SUPPORTING INFORMATION

Trialkyl Phosphites and Diaryliodonium Salts as Co-Initiators in a System for Radical-Promoted Visible-Light-Induced Cationic Polymerization

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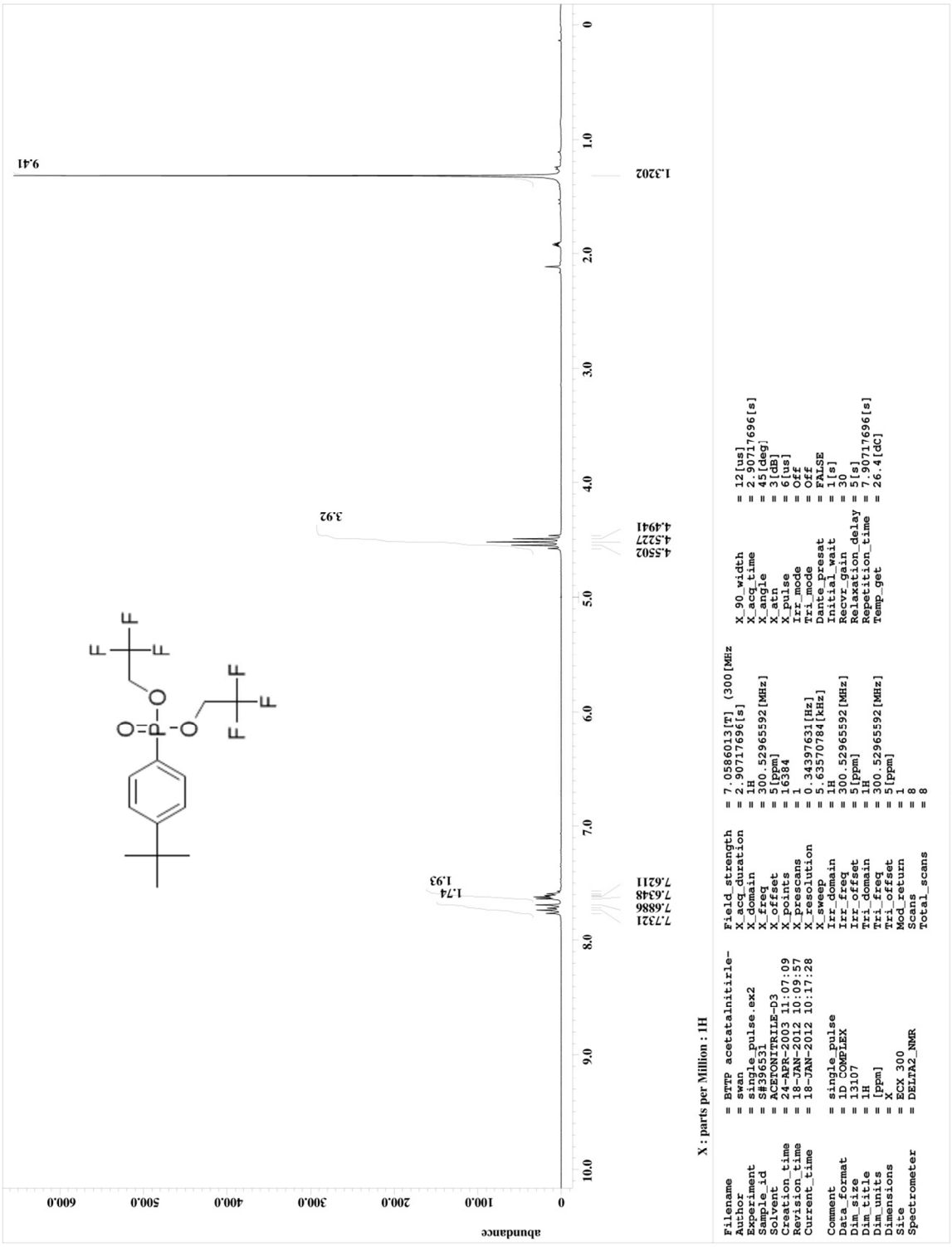
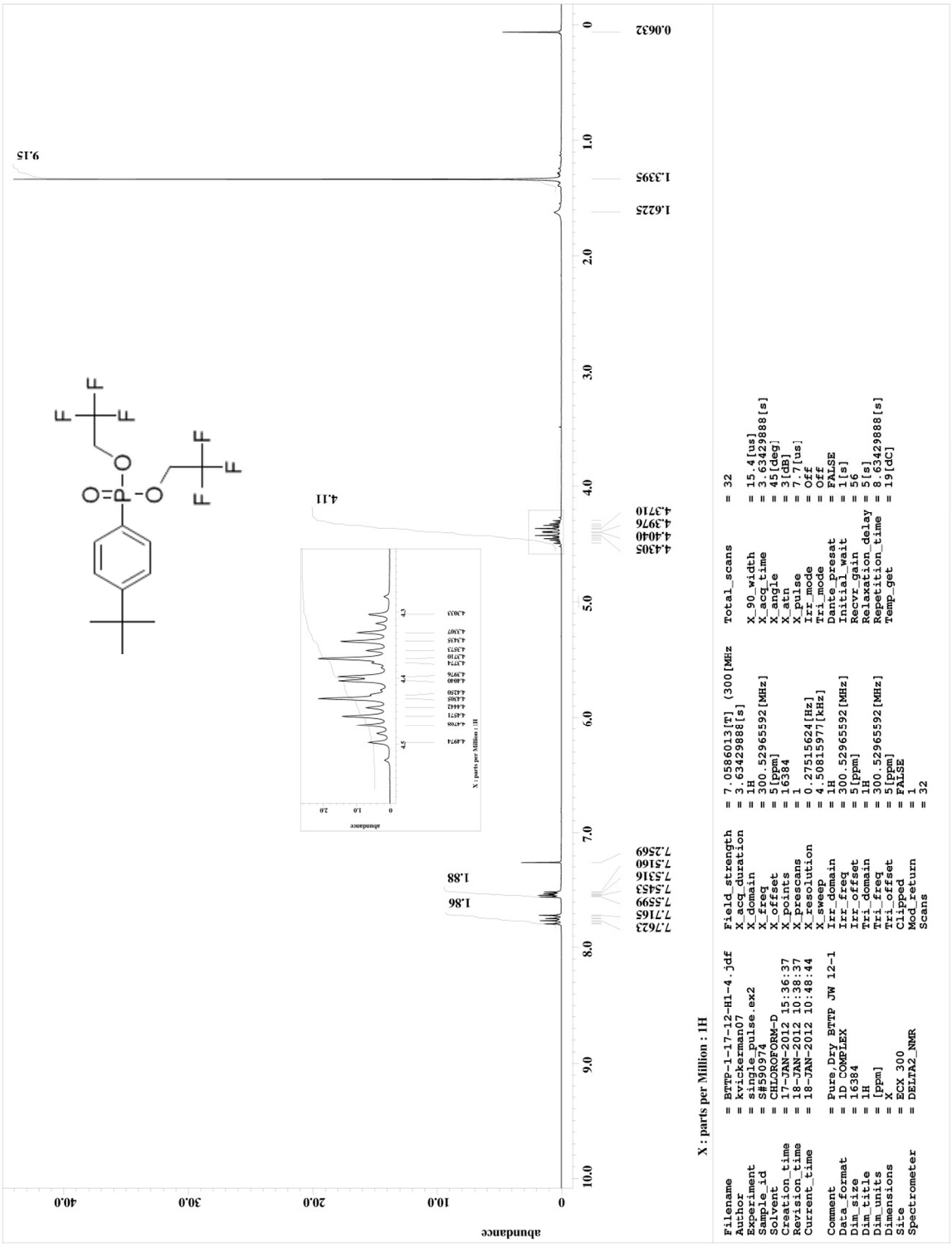
1. ^{1}H NMR Spectrum of bis(2,2,2-trifluoroethyl) *tert*-butylphenylphosphonate (CD_3CN).

