catalysts

Supplementary Materials: Synthesis, Structure and 1,3-Butadiene Polymerization Behavior of Phosphine Vanadium(III) Complexes

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Table S1. Cartesian coordinates of the modelled compounds at their UM06/6-311G(d) optimized geometry.

complex 1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.000002	-0.131273	-0.000007
2	15	0	2.436210	-0.247619	-0.696932
3	15	0	-2.436205	-0.247615	0.696931
4	17	0	0.000005	-2.373462	0.000009
5	17	0	0.515748	0.993623	1.870182
6	17	0	-0.515751	0.993566	-1.870229
7	6	0	3.440951	-1.262731	0.434097
8	6	0	3.808442	-0.717480	1.665335
9	1	0	3.532365	0.307875	1.907979
10	6	0	4.519279	-1.477510	2.579204
11	1	0	4.803176	-1.044208	3.535365
12	6	0	4.862264	-2.789398	2.278076
13	1	0	5.418522	-3.385729	2.997764
14	6	0	4.488477	-3.340155	1.061870
15	1	0	4.747749	-4.369636	0.825666
16	6	0	3.777353	-2.581860	0.142209
17	1	0	3.477970	-3.031522	-0.801983
18	6	0	3.411505	1.287715	-0.879608
19	6	0	4.796676	1.226238	-1.038413
20	1	0	5.304713	0.262957	-1.003118
21	6	0	5.531129	2.385822	-1.221795
22	1	0	6.610702	2.330381	-1.341996
23	6	0	4.888335	3.617386	-1.247687
24	1	0	5.465546	4.528396	-1.389327
25	6	0	3.512910	3.685706	-1.089484
26	1	0	3.008131	4.648655	-1.106167
27	6	0	2.773763	2.524748	-0.904554
28	1	0	1.694253	2.585354	-0.782017
29	6	0	2.611941	-1.027056	-2.340693

30	1	0	2.184262	-0.338248	-3.075639
31	1	0	2.044495	-1.961522	-2.382860
32	1	0	3.660579	-1.214463	-2.593924
33	6	0	-3.411496	1.287721	0.879613
34	6	0	-4.796667	1.226246	1.038426
35	1	0	-5.304705	0.262966	1.003136
36	6	0	-5.531116	2.385831	1.221812
37	1	0	-6.610689	2.330392	1.342020
38	6	0	-4.888320	3.617394	1.247697
39	1	0	-5.465528	4.528405	1.389340
40	6	0	-3.512896	3.685712	1.089486
41	1	0	-3.008115	4.648660	1.106164
42	6	0	-2.773752	2.524753	0.904553
43	1	0	-1.694243	2.585356	0.782010
44	6	0	-3.440958	-1.262725	-0.434091
45	6	0	-3.808453	-0.717474	-1.665326
46	1	0	-3.532372	0.307880	-1.907974
47	6	0	-4.519303	-1.477500	-2.579189
48	1	0	-4.803203	-1.044197	-3.535349
49	6	0	-4.862294	-2.789385	-2.278057
50	1	0	-5.418562	-3.385714	-2.997740
51	6	0	-4.488502	-3.340143	-1.061853
52	1	0	-4.747779	-4.369622	-0.825645
53	6	0	-3.777366	-2.581851	-0.142197
54	1	0	-3.477979	-3.031514	0.801992
55	6	0	-2.611926	-1.027050	2.340693
56	1	0	-2.044478	-1.961516	2.382856
57	1	0	-3.660562	-1.214460	2.593931
58	1	0	-2.184243	-0.338241	3.075636

complex 1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.029391	-0.042944	0.564122
2	15	0	-2.516728	-0.018165	0.535009
3	15	0	2.582942	0.030595	0.591455
4	17	0	0.052831	0.172423	-1.663695
5	17	0	0.083291	1.709814	1.973849
6	17	0	-0.086165	-2.073770	1.504600
7	6	0	-3.366658	1.379478	-0.283001

