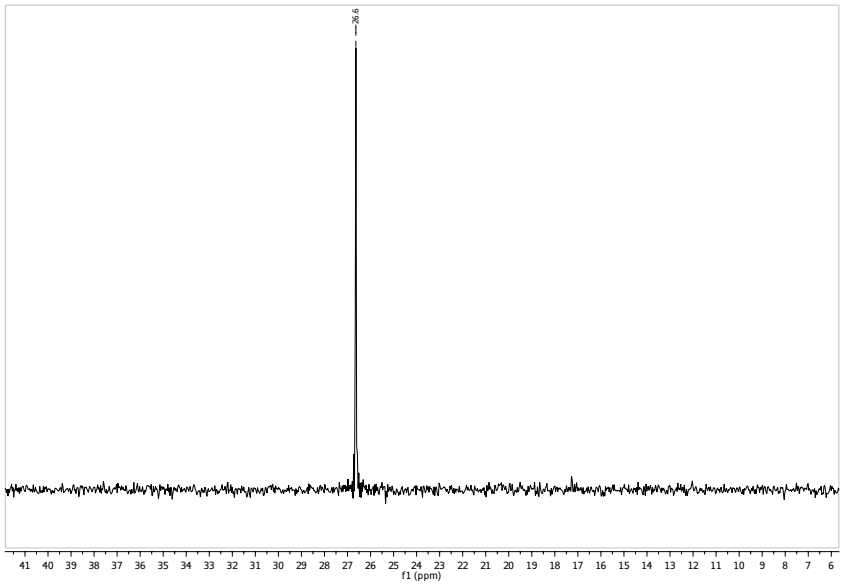


Fig. 10 $^{31}P\{^{1}H\}$ spectrum of tmbitianp

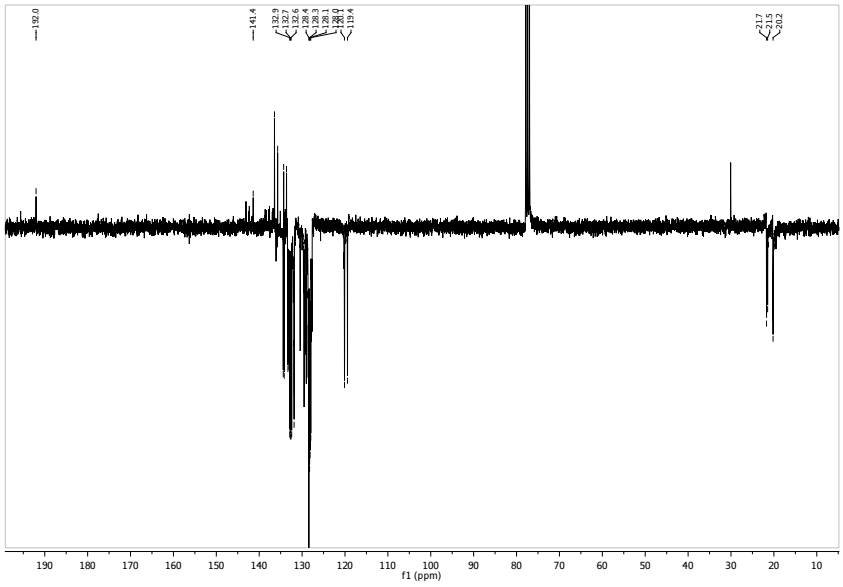
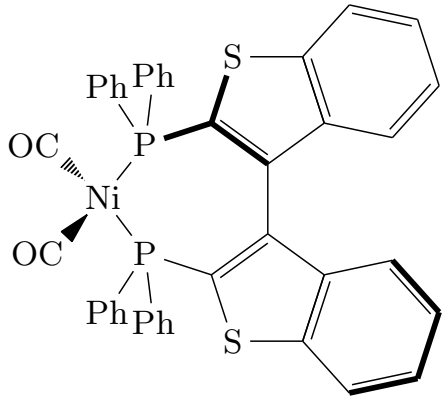