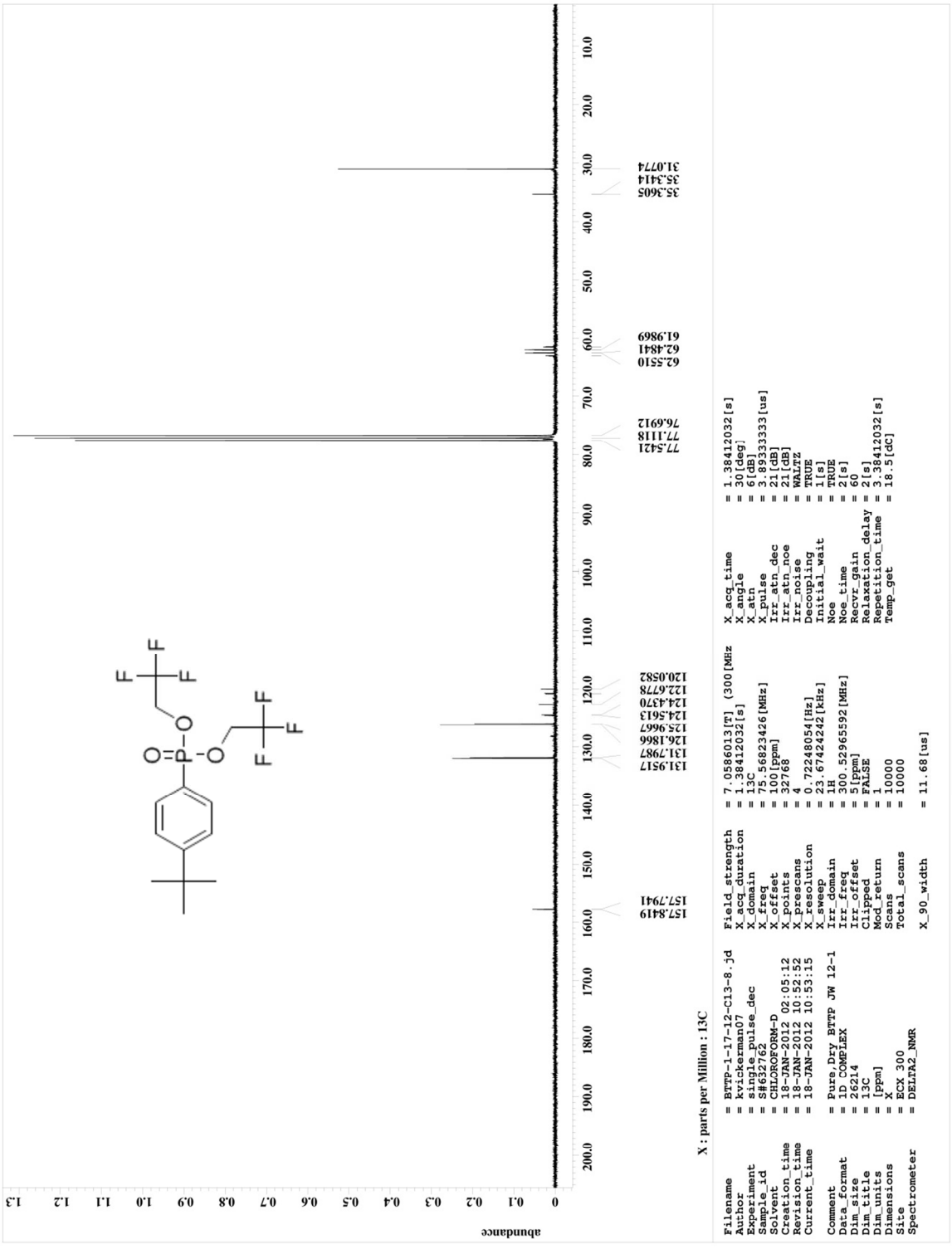


S-1

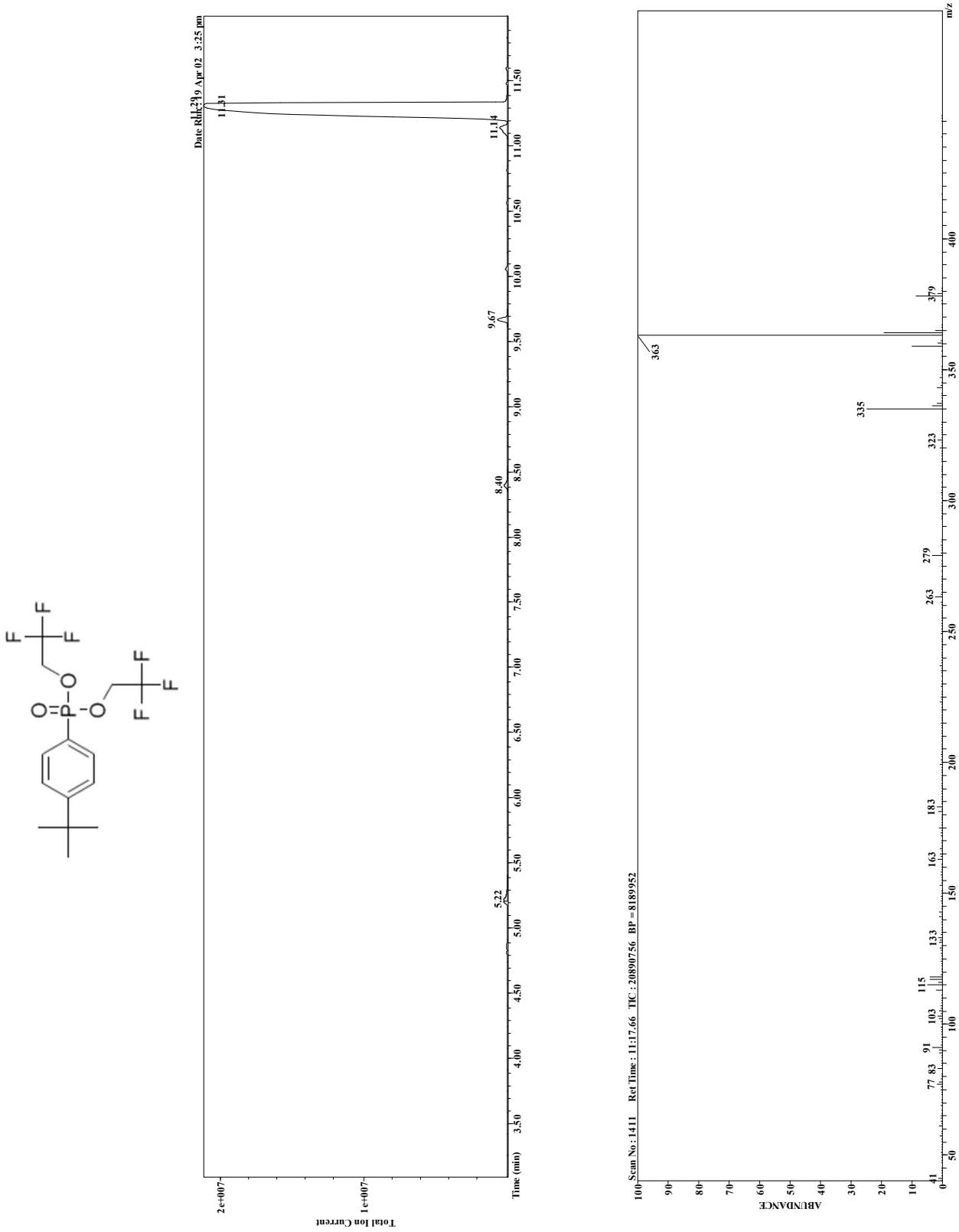
2. ^{1}H NMR Spectrum of bis(2,2,2-trifluoroethyl) *tert*-butylphenylphosphonate (2a). ($CDCl_3$)