8	6	0	-2.763313	2.636055	-0.249483
9	1	0	-1.781796	2.759894	0.205348
10	6	0	-3.407285	3.735759	-0.798298
11	1	0	-2.925253	4.710083	-0.770932
12	6	0	-4.654401	3.590637	-1.387318
13	1	0	-5.155291	4.452650	-1.822278
14	6	0	-5.261608	2.342695	-1.424297
15	1	0	-6.239686	2.224536	-1.885299
16	6	0	-4.623644	1.242323	-0.873112
17	1	0	-5.104485	0.266504	-0.907991
18	6	0	-3.167432	-1.511806	-0.281996
19	6	0	-3.571174	-2.628372	0.447460
20	1	0	-3.574184	-2.604927	1.535003
21	6	0	-3.956624	-3.790429	-0.204991
22	1	0	-4.271532	-4.654410	0.375606
23	6	0	-3.933745	-3.852239	-1.590082
24	1	0	-4.235051	-4.764454	-2.100044
25	6	0	-3.513577	-2.750868	-2.323571
26	1	0	-3.478452	-2.798223	-3.409481
27	6	0	-3.126223	-1.588927	-1.675801
28	1	0	-2.779345	-0.736108	-2.256913
29	6	0	-3.213460	0.001660	2.240524
30	1	0	-2.776910	-0.855891	2.769350
31	1	0	-2.761957	0.889322	2.704081
32	6	0	3.156088	1.605403	-0.133994
33	6	0	3.238956	1.725342	-1.522230
34	1	0	3.010063	0.869787	-2.154749
35	6	0	3.605755	2.930182	-2.098989
36	1	0	3.669210	3.011001	-3.181641
37	6	0	3.884493	4.030648	-1.299481
38	1	0	4.171019	4.976363	-1.754052
39	6	0	3.789429	3.923128	0.079627
40	1	0	3.997982	4.784025	0.710760
41	6	0	3.422853	2.717996	0.661953
42	1	0	3.338080	2.656101	1.744402
43	6	0	3.527372	-1.237507	-0.324480
44	6	0	2.895097	-2.401342	-0.752785
45	1	0	1.828801	-2.537934	-0.583417
46	6	0	3.623552	-3.394929	-1.394189
47	1	0	3.121459	-4.299684	-1.728257
48	6	0	4.983286	-3.232570	-1.607810
49	1	0	5.552009	-4.011337	-2.111110
50	6	0	5.620955	-2.073532	-1.181441

51	1	0	6.687442	-1.943110	-1.350810
52	6	0	4.897152	-1.080672	-0.542475
53	1	0	5.397071	-0.167117	-0.222389
54	6	0	3.357900	-0.006152	2.265696
55	1	0	4.394826	0.344626	2.172062
56	1	0	2.818092	0.724439	2.881044
57	6	0	-4.725329	0.041365	2.355950
58	1	0	-5.134037	0.951827	1.905708
59	1	0	-5.031486	0.030114	3.407543
60	1	0	-5.203760	-0.813032	1.864698
61	6	0	3.297248	-1.383515	2.902392
62	1	0	2.266326	-1.736298	3.009115
63	1	0	3.747663	-1.362979	3.899971
64	1	0	3.840750	-2.127338	2.309381

complex 1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.023517	-0.230745	0.294608
2	17	0	-0.728702	1.135075	1.938224
3	17	0	0.086521	0.310447	-1.881733
4	17	0	0.534558	-2.318933	0.878690
5	15	0	-2.425561	-0.922326	-0.097721
6	15	0	2.320192	0.714112	0.746615
7	6	0	-3.177241	-1.827906	1.315177
8	1	0	-2.523154	-2.691227	1.493887
9	1	0	-3.047297	-1.189082	2.197888
10	6	0	-4.624211	-2.247809	1.134353
11	1	0	-5.271416	-1.392372	0.912074
12	1	0	-5.008348	-2.724748	2.042309
13	1	0	-4.740806	-2.969718	0.318607
14	6	0	-2.738383	-1.992658	-1.563358
15	1	0	-3.823065	-2.054236	-1.724168
16	1	0	-2.315579	-1.464886	-2.426459
17	6	0	-2.105534	-3.368823	-1.450128
18	1	0	-1.018506	-3.305920	-1.336812
19	1	0	-2.312355	-3.957843	-2.349392
20	1	0	-2.487650	-3.936860	-0.594598
21	6	0	-3.514011	0.517930	-0.373844
22	6	0	-4.027152	1.230452	0.711524