Fig. 11 $^{13}C\{^{1}H\}$ spectrum of tmbitianp

4.4 bitianp



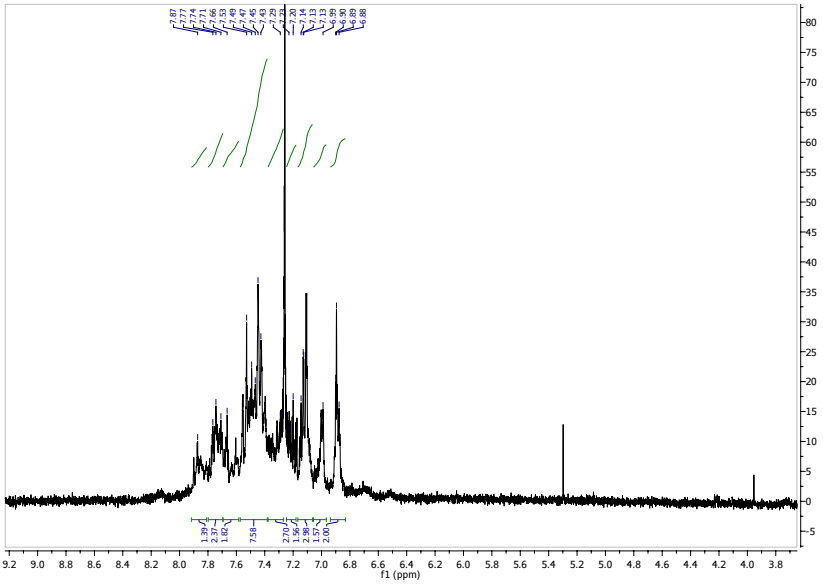


Fig. 12 ^{1}H spectrum of bitianp

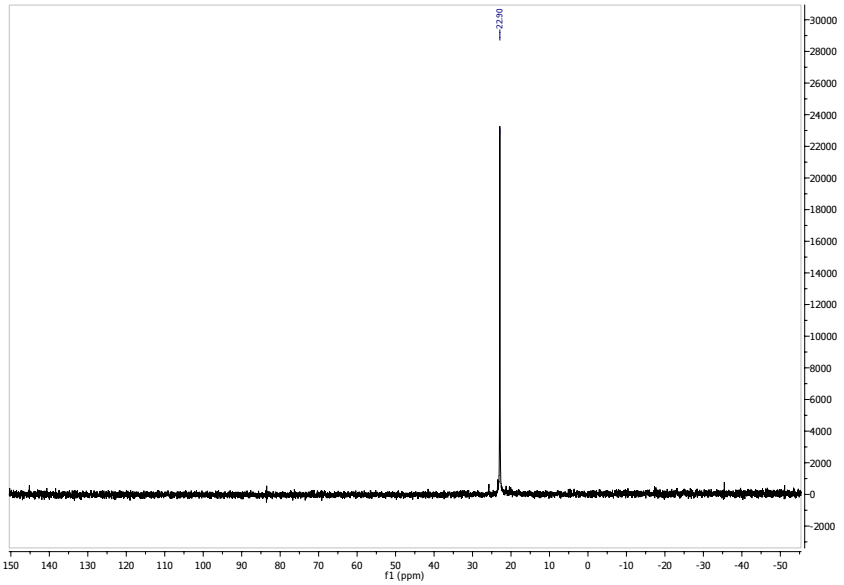


Fig. 13 $^{31}P\{^{1}H\}$ spectrum of bitianp

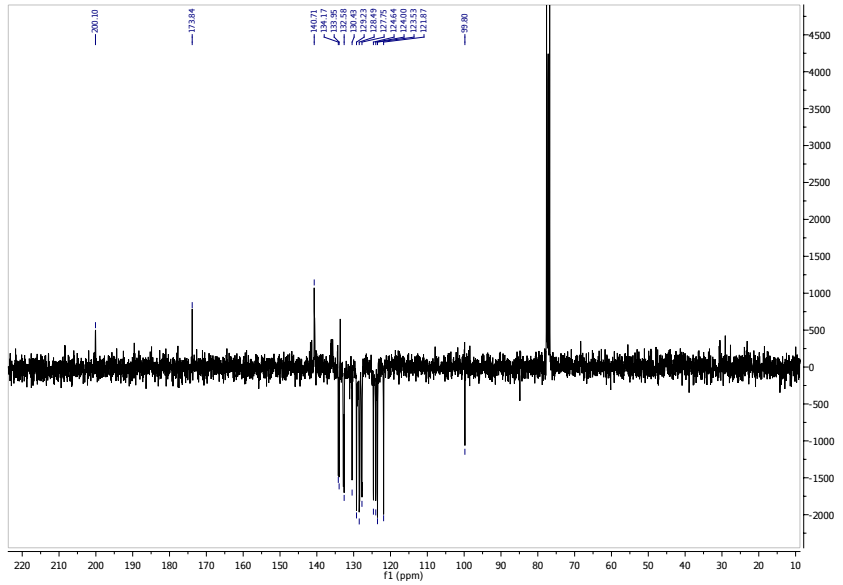
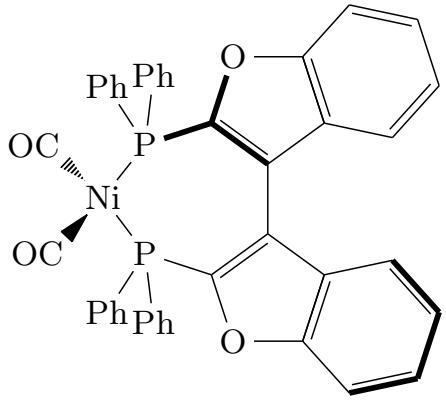