3. ^{13}C NMR Spectrum of bis(2,2,2-trifluoroethyl) *tert*-butylphenylphosphonate (2a).



4. GC-MS TIC chromatogram and EI-MS of bis(2,2,2-trifluoroethyl) *tert*-butylphenylphosphonate (2a).



5. Computational method, total energies, and Cartesian coordinates (in Å).

Computational Method. Calculations were carried out on a personal computer using HyperChem™ 8.0.9 (HyperCube Inc, 1115 NW 4th St., Gainesville, FL 32608, USA). The MNDO/d semi-empirical method was used for geometry optimization using a conjugate-gradient (Polak-Ribiere) search algorithm and a termination condition of 0.001 kcal/(Å mol). Total energies and HOMO energies for the optimized structures were determined by DFT calculations (SCF convergence limit = 0.01) using the B3-LYP combination potential in conjunction with both the 6-31G(d,p) and DZVP basis sets. All calculations for non-radical species used the restricted Hartree-Fock (RHF) approximation while those on radicals used UHF.

Triphenylphosphine (Ph_3P).

Total energy (kcal/mol) = −61034.4 (MNDO/d); −649976.5 (6-31G(d,p)); −649987.4 (DZVP)

atom	atom	X	Y	Z
1	C	3.016	-1.717	1.541
2	C	3.568	-1.601	0.253
3	C	3.691	-0.337	-0.352
4	C	3.269	0.838	0.329
5	C	2.717	0.703	1.625
6	C	2.590	-0.565	2.224
7	H	2.919	-2.698	2.008
8	H	3.899	-2.493	-0.280
9	H	4.118	-0.278	-1.358
10	H	2.161	-0.652	3.222
11	P	3.409	2.379	-0.608
12	C	5.936	2.669	0.736
13	C	5.076	3.024	-0.331
14	C	5.567	3.909	-1.329
15	C	6.874	4.423	-1.253
16	C	7.716	4.059	-0.187
17	C	7.245	3.182	0.805
18	H	5.606	1.994	1.528
19	H	8.730	4.456	-0.130
20	H	7.895	2.896	1.632
21	H	7.237	5.103	-2.024
22	H	2.379	1.574	2.190
23	H	4.938	4.204	-2.174
24	C	-0.040	4.447	0.044
25	C	0.930	3.531	-0.403
26	C	2.251	3.558	0.123
27	C	2.565	4.532	1.102
28	C	1.592	5.450	1.542
29	C	0.289	5.408	1.016
30	H	-1.050	4.412	-0.367
31	H	0.647	2.799	-1.165
32	H	3.564	4.594	1.538
33	H	1.851	6.195	2.294
34	H	-0.463	6.119	1.359

Tetraphenylphosphonium (Ph_4P^+).