23	1	0	-3.814110	0.910321	1.729037
24	6	0	-4.799463	2.362733	0.508024
25	1	0	-5.194814	2.904668	1.364020
26	6	0	-5.059547	2.808642	-0.780295
27	1	0	-5.663250	3.699341	-0.938407
28	6	0	-4.537754	2.119481	-1.864261
29	1	0	-4.726780	2.468926	-2.876681
30	6	0	-3.767295	0.983319	-1.664091
31	1	0	-3.354550	0.466914	-2.527399
32	6	0	2.972498	0.381377	2.441960
33	1	0	3.763705	1.117076	2.646102
34	1	0	2.147459	0.606003	3.131677
35	6	0	3.487838	-1.032051	2.641489
36	1	0	2.711685	-1.779357	2.451364
37	1	0	3.840276	-1.171642	3.668781
38	1	0	4.327888	-1.249665	1.972429
39	6	0	2.336985	2.556591	0.727335
40	1	0	1.641170	2.865540	1.518632
41	1	0	3.333645	2.897147	1.039192
42	6	0	1.946097	3.161356	-0.608030
43	1	0	2.582224	2.793460	-1.421393
44	1	0	2.037652	4.252069	-0.580694
45	1	0	0.911506	2.922710	-0.873901
46	6	0	3.706130	0.230071	-0.344081
47	6	0	4.938383	0.882400	-0.284924
48	1	0	5.083106	1.725680	0.389139
49	6	0	5.831314	-0.611732	-1.941046
50	1	0	6.659691	-0.938376	-2.565661
51	6	0	4.613301	-1.270719	-2.001793
52	1	0	4.481901	-2.115838	-2.673213
53	6	0	3.554462	-0.852484	-1.207236
54	1	0	2.601011	-1.374041	-1.263048
55	6	0	5.993768	0.466415	-1.080453
56	1	0	6.948654	0.984765	-1.028718

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complex 2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.042753	-0.005469	-0.054352
2	15	0	-2.627614	0.115390	-0.053154
3	15	0	2.541926	0.094638	-0.058047
4	17	0	0.000234	1.367109	1.731852
5	17	0	-0.042515	0.855247	-2.135850
6	17	0	-0.084421	-2.235237	0.213996
7	6	0	-3.171447	1.690252	-0.854415
8	1	0	-2.794479	1.596268	-1.884383
9	6	0	-2.553616	2.964936	-0.241611
10	1	0	-2.320887	2.840814	0.822304
11	1	0	-1.599393	3.197280	-0.727825
12	6	0	-3.606278	4.073053	-0.445213
13	1	0	-3.178512	4.988091	-0.867536
14	1	0	-4.048889	4.351925	0.520045
15	6	0	-4.681349	3.456664	-1.337664
16	1	0	-4.398588	3.544172	-2.396376
17	1	0	-5.662135	3.931643	-1.223810
18	6	0	-4.668805	1.989791	-0.931137
19	1	0	-5.139841	1.880733	0.056874
20	1	0	-5.207124	1.337948	-1.629270
21	6	0	-3.531696	-1.155777	-1.045654
22	1	0	-4.570634	-0.804810	-1.127338
23	6	0	-2.994841	-1.316766	-2.472825
24	1	0	-3.288752	-0.492928	-3.133990
25	1	0	-1.896765	-1.355071	-2.475041
26	6	0	-3.551349	-2.671509	-2.885329
27	1	0	-3.083935	-3.071801	-3.791481
28	1	0	-4.630573	-2.587877	-3.083102
29	6	0	-3.299827	-3.526712	-1.649195
30	1	0	-2.252291	-3.855762	-1.643495
31	1	0	-3.920053	-4.428503	-1.612088
32	6	0	-3.545834	-2.586921	-0.457189
33	1	0	-2.777110	-2.734606	0.306546
34	1	0	-4.511542	-2.785273	0.024085
35	6	0	-3.420731	0.123453	1.625789
36	1	0	-3.255439	1.151881	1.980324
37	6	0	-2.735232	-0.816813	2.634447
38	1	0	-2.468523	-1.774888	2.168064