Fig. 14 $^{13}C\{^{1}H\}$ spectrum of bitianp

4.5 bifurp



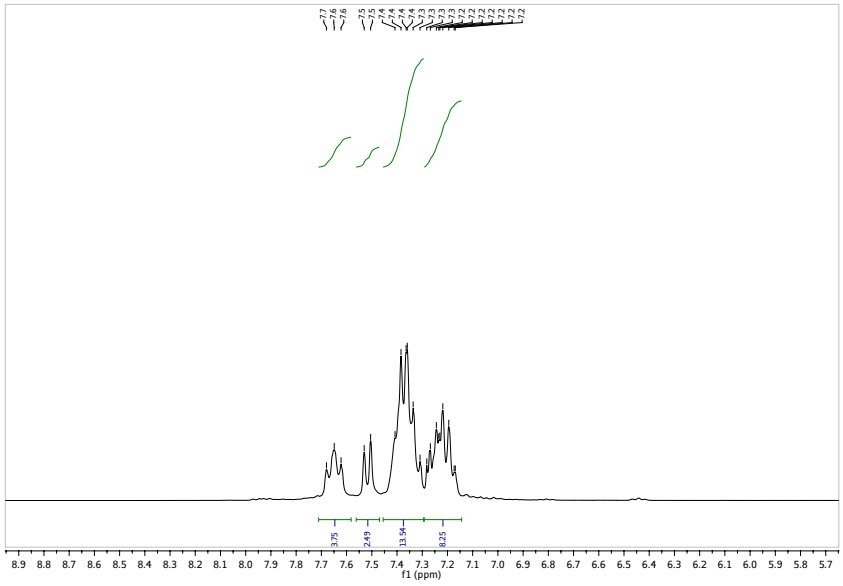


Fig. 15 ^{1}H spectrum of bifurp

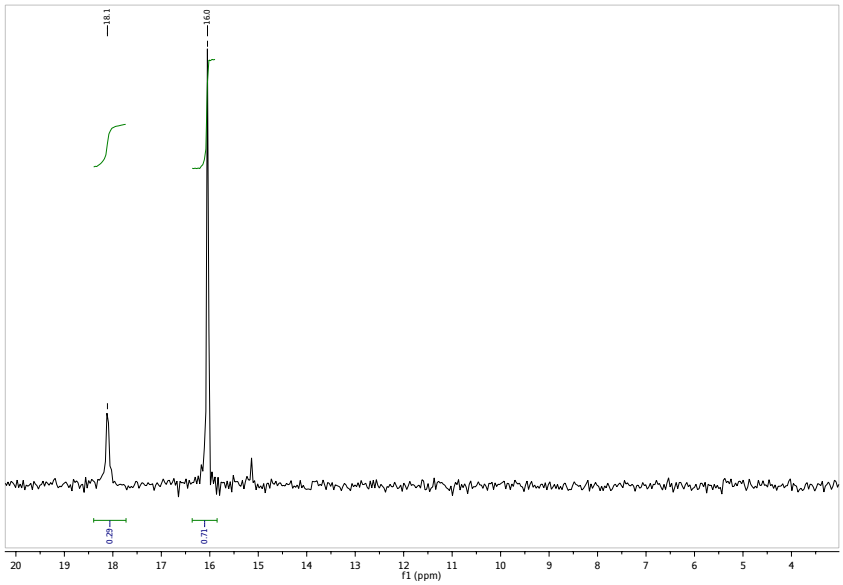


Fig. 16 $^{31}P\{^{1}H\}$ spectrum of bifurp

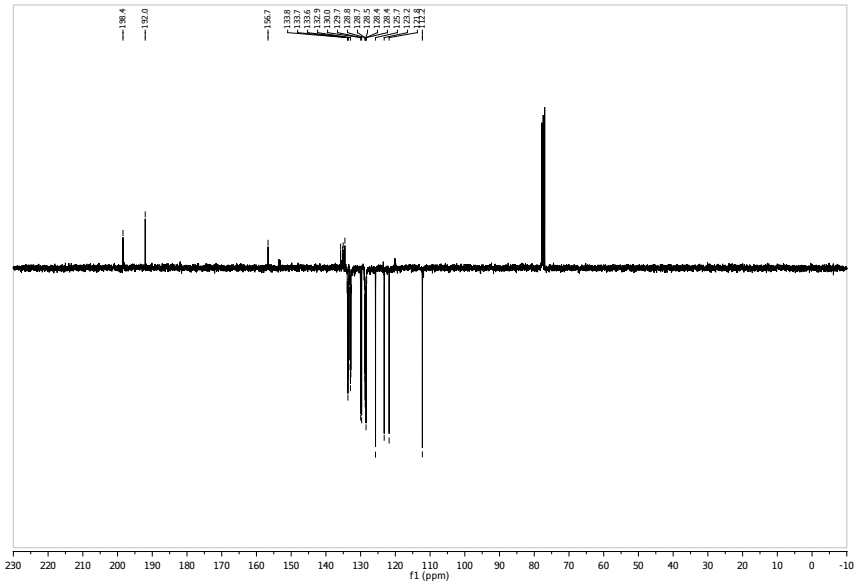
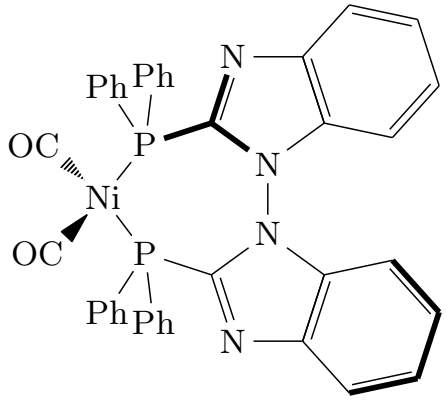