Total energy (kcal/mol) = −80214.0 (MNDO/d); −795128.7 (6-31G(d,p)); −795141.6 (DZVP)

atom	atom	X	Y	Z	atom	atom	X	Y	Z
1	C	13.114	-0.765	1.589	40	C	12.661	6.606	-1.246
2	C	12.620	0.472	2.032	41	H	10.508	6.522	-1.481
3	C	12.825	1.665	1.275	42	H	10.181	4.732	0.157
4	C	13.532	1.550	0.049	43	H	14.498	4.650	0.866
5	C	14.027	0.308	-0.392	44	H	14.775	6.454	-0.778
6	C	13.823	-0.852	0.374	45	H	12.795	7.408	-1.974
7	H	12.946	-1.662	2.186					
8	H	12.070	0.492	2.978					
9	H	13.707	2.416	-0.595					
10	H	14.570	0.249	-1.337					
11	H	14.207	-1.814	0.031					
12	C	14.420	4.806	5.592					
13	C	14.710	3.522	5.101					
14	C	14.028	3.018	3.978					
15	C	13.029	3.784	3.319					
16	C	12.758	5.090	3.829					
17	C	13.441	5.590	4.948					
18	H	14.949	5.196	6.463					
19	H	15.470	2.910	5.590					
20	H	14.304	2.019	3.630					
21	H	13.215	6.591	5.320					
22	P	12.149	3.208	1.873					
23	C	9.835	3.195	3.497					
24	C	10.432	2.881	2.247					
25	C	9.614	2.237	1.269					
26	C	8.267	1.941	1.529					
27	C	7.694	2.273	2.773					
28	C	8.483	2.898	3.754					
29	H	10.406	3.666	4.301					
30	H	6.646	2.044	2.973					
31	H	8.050	3.153	4.722					
32	H	7.662	1.451	0.765					
33	H	12.011	5.736	3.356					
34	H	10.019	1.957	0.292					
35	C	11.377	6.106	-0.969					
36	C	11.202	5.072	-0.030					
37	C	12.311	4.504	0.652					
38	C	13.605	5.035	0.362					
39	C	13.775	6.067	-0.573					

Tetraphenylphosphoranyl ($Ph_4P^{\bullet}$).

Total energy (kcal/mol) = −80325.9 (MNDO/d); −795186.5 (6-31G(d,p)); −795205.4 (DZVP)

atom	atom	X	Y	Z	atom	atom	X	Y	Z
1	C	11.861	-0.445	4.173	40	C	11.919	3.061	-2.681
2	C	11.656	0.871	3.693	41	H	10.563	1.382	-2.427
3	C	12.310	1.333	2.516	42	H	10.639	1.417	0.038
4	C	13.185	0.440	1.843	43	H	13.363	4.835	-0.136
5	C	13.393	-0.877	2.321	44	H	13.270	4.759	-2.593
6	C	12.730	-1.323	3.487	45	H	11.878	3.040	-3.769
7	H	11.348	-0.782	5.074					
8	H	10.982	1.522	4.255					
9	H	13.719	0.745	0.941					
10	H	14.066	-1.548	1.788					
11	H	12.889	-2.336	3.854					
12	C	15.765	4.963	4.021					
13	C	15.900	4.275	2.795					
14	C	14.764	3.732	2.151					
15	C	13.460	3.879	2.706					
16	C	13.348	4.556	3.959					
17	C	14.486	5.097	4.603					
18	H	16.641	5.382	4.515					
19	H	16.885	4.157	2.343					
20	H	14.923	3.190	1.217					
21	H	14.372	5.617	5.554					
22	P	11.965	3.114	2.001					
23	C	9.324	3.942	2.582					
24	C	10.612	4.409	2.196					
25	C	10.774	5.800	1.953					
26	C	9.689	6.697	2.099					
27	C	8.419	6.218	2.489					
28	C	8.237	4.838	2.730					
29	H	9.144	2.881	2.770					
30	H	7.584	6.908	2.603					
31	H	7.260	4.461	3.029					
32	H	9.835	7.760	1.910					
33	H	12.381	4.670	4.455					
34	H	11.740	6.209	1.649					
35	C	11.180	2.126	-1.923					
36	C	11.236	2.151	-0.510					
37	C	12.043	3.106	0.181					
38	C	12.760	4.054	-0.602					
39	C	12.705	4.027	-2.016					

Trimethyl phosphite ($P(OMe)_3$).