39	1	0	-1.809130	-0.388168	3.029195
40	6	0	-3.809293	-1.048464	3.685448
41	1	0	-3.916098	-0.153110	4.316082
42	1	0	-3.590258	-1.891986	4.348951
43	6	0	-5.060337	-1.248255	2.842625
44	1	0	-5.993850	-1.154199	3.407903
45	1	0	-5.046540	-2.259569	2.412007
46	6	0	-4.935677	-0.200047	1.730521
47	1	0	-5.489219	0.708577	1.998104
48	1	0	-5.374969	-0.555881	0.792751
49	6	0	3.100489	1.669472	-0.855456
50	1	0	2.594100	1.636992	-1.831197
51	6	0	2.619567	2.945247	-0.152466
52	1	0	2.781489	2.889427	0.934109
53	1	0	1.550723	3.130637	-0.304368
54	6	0	3.525535	4.015208	-0.742545
55	1	0	3.220757	4.228817	-1.777522
56	1	0	3.497604	4.961320	-0.191151
57	6	0	4.892840	3.344107	-0.722568
58	1	0	5.302875	3.395047	0.296546
59	1	0	5.625533	3.821882	-1.381632
60	6	0	4.615817	1.881418	-1.101697
61	1	0	4.849055	1.693506	-2.156983
62	1	0	5.251035	1.200617	-0.526978
63	6	0	3.500405	-1.164297	-1.011024
64	1	0	4.546081	-0.816386	-1.048230
65	6	0	3.000449	-1.335642	-2.446820
66	1	0	1.913372	-1.495773	-2.437147
67	1	0	3.183605	-0.459946	-3.080094
68	6	0	3.722859	-2.596543	-2.936807
69	1	0	4.628495	-2.326047	-3.492853
70	1	0	3.097620	-3.172491	-3.626856
71	6	0	4.085103	-3.394408	-1.666603
72	1	0	5.174799	-3.465517	-1.559235
73	1	0	3.708521	-4.422173	-1.692279
74	6	0	3.494500	-2.602484	-0.495793
75	1	0	2.463241	-2.921178	-0.300951
76	1	0	4.060568	-2.736328	0.433312
77	6	0	3.231472	0.097896	1.655158
78	1	0	2.821290	1.018491	2.093994
79	6	0	4.749973	0.120520	1.853166
80	1	0	5.253758	-0.582750	1.173262
81	1	0	5.183234	1.112655	1.679849

82	6	0	4.906761	-0.364297	3.288394
83	1	0	5.934986	-0.644822	3.542749
84	1	0	4.605137	0.435406	3.980387
85	6	0	3.923984	-1.526651	3.365678
86	1	0	3.642890	-1.785300	4.391755
87	1	0	4.388442	-2.423487	2.932002
88	6	0	2.721791	-1.089125	2.514745
89	1	0	1.880496	-0.758371	3.134455
90	1	0	2.337013	-1.918629	1.911958

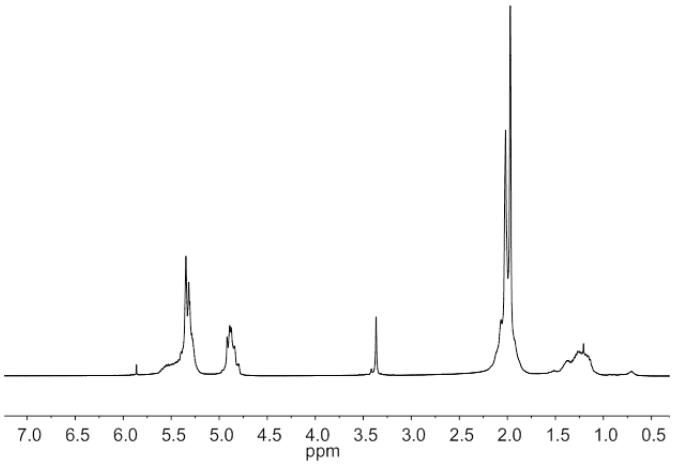

Figure S1. ^{1}H NMR spectrum of poly(1,3-butadiene) (Table 2, entry 4).