Fig. 17 $^{13}C\{^{1}H\}$ spectrum of bifurp

4.6 bimip



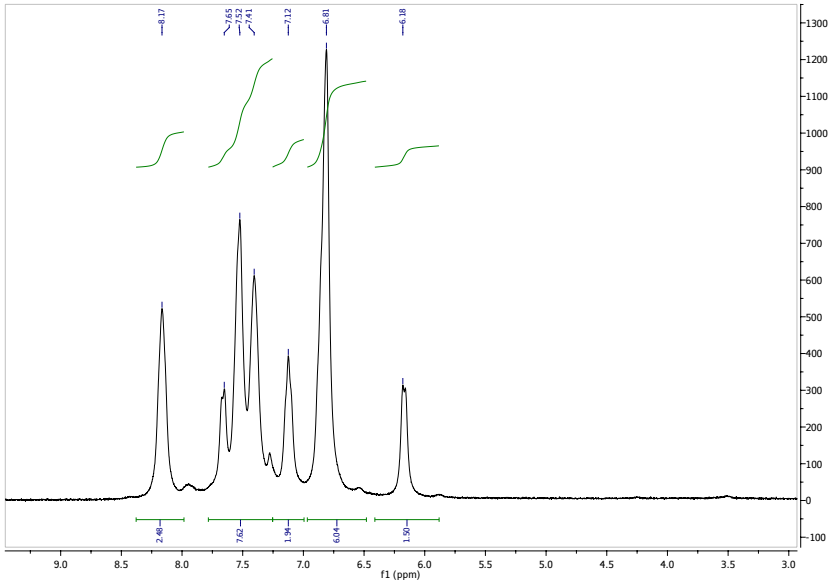


Fig. 18 ^{1}H spectrum of bimip

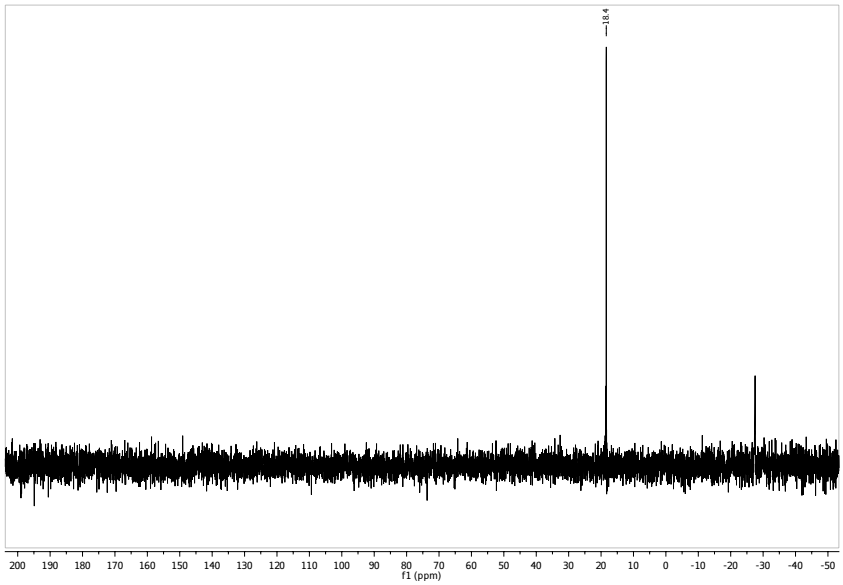


Fig. 19 $^{31}P\{^{1}H\}$ spectrum of bimip

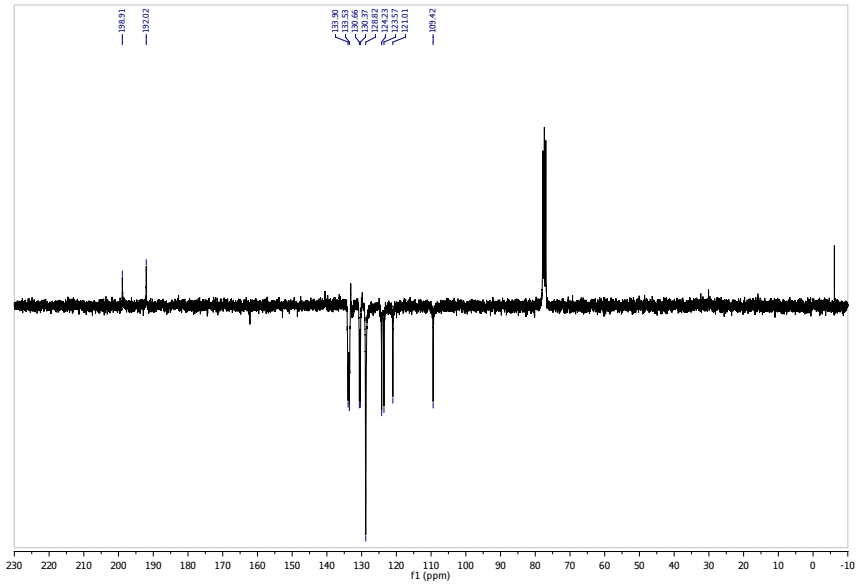


Fig. 20 $^{13}C\{^{1}H\}$ spectrum of bimip

5 Optimized structures of the complexes

5.1 bitiop

Table 3 XYZ coordinates of the optimized structure of the bitiop complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	16	4.465558	-0.913286	-3.116779
2	16	4.466001	0.916590	3.118087
3	15	1.485069	-1.631708	0.000000
4	15	1.485524	1.631708	0.000000
5	6	2.994443	-1.558358	-2.424277
6	6	2.896254	-1.222870	-1.094581
7	6	3.973775	-0.343050	-0.654769
8	6	4.916279	-0.124241	-1.629307
9	6	2.031564	-2.279327	-3.322255
10	1	2.209121	-3.359757	-3.350029
11	1	2.107250	-1.898239	-4.345393
12	1	1.004622	-2.125408	-2.982022
13	6	6.148704	0.721424	-1.557861
14	1	6.106819	1.353579	-0.667103
15	1	6.237778	1.370719	-2.434208
16	1	7.057992	0.110939	-1.495331
17	6	2.995688	1.562404	2.424425
18	6	2.896745	1.224222	1.095463
19	6	3.973480	0.342425	0.657228
20	6	4.915427	0.123810	1.632268
21	6	2.034490	2.286880	3.321406
22	1	1.006827	2.131508	2.984033
23	1	2.212020	3.367414	3.344319
24	1	2.112378	1.910031	4.345945
25	6	6.146576	-0.723815	1.562052
26	1	6.102924	-1.358073	0.672866
27	1	6.235265	-1.371172	2.439844
28	1	7.056763	-0.114903	1.497336
29	6	0.897643	-3.289901	-0.542864
30	6	-0.482773	-3.520100	-0.556815
31	1	-1.157001	-2.708826	-0.299162
32	6	-0.990351	-4.773452	-0.905727
33	1	-2.064137	-4.936790	-0.913933
34	6	-0.119971	-5.808280	-1.246249
35	1	-0.512260	-6.782660	-1.522986
36	6	1.260571	-5.587451	-1.233629
37	1	1.943005	-6.388996	-1.501915
38	6	1.766109	-4.338454	-0.880485
39	1	2.838181	-4.174598	-0.890652
40	6	2.320293	-2.081627	1.582757
41	6	3.487057	-2.859263	1.602866
42	1	3.971373	-3.129678	0.670788
43	6	4.051919	-3.259853	2.810561
44	1	4.956977	-3.860875	2.809159
45	6	3.460720	-2.882736	4.019700
46	1	3.902187	-3.193208	4.962384
47	6	2.308126	-2.099236	4.009411
48	1	1.847957	-1.791453	4.944012
49	6	1.741775	-1.699526	2.796863
50	1	0.848586	-1.086271	2.797583
51	6	2.321146	2.081846	-1.582353
52	6	3.490643	2.855373	-1.601733
53	1	3.977208	3.121016	-0.669434
54	6	4.055416	3.257582	-2.808928
55	1	4.962516	3.855513	-2.806840
56	6	3.461549	2.885927	-4.018427
57	1	3.902904	3.197628	-4.960757
58	6	2.306447	2.106104	-4.008968
59	1	1.844182	1.802458	-4.943890
60	6	1.740088	1.704919	-2.796891
61	1	0.844717	1.094837	-2.798480
62	6	0.896392	3.289835	0.541709
63	6	1.764047	4.341050	0.873107
64	1	2.836560	4.179962	0.877898
65	6	1.257348	5.589506	1.226481
66	1	1.939230	6.393139	1.489880
67	6	-0.123636	5.807159	1.245514
68	1	-0.516834	6.781121	1.522434
69	6	-0.993229	4.769766	0.910923
70	1	-2.067340	4.930642	0.923919
71	6	-0.484427	3.516995	0.561686
72	1	-1.157981	2.703834	0.308409
73	28	0.000000	0.000000	0.000000
74	6	-0.956469	-0.080558	-1.474774
75	6	-0.957147	0.080519	1.474341
76	8	-1.613754	-0.146274	-2.431372
77	8	-1.614854	0.145995	2.430669