Total energy (kcal/mol) = −37244.5 (MNDO/d); −430801.1 (6-31G(d,p)); −430824.0 (DZVP)

atom	atom	X	Y	Z
1	P	-0.983	-0.448	0.771
2	O	0.430	-1.271	0.880
3	O	-0.501	1.003	0.114
4	O	-1.773	-1.125	-0.543
5	C	1.570	-1.514	0.100
6	C	-2.845	-2.019	-0.589
7	C	-1.197	2.193	-0.123
8	H	2.141	-2.344	0.584
9	H	1.316	-1.824	-0.943
10	H	2.230	-0.614	0.050
11	H	-3.157	-2.129	-1.656
12	H	-2.564	-3.030	-0.202
13	H	-3.727	-1.656	-0.005
14	H	-0.447	2.992	-0.336
15	H	-1.878	2.107	-1.006
16	H	-1.807	2.514	0.758

Trimethoxyphenylphosphonium ($PhP^{+}(OMe)_3$).

Total energy (kcal/mol) = −56411.6 (MNDO/d); −575940.3 (6-31G(d,p)); −575963.7 (DZVP)

atom	atom	X	Y	Z
1	P	-2.118	-1.293	-0.023
2	O	-3.571	-1.937	0.200
3	O	-1.123	-1.976	1.044
4	O	-1.616	-1.766	-1.475
5	C	-0.977	-2.213	2.442
6	C	-0.486	-1.760	-2.344
7	C	-4.630	-2.629	-0.460
8	H	0.059	-2.597	2.591
9	H	-1.117	-1.270	3.020
10	H	-0.787	-2.322	-3.258
11	H	-0.214	-0.714	-2.616
12	H	-5.459	-2.714	0.280
13	H	-4.976	-2.057	-1.352
14	C	-2.140	3.311	0.381
15	C	-0.932	2.588	0.462
16	C	-0.935	1.191	0.342
17	C	-2.152	0.470	0.139
18	C	-3.359	1.221	0.056
19	C	-3.350	2.623	0.177
20	H	-2.136	4.398	0.475
21	H	0.009	3.118	0.618
22	H	0.026	0.670	0.409
23	H	-4.324	0.733	-0.104
24	H	-4.288	3.176	0.112
25	H	-4.291	-3.644	-0.769
26	H	0.383	-2.263	-1.860
27	H	-1.716	-2.975	2.780

Trimethoxyphenylphosphoranyl ($PhP^{\bullet}(OMe)_3$).

Total energy (kcal/mol) = −56541.2 (MNDO/d); −576002.3 (6-31G(d,p)); −576030.9 (DZVP)

atom	atom	X	Y	Z
1	P	-2.015	-1.480	-0.314
2	O	-3.447	-2.193	0.182
3	O	-0.842	-2.070	0.702
4	O	-1.348	-1.657	-1.826
5	C	-0.742	-2.724	1.932
6	C	-0.279	-1.391	-2.678
7	C	-4.753	-2.084	0.640
8	H	0.337	-2.755	2.220
9	H	-1.305	-2.195	2.740
10	H	-0.573	-1.660	-3.723
11	H	0.007	-0.310	-2.664
12	H	-4.836	-1.377	1.503
13	H	-5.439	-1.726	-0.168
14	C	-2.434	3.157	0.357
15	C	-1.516	2.432	1.148
16	C	-1.367	1.035	0.972
17	C	-2.134	0.330	0.004
18	C	-3.051	1.083	-0.791
19	C	-3.201	2.478	-0.616
20	H	-2.548	4.232	0.494
21	H	-0.918	2.949	1.898
22	H	-0.639	0.523	1.603
23	H	-3.659	0.595	-1.558
24	H	-3.909	3.029	-1.234
25	H	-5.109	-3.088	0.979
26	H	0.621	-1.993	-2.402
27	H	-1.120	-3.774	1.868

Dimethyl phenylphosphinite ($PhP(OMe)_2$).

Total energy (kcal/mol) = −45171.0 (MNDO/d); −503857.3 (6-31G(d,p)); −503857.9 (DZVP)

atom	atom	X	Y	Z
1	P	-0.769	0.160	-0.422
2	O	-1.376	0.239	-1.967
3	O	-2.037	-0.587	0.375
4	C	-1.237	-0.724	-2.978
5	C	-1.965	-1.364	1.537
6	H	-1.568	-0.254	-3.936
7	H	-0.180	-1.068	-3.106
8	H	-1.876	-1.622	-2.791
9	H	-1.755	-0.743	2.443
10	H	-2.957	-1.858	1.677
11	H	-1.185	-2.164	1.475
12	C	-0.869	1.903	0.089
13	C	0.331	2.497	0.558
14	C	0.351	3.839	0.980
15	C	-0.824	4.609	0.939
16	C	-2.020	4.034	0.476
17	C	-2.045	2.691	0.053
18	H	1.262	1.922	0.598
19	H	1.281	4.283	1.338
20	H	-0.808	5.649	1.266
21	H	-2.933	4.630	0.442
22	H	-2.991	2.275	-0.304

Dimethoxydiphenylphosphonium ($Ph_2P^+(OMe)_2$).