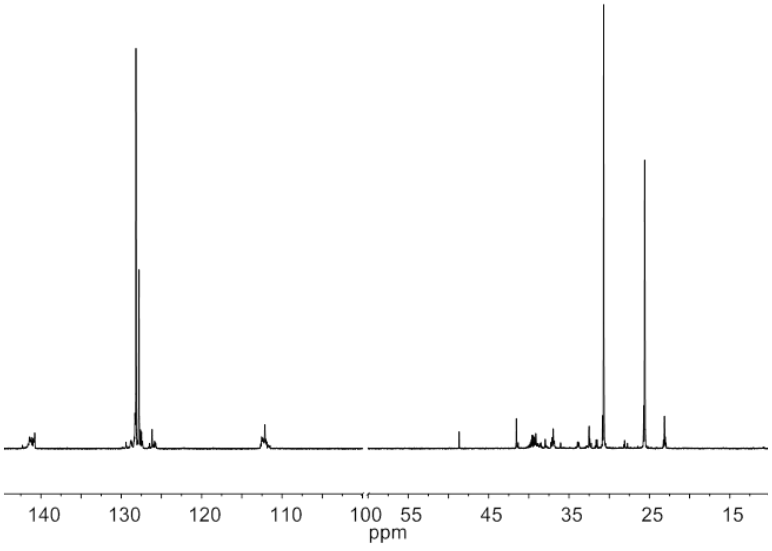

Figure S2. ^{13}C NMR spectrum of poly(1,3-butadiene) (Table 2, entry 4).

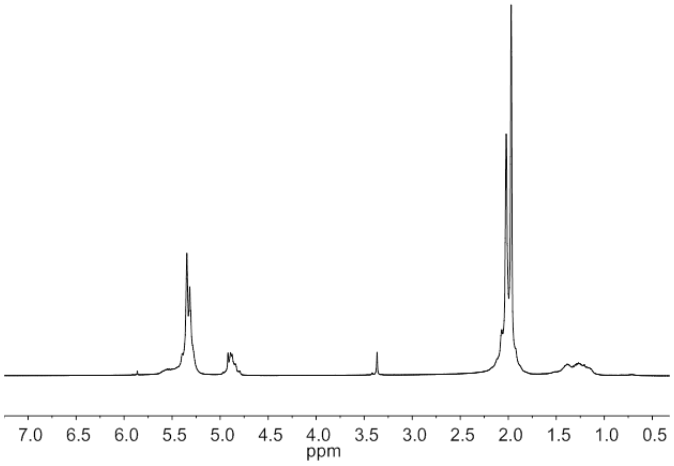

Figure S3. ^{1}H NMR spectrum of poly(1,3-butadiene) (Table 2, entry 14).

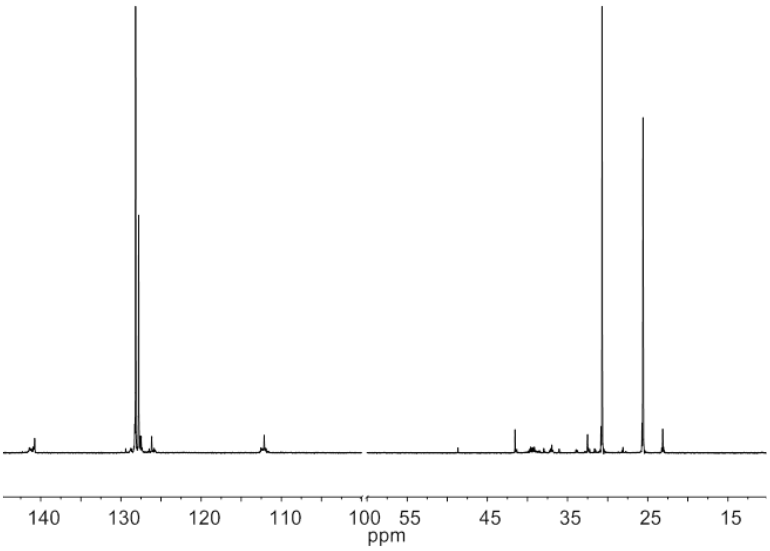

Figure S4. ^{13}C NMR spectrum of poly(1,3-butadiene) (Table 2, entry 14).