5.2 binap

Table 4 XYZ coordinates of the optimized structure of the binap complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	15	1.496202	-1.655560	0.000000
2	15	1.446350	1.655560	0.000000
3	6	3.907711	-0.245140	-0.518802
4	6	4.978118	0.196970	-1.362071
5	6	5.116004	-0.348160	-2.677039
6	6	4.198645	-1.337910	-3.102946
7	1	4.308618	-1.765652	-4.096137
8	6	3.183217	-1.758211	-2.279622
9	1	2.499807	-2.520910	-2.631399
10	6	3.011945	-1.214319	-0.979397
11	6	5.906472	1.191509	-0.947773
12	1	5.805611	1.625122	0.039952
13	6	6.914820	1.613655	-1.783199
14	1	7.611188	2.375945	-1.445772
15	6	7.046127	1.071802	-3.083685
16	1	7.843768	1.417194	-3.734969
17	6	6.161644	0.112561	-3.519078
18	1	6.248165	-0.309300	-4.517032
19	6	3.791523	0.330252	0.860300
20	6	4.733151	-0.084309	1.861958
21	6	4.568577	0.362750	3.211064
22	6	3.476976	1.211026	3.524296
23	1	3.335566	1.527671	4.554314
24	6	2.612851	1.632584	2.547127
25	1	1.784615	2.281271	2.808323
26	6	2.776651	1.224454	1.193689
27	6	5.486894	-0.060463	4.205890
28	1	5.340893	0.284622	5.226179
29	6	6.541388	-0.885675	3.888329
30	1	7.241881	-1.200081	4.656498
31	6	6.709980	-1.329033	2.556539
32	1	7.539160	-1.985628	2.308998
33	6	5.825418	-0.947309	1.573194
34	1	5.958283	-1.309334	0.561294
35	6	2.209142	-2.221836	1.592217
36	6	1.602718	-1.866777	2.801895
37	1	0.710510	-1.253275	2.797821
38	6	2.149622	-2.285046	4.015362
39	1	1.676443	-1.989943	4.947438
40	6	3.304776	-3.066023	4.031539
41	1	3.737150	-3.381315	4.976610
42	6	3.909798	-3.435545	2.828405
43	1	4.816976	-4.031722	2.834194
44	6	3.367529	-3.013426	1.617887
45	1	3.858890	-3.276357	0.686049
46	6	0.889036	-3.215255	-0.773494
47	6	1.047066	-4.474482	-0.179243
48	1	1.569473	-4.568812	0.765036
49	6	0.526038	-5.617690	-0.789169
50	1	0.652674	-6.584175	-0.309484
51	6	-0.152040	-5.522609	-2.003719
52	1	-0.554850	-6.413443	-2.476869
53	6	-0.320173	-4.271868	-2.602835
54	1	-0.855104	-4.183211	-3.543967
55	6	0.184320	-3.128883	-1.986669
56	1	0.025118	-2.161132	-2.449512
57	6	0.835256	3.296382	0.557137
58	6	1.664152	4.300584	1.081546
59	1	2.718142	4.104973	1.249064
60	6	1.138415	5.546179	1.419999
61	1	1.789849	6.311527	1.832229
62	6	-0.220780	5.809197	1.231125
63	1	-0.628558	6.780835	1.494706
64	6	-1.053036	4.817822	0.710653
65	1	-2.111799	5.012879	0.566952
66	6	-0.528237	3.567272	0.380981
67	1	-1.176311	2.788815	-0.011145
68	6	2.306906	2.082391	-1.567713
69	6	3.318446	3.051357	-1.619782
70	1	3.634279	3.559121	-0.715258
71	6	3.948943	3.351636	-2.824267
72	1	4.745221	4.089596	-2.845735
73	6	3.574752	2.689565	-3.995243
74	1	4.074460	2.917001	-4.932314
75	6	2.563227	1.730317	-3.954541
76	1	2.271455	1.204330	-4.858940
77	6	1.932564	1.429882	-2.747855
78	1	1.162820	0.667653	-2.714602
79	28	0.000000	0.000000	0.000000
80	6	-1.006700	-0.015104	-1.442394
81	6	-0.943479	0.046528	1.483855
82	8	-1.708437	0.006065	-2.368995
83	8	-1.611974	0.114003	2.431877