Total energy (kcal/mol) = −64337.5 (MNDO/d); −648995.8 (6-31G(d,p)); −649015.7 (DZVP)

atom	atom	X	Y	Z
1	C	6.475	-0.826	-2.390
2	C	5.123	-1.311	-2.390
3	C	4.834	-2.682	-2.390
4	C	5.878	-3.629	-2.390
5	C	7.209	-3.183	-2.390
6	C	7.501	-1.805	-2.390
7	H	4.272	-0.621	-2.390
8	H	3.795	-3.018	-2.390
9	H	5.652	-4.697	-2.391
10	H	8.027	-3.905	-2.390
11	H	8.556	-1.534	-2.390
12	P	6.665	0.947	-2.390
13	O	5.821	1.544	-1.143
14	O	5.821	1.544	-3.637
15	C	5.830	1.537	0.279
16	C	5.830	1.538	-5.058
17	H	4.960	2.152	0.605
18	H	5.723	0.498	0.669
19	H	6.774	1.985	0.669
20	H	4.959	2.153	-5.384
21	H	6.773	1.986	-5.449
22	H	5.722	0.499	-5.449
23	C	8.273	1.717	-2.390
24	C	8.280	3.153	-2.390
25	C	9.476	3.883	-2.390
26	C	10.717	3.215	-2.390
27	C	10.740	1.811	-2.390
28	C	9.539	1.076	-2.390
29	H	7.346	3.726	-2.390
30	H	9.446	4.974	-2.390
31	H	11.649	3.783	-2.390
32	H	11.694	1.280	-2.391
33	H	9.635	-0.009	-2.391

Dimethoxydiphenylphosphoranyl ($Ph_2P^{\bullet}(OMe)_2$).

Total energy (kcal/mol) = −64461.2 (MNDO/d); −649065.0 (6-31G(d,p)); −649092.0 (DZVP)

atom	atom	X	Y	Z
1	C	6.301	-0.962	-2.390
2	C	4.945	-1.394	-2.390
3	C	4.618	-2.771	-2.390
4	C	5.642	-3.745	-2.390
5	C	6.994	-3.334	-2.390
6	C	7.317	-1.955	-2.390
7	H	4.124	-0.673	-2.390
8	H	3.573	-3.081	-2.390
9	H	5.391	-4.805	-2.390
10	H	7.789	-4.079	-2.390
11	H	8.374	-1.680	-2.390
12	P	6.777	0.868	-2.390
13	O	5.889	1.495	-1.139
14	O	5.889	1.496	-3.641
15	C	6.005	1.413	0.256
16	C	6.005	1.414	-5.035
17	H	5.168	2.005	0.698
18	H	5.925	0.360	0.622
19	H	6.971	1.840	0.622
20	H	5.167	2.006	-5.477
21	H	6.970	1.841	-5.402
22	H	5.924	0.361	-5.402
23	C	8.344	1.926	-2.390
24	C	8.298	3.349	-2.390
25	C	9.488	4.116	-2.390
26	C	10.747	3.475	-2.390
27	C	10.811	2.064	-2.390
28	C	9.619	1.299	-2.390
29	H	7.345	3.883	-2.390
30	H	9.432	5.205	-2.390
31	H	11.663	4.066	-2.390
32	H	11.778	1.562	-2.390
33	H	9.711	0.212	-2.390

Tris(2,2,2-trifluoroethyl) phosphite ($P(OTfe)_3$).

Total energy (kcal/mol) = −144662.7 (MNDO/d); −1065036.0 (6-31G(d,p)); −1065227.1 (DZVP)

atom	atom	X	Y	Z
1	P	3.735	4.667	5.914
2	O	2.930	6.104	5.891
3	O	2.526	3.575	5.553
4	O	4.602	4.633	4.471
5	C	2.451	2.218	5.271
6	C	0.890	1.784	5.313
7	C	5.865	5.058	4.089
8	C	6.229	4.354	2.676
9	C	1.881	6.765	5.257
10	C	2.036	8.351	5.543
11	H	2.850	1.982	4.252
12	H	3.005	1.598	6.021
13	F	0.749	0.467	5.016
14	F	0.324	1.964	6.530
15	F	0.127	2.462	4.423
16	H	5.900	6.168	3.944
17	H	6.656	4.775	4.831
18	F	7.466	4.723	2.257
19	F	6.237	3.001	2.747
20	F	5.373	4.687	1.681
21	H	1.884	6.607	4.149
22	H	0.893	6.430	5.661
23	F	1.971	8.664	6.858
24	F	3.203	8.860	5.077
25	F	1.045	9.049	4.933

Tris(2,2,2-trifluoroethoxy)phenylphosphonium ($PhP^{+}(OTfe)_3$).