5.3 tmbitianp

Table 5 XYZ coordinates of the optimized structure of the tmbitianp complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	6	2.932900	-1.254343	1.002152
2	6	3.889292	-0.327841	0.652308
3	6	4.832504	-0.049490	1.722760
4	6	5.928555	0.853397	1.774638
5	6	6.649706	0.928464	2.961116
6	1	7.483742	1.624857	3.012436
7	6	6.349136	0.163310	4.106398
8	6	5.277255	-0.719514	4.058508
9	1	5.013942	-1.318355	4.925666
10	6	4.536501	-0.811066	2.877830
11	6	2.922017	1.256678	-1.013968
12	6	3.882247	0.329386	-0.677061
13	6	4.813217	0.053761	-1.758633
14	6	5.907069	-0.850453	-1.826923
15	6	6.611194	-0.926140	-3.023602
16	1	7.442536	-1.624888	-3.086623
17	6	6.297159	-0.158616	-4.163618
18	6	5.228594	0.727128	-4.099230
19	1	4.954429	1.327887	-4.961671
20	6	4.504288	0.818249	-2.908496
21	6	2.240347	-2.168817	-1.576840
22	6	3.281417	-3.110260	-1.593986
23	1	3.594568	-3.583061	-0.668219
24	6	3.924724	-3.428955	-2.786337
25	1	4.736717	-4.150093	-2.785407
26	6	3.542483	-2.803008	-3.975638
27	1	4.058734	-3.035482	-4.902294
28	6	2.507690	-1.869408	-3.966922
29	1	2.212792	-1.371865	-4.885909
30	6	1.854939	-1.557336	-2.773575
31	1	1.063699	-0.817535	-2.769314
32	6	0.840460	-3.227838	0.750217
33	6	0.850690	-4.455082	0.074568
34	1	1.268945	-4.523968	-0.922578
35	6	0.316322	-5.596449	0.675619
36	1	0.328184	-6.539856	0.137246
37	6	-0.228602	-5.528454	1.957568
38	1	-0.640258	-6.418651	2.424126
39	6	-0.256114	-4.305953	2.632869
40	1	-0.691697	-4.238918	3.625464
41	6	0.259796	-3.161886	2.028336
42	1	0.200262	-2.211519	2.547775
43	6	2.245170	2.157987	1.576138
44	6	1.857435	1.544531	2.771122
45	1	1.058178	0.813353	2.765198
46	6	2.516278	1.844885	3.964047
47	1	2.219645	1.345289	4.881350
48	6	3.560445	2.768048	3.973905
49	1	4.082486	2.990363	4.899794
50	6	3.943766	3.397453	2.786845
51	1	4.761955	4.111494	2.787203
52	6	3.293288	3.091296	1.594964
53	1	3.606004	3.567947	0.671045
54	6	0.832774	3.233217	-0.735435
55	6	0.237898	3.177130	-2.007545
56	1	0.171746	2.231137	-2.533704
57	6	-0.283832	4.325875	-2.598051
58	1	-0.730683	4.266053	-3.586093
59	6	-0.248299	5.543477	-1.914460
60	1	-0.664940	6.437092	-2.369911
61	6	0.311623	5.601960	-0.638485
62	1	0.330467	6.541485	-0.093553
63	6	0.852238	4.456065	-0.051871
64	1	1.282521	4.518129	0.940604
65	15	1.452646	-1.665124	0.000000
66	15	1.449646	1.665124	0.000000
67	16	3.140638	-1.845789	2.642309
68	16	3.111854	1.852862	-2.654948
69	6	6.335684	1.727792	0.614308
70	1	6.809190	1.151534	-0.187374
71	1	5.478255	2.237183	0.170420
72	1	7.050326	2.485276	0.948984
73	6	6.331169	-1.726059	-0.673350
74	1	6.820523	-1.151148	0.119986
75	1	5.480287	-2.233388	-0.214947
76	1	7.038061	-2.485031	-1.020760
77	6	7.103899	-0.319001	-5.428278
78	1	8.169047	-0.129960	-5.248125
79	1	7.022438	-1.339626	-5.822617
80	1	6.765733	0.370069	-6.207847
81	6	7.174940	0.322110	5.358999
82	1	8.234427	0.113886	5.166714
83	1	7.115389	1.347453	5.744776
84	1	6.836168	-0.354344	6.149280
85	28	0.000000	0.000000	0.000000
86	6	-0.966845	0.020934	-1.472133
87	6	-0.967755	-0.019734	1.471565
88	8	-1.630085	0.049557	-2.424980
89	8	-1.631392	-0.044653	2.424233

5.4 bitianp

Table 6 XYZ coordinates of the optimized structure of the bitianp complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	6	3.008601	-1.250157	0.903291
2	6	3.953510	-0.357585	0.456240
3	6	5.042191	-0.177531	1.387837
4	6	6.171690	0.650412	1.271199
5	1	6.312966	1.241539	0.371885
6	6	7.085398	0.705950	2.313833
7	1	7.959661	1.344681	2.230308
8	6	6.888015	-0.049518	3.484575
9	1	7.611347	0.011810	4.292247
10	6	5.777301	-0.875944	3.622644
11	1	5.624493	-1.456618	4.527070
12	6	4.862669	-0.936580	2.568031
13	6	2.853263	1.268070	-1.111527
14	6	3.844352	0.357173	-0.832027
15	6	4.716866	0.112858	-1.958922
16	6	5.838265	-0.730183	-2.036692
17	1	6.147036	-1.293902	-1.162402
18	6	6.529303	-0.835085	-3.235349
19	1	7.396671	-1.485137	-3.301346
20	6	6.113342	-0.116901	-4.371085
21	1	6.664285	-0.216411	-5.301660
22	6	5.003400	0.720466	-4.320033
23	1	4.680792	1.272080	-5.197636
24	6	4.313003	0.828957	-3.110397
25	6	2.197119	-2.200463	-1.593239
26	6	3.288476	-3.083976	-1.616005
27	1	3.679687	-3.482688	-0.684758
28	6	3.886549	-3.433451	-2.822935
29	1	4.734620	-4.111795	-2.828504
30	6	3.413948	-2.890745	-4.020999
31	1	3.895966	-3.145521	-4.960121
32	6	2.333318	-2.011301	-4.005530
33	1	1.968133	-1.577176	-4.931478
34	6	1.723715	-1.670630	-2.796834
35	1	0.893752	-0.975029	-2.790064
36	6	0.904902	-3.199007	0.825706
37	6	0.904702	-4.447591	0.191243
38	1	1.277511	-4.542404	-0.822138
39	6	0.422642	-5.575593	0.858052
40	1	0.423833	-6.537322	0.353054
41	6	-0.055267	-5.471309	2.164398
42	1	-0.425824	-6.351401	2.681780
43	6	-0.066270	-4.227765	2.800722
44	1	-0.446874	-4.134929	3.813611
45	6	0.397064	-3.097095	2.131761
46	1	0.355719	-2.130430	2.622812
47	6	2.351928	2.025711	1.567749
48	6	1.881480	1.475346	2.765043
49	1	0.996416	0.850082	2.756960
50	6	2.555902	1.707959	3.964211
51	1	2.186452	1.261836	4.882977
52	6	3.705685	2.496614	3.979079
53	1	4.238205	2.668061	4.909919
54	6	4.177912	3.055669	2.789527
55	1	5.081608	3.657654	2.790648
56	6	3.507626	2.819498	1.592452
57	1	3.909024	3.222824	0.669401
58	6	0.867010	3.294526	-0.585624
59	6	-0.517705	3.508385	-0.607761
60	1	-1.182837	2.700253	-0.318646
61	6	-1.039189	4.741644	-1.000282
62	1	-2.114563	4.892783	-1.013080
63	6	-0.179899	5.772821	-1.380520
64	1	-0.583821	6.731771	-1.692063
65	6	1.202188	5.569122	-1.362736
66	1	1.875095	6.368203	-1.660049
67	6	1.724000	4.340020	-0.963613
68	1	2.798545	4.197207	-0.960465
69	15	1.465215	-1.657778	0.000000
70	15	1.458492	1.657778	0.000000
71	16	3.391286	-1.893018	2.494659
72	16	2.895769	1.814761	-2.783843
73	28	0.000000	0.000000	0.000000
74	6	-0.968519	0.025331	-1.473280
75	6	-0.987613	-0.054653	1.456916
76	8	-1.651539	0.061192	-2.410887
77	8	-1.669122	-0.104206	2.395830

5.5 bifurp1

Table 7 XYZ coordinates of the optimized structure of the lowest-energy bifurp complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	6	4.265753	-1.195655	-2.751081
2	6	4.830422	-0.336458	-1.789873
3	6	6.002892	0.362946	-2.103239
4	6	6.566776	0.168576	-3.360867
5	6	5.981282	-0.702426	-4.299946
6	6	4.810776	-1.405244	-4.009907
7	6	2.942178	-1.266410	-0.984353
8	6	3.940621	-0.389189	-0.651730
9	1	6.448157	1.043478	-1.384428
10	1	7.474854	0.700790	-3.628255
11	1	6.447833	-0.829385	-5.272127
12	1	4.345480	-2.074627	-4.725224
13	6	3.954991	0.389733	0.587194
14	6	4.867959	0.327790	1.706476
15	6	2.960743	1.259607	0.949574
16	6	4.319027	1.172327	2.689213
17	6	6.051014	-0.367801	1.987203
18	6	4.887251	1.368493	3.939806
19	6	6.638381	-0.186747	3.235966
20	1	6.487284	-1.034918	1.250454
21	6	6.066337	0.667715	4.198158
22	1	4.432637	2.026121	4.672702
23	1	7.554762	-0.716894	3.478001
24	1	6.550993	0.784022	5.162782
25	15	1.451594	-1.663210	0.000000
26	15	1.448906	1.663210	0.000000
27	6	2.279613	-2.090647	1.581668
28	6	1.888303	-1.456183	2.764241
29	6	3.366367	-2.978959	1.607227
30	6	2.577250	-1.695332	3.954394
31	1	1.060011	-0.757519	2.750786
32	6	4.045709	-3.225290	2.796841
33	1	3.689031	-3.463996	0.690789
34	6	3.655745	-2.578188	3.972576
35	1	2.275431	-1.182395	4.862598
36	1	4.889425	-3.909115	2.804978
37	1	4.199552	-2.754513	4.895794
38	6	0.888721	-3.250317	-0.716964
39	6	0.808839	-4.427111	0.037500
40	6	0.433971	-3.251389	-2.045384
41	6	0.293686	-5.592545	-0.533919
42	1	1.146791	-4.436757	1.067998
43	6	-0.066110	-4.419491	-2.614973
44	1	0.468994	-2.338582	-2.630888
45	6	-0.138704	-5.593462	-1.859923
46	1	0.232587	-6.499541	0.060679
47	1	-0.407532	-4.411916	-3.646020
48	1	-0.536880	-6.501663	-2.302981
49	6	2.251389	2.115305	-1.588758
50	6	1.866308	1.474391	-2.769611
51	6	3.321548	3.023388	-1.618340
52	6	2.544016	1.728323	-3.963255
53	1	1.052039	0.759299	-2.752202
54	6	3.990179	3.283776	-2.811049
55	1	3.638804	3.513702	-0.702796
56	6	3.605754	2.631057	-3.985649
57	1	2.247479	1.210631	-4.870444
58	1	4.820623	3.983668	-2.822953
59	1	4.141242	2.818845	-4.911513
60	6	0.893418	3.240472	0.744050
61	6	0.487859	3.233548	2.088178
62	6	0.765843	4.415909	-0.005763
63	6	-0.010527	4.392906	2.676782
64	1	0.562665	2.322030	2.671802
65	6	0.253386	5.572654	0.585333
66	1	1.064212	4.430845	-1.048281
67	6	-0.130032	5.565966	1.926270
68	1	-0.313066	4.379416	3.719846
69	1	0.155801	6.478739	-0.005791
70	1	-0.526162	6.467393	2.384706
71	8	3.113157	-1.765771	-2.258262
72	8	3.155741	1.744914	2.225518
73	28	0.000000	0.000000	0.000000
74	6	-0.965152	-0.071733	-1.475046
75	6	-0.970961	0.069079	1.471767
76	8	-1.632678	0.155652	2.420806
77	8	-1.622363	-0.159956	-2.427213

5.6 bifurp2

Table 8 XYZ coordinates of the optimized structure of the less stable bifurp complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	6	5.222883	-2.045845	0.948418
2	6	5.053715	-0.873039	1.701258
3	6	6.164047	-0.317689	2.356285
4	6	7.385944	-0.974795	2.249952
5	6	7.517897	-2.161232	1.501802
6	6	6.432457	-2.719455	0.828494
7	6	3.106447	-1.421937	0.691694
8	6	3.661928	-0.488161	1.533647
9	1	6.071409	0.599507	2.927339
10	1	8.258001	-0.564621	2.750027
11	1	8.486562	-2.647858	1.441763
12	1	6.520131	-3.623624	0.236298
13	6	3.063422	0.683971	2.166475
14	6	3.232219	1.079081	3.554348
15	6	2.268182	1.645535	1.595002
16	6	2.496932	2.267992	3.704143
17	6	3.878367	0.537407	4.676509
18	6	2.385651	2.965262	4.899590
19	6	3.779131	1.218589	5.886346
20	1	4.435255	-0.390252	4.603106
21	6	3.048351	2.417108	5.997450
22	1	1.807340	3.880011	4.968503
23	1	4.271615	0.815642	6.766201
24	1	2.992269	2.920981	6.957418
25	15	1.438106	-1.674229	0.000000
26	15	1.398423	1.674229	0.000000
27	6	0.973855	-3.272149	0.787081
28	6	-0.057462	-3.299122	1.732597
29	6	1.659075	-4.459291	0.482717
30	6	-0.400611	-4.493981	2.368354
31	1	-0.591863	-2.387213	1.973642
32	6	1.312534	-5.650791	1.115527
33	1	2.459026	-4.447131	-0.248958
34	6	0.282035	-5.670464	2.059919
35	1	-1.203610	-4.503061	3.099575
36	1	1.846279	-6.565143	0.872353
37	1	0.012475	-6.601167	2.550915
38	6	1.845149	-2.174906	-1.718780
39	6	0.925558	-2.975688	-2.413004
40	6	2.967135	-1.679741	-2.392610
41	6	1.135374	-3.289260	-3.754160
42	1	0.048456	-3.360280	-1.900628
43	6	3.172625	-1.993663	-3.736385
44	1	3.678638	-1.043868	-1.879667
45	6	2.262133	-2.799511	-4.419920
46	1	0.419028	-3.914667	-4.279156
47	1	4.045340	-1.597874	-4.247218
48	1	2.425576	-3.042573	-5.465930
49	6	2.733058	1.637427	-1.252344
50	6	2.325692	1.563127	-2.592798
51	6	4.099673	1.656467	-0.950388
52	6	3.270448	1.518522	-3.614485
53	1	1.266714	1.523858	-2.832703
54	6	5.045012	1.585954	-1.975612
55	1	4.428857	1.717941	0.080372
56	6	4.633487	1.521004	-3.307738
57	1	2.943122	1.458792	-4.647979
58	1	6.102986	1.586371	-1.729787
59	1	5.370748	1.468543	-4.103550
60	6	0.782967	3.394973	-0.084687
61	6	-0.594751	3.621509	0.000221
62	6	1.657518	4.480645	-0.234423
63	6	-1.096267	4.923167	-0.055853
64	1	-1.268047	2.775890	0.107505
65	6	1.155433	5.778557	-0.290411
66	1	2.726980	4.308158	-0.312035
67	6	-0.222216	6.000909	-0.200541
68	1	-2.166964	5.092773	0.009769
69	1	1.836000	6.617195	-0.406068
70	1	-0.611724	7.013817	-0.247560
71	8	4.046462	-2.386364	0.344857
72	8	1.911261	2.612284	2.512511
73	28	0.000000	0.000000	0.000000
74	6	-0.880477	-0.106225	-1.527583
75	6	-0.958103	0.088589	1.482335
76	8	-1.609161	0.147126	2.440943
77	8	-1.437662	-0.161250	-2.542779

5.7 bimip

Table 9 XYZ coordinates of the optimized structure of the bimip complex

Center Number	Atomic Number	Coordinates (Ångstroms) X	Y	Z
1	6	4.311820	-0.996753	-2.624794
2	6	4.721753	-0.113783	-1.603008
3	6	5.831941	0.717217	-1.707809
4	6	6.538007	0.647697	-2.906831
5	6	6.144985	-0.219827	-3.945882
6	6	5.034969	-1.051010	-3.821136
7	6	2.889449	-1.296753	-1.016909
8	1	6.120187	1.388108	-0.906357
9	1	7.408969	1.280975	-3.045219
10	1	6.725361	-0.239525	-4.863372
11	1	4.730367	-1.720968	-4.618668
12	6	4.695227	0.119881	1.651813
13	6	2.871862	1.301784	1.036070
14	6	4.266887	1.001009	2.667683
15	6	5.805184	-0.708919	1.774725
16	6	4.969492	1.055882	3.876156
17	6	6.490412	-0.639276	2.985822
18	1	6.108874	-1.378571	0.978002
19	6	6.078648	0.226531	4.019016
20	1	4.649874	1.724671	4.668792
21	1	7.360095	-1.271070	3.138329
22	1	6.643381	0.246258	4.946218
23	15	1.408849	-1.684310	0.000000
24	15	1.404376	1.684310	0.000000
25	6	2.238114	-2.176020	1.556536
26	6	1.896160	-1.541154	2.754341
27	6	3.266561	-3.132440	1.551125
28	6	2.574011	-1.853962	3.933557
29	1	1.115043	-0.789944	2.761564
30	6	3.933509	-3.450342	2.730691
31	1	3.544959	-3.621782	0.622068
32	6	3.590218	-2.807780	3.923480
33	1	2.312257	-1.343763	4.855342
34	1	4.731162	-4.187175	2.718328
35	1	4.123216	-3.043798	4.839565
36	6	0.814597	-3.238388	-0.753879
37	6	0.634278	-4.401705	0.004327
38	6	0.423268	-3.223811	-2.101744
39	6	0.084884	-5.542555	-0.584056
40	1	0.921308	-4.420880	1.049930
41	6	-0.112355	-4.368425	-2.686307
42	1	0.546199	-2.322513	-2.690773
43	6	-0.283403	-5.530713	-1.929153
44	1	-0.052419	-6.440026	0.012184
45	1	-0.401866	-4.351854	-3.732956
46	1	-0.707394	-6.420245	-2.385951
47	6	2.246164	2.157020	-1.555313
48	6	1.910699	1.510009	-2.748446
49	6	3.274863	3.113002	-1.553899
50	6	2.596103	1.809480	-3.926696
51	1	1.128317	0.760021	-2.751623
52	6	3.949410	3.417779	-2.732655
53	1	3.547924	3.612593	-0.628749
54	6	3.613345	2.762358	-3.920454
55	1	2.339639	1.289692	-4.844603
56	1	4.747459	4.154191	-2.723258
57	1	4.152541	2.987791	-4.835553
58	6	0.799865	3.248192	0.724157
59	6	0.412931	3.264812	2.073363
60	6	0.599009	4.387367	-0.065274
61	6	-0.140446	4.416495	2.627017
62	1	0.554847	2.383302	2.687461
63	6	0.032612	5.535049	0.492659
64	1	0.882654	4.381973	-1.112008
65	6	-0.332905	5.554272	1.838447
66	1	-0.427217	4.424288	3.674537
67	1	-0.120683	6.413237	-0.127895
68	1	-0.771164	6.448744	2.271512
69	7	3.133735	1.705439	2.255156
70	7	3.785585	0.326628	0.619767
71	7	3.794978	-0.319951	-0.586594
72	7	3.172640	-1.702327	-2.230574
73	28	0.000000	0.000000	0.000000
74	6	-0.966425	-0.081028	-1.477636
75	6	-0.963532	0.081589	1.479717
76	8	-1.618104	0.167283	2.432210
77	8	-1.622632	-0.162826	-2.429374