Total energy (kcal/mol) = −163804.7 (MNDO/d); −1210158.2 (6-31G(d,p)); −1210347.4 (DZVP)

atom	atom	X	Y	Z
1	P	-1.244	-0.390	0.059
2	O	-1.043	1.197	-0.198
3	O	-0.559	-1.160	-1.180
4	O	-0.339	-0.729	1.354
5	C	0.518	-1.979	-1.601
6	C	0.446	-2.070	-3.218
7	C	-0.006	-0.360	2.678
8	C	0.924	-1.542	3.284
9	C	-1.269	2.250	-1.113
10	C	-0.899	3.633	-0.353
11	H	1.496	-1.535	-1.294
12	H	0.419	-3.002	-1.161
13	F	1.473	-2.808	-3.692
14	F	-0.699	-2.647	-3.646
15	F	0.520	-0.851	-3.799
16	H	0.562	0.603	2.679
17	H	-0.925	-0.251	3.303
18	F	1.304	-1.241	4.544
19	F	0.273	-2.727	3.328
20	F	2.047	-1.732	2.555
21	H	-0.613	2.131	-2.010
22	H	-2.338	2.276	-1.437
23	F	-1.099	4.688	-1.172
24	F	-1.664	3.825	0.748
25	F	0.391	3.668	0.048
26	C	-5.661	-1.553	0.650
27	C	-5.145	-0.371	1.225
28	C	-3.802	-0.021	1.038
29	C	-2.925	-0.845	0.260
30	C	-3.467	-2.039	-0.304
31	C	-4.817	-2.382	-0.111
32	H	-6.709	-1.821	0.798
33	H	-5.797	0.273	1.820
34	H	-3.444	0.902	1.506
35	H	-2.851	-2.720	-0.899
36	H	-5.209	-3.299	-0.556

Tris(2,2,2-trifluoroethoxy)phenylphosphoranyl ($PhP^{\bullet}(OTfe)_3$).

Total energy (kcal/mol) = −163963.6 (MNDO/d); −1210244.0 (6-31G(d,p)); −1210441.6 (DZVP)

atom	atom	X	Y	Z
1	P	-1.064	-0.480	0.086
2	O	-0.822	1.172	-0.008
3	O	-0.618	-1.110	-1.413
4	O	-0.347	-0.962	1.525
5	C	-0.869	-1.954	-2.474
6	C	0.074	-1.541	-3.726
7	C	-0.310	-0.897	2.906
8	C	0.624	-2.095	3.469
9	C	0.103	2.057	-0.543
10	C	-0.096	3.498	0.174
11	H	-0.640	-3.017	-2.208
12	H	-1.934	-1.898	-2.816
13	F	-0.149	-2.350	-4.793
14	F	-0.146	-0.275	-4.158
15	F	1.397	-1.629	-3.451
16	H	0.125	0.074	3.256
17	H	-1.327	-1.009	3.361
18	F	0.675	-2.074	4.826
19	F	0.170	-3.326	3.127
20	F	1.905	-2.020	3.038
21	H	1.159	1.727	-0.371
22	H	-0.052	2.193	-1.643
23	F	0.804	4.398	-0.295
24	F	-1.321	4.033	-0.043
25	F	0.075	3.450	1.517
26	C	-5.669	-1.162	0.560
27	C	-5.199	0.126	0.229
28	C	-3.811	0.367	0.082
29	C	-2.863	-0.678	0.267
30	C	-3.360	-1.978	0.596
31	C	-4.745	-2.215	0.741
32	H	-6.737	-1.345	0.674
33	H	-5.905	0.944	0.085
34	H	-3.500	1.380	-0.179
35	H	-2.679	-2.821	0.742
36	H	-5.099	-3.214	0.995

Tris(2-chloroethyl) phosphite ($P(OC_2H_4Cl)_3$).

Total energy (kcal/mol) = −65407.4 (MNDO/d); −1369846.1 (6-31G(d,p)); −1369817.7 (DZVP)

atom	atom	X	Y	Z
1	P	1.439	5.193	7.339
2	O	1.400	5.018	8.969
3	O	1.244	3.636	6.744
4	O	-0.070	5.825	7.015
5	C	2.157	2.789	6.099
6	C	1.422	1.470	5.719
7	C	-0.624	6.366	5.843
8	C	-2.002	6.996	6.197
9	C	0.542	4.518	9.968
10	C	1.284	4.599	11.333
11	H	2.569	3.279	5.176
12	H	3.030	2.563	6.768
13	H	1.044	0.929	6.615
14	H	0.574	1.649	5.020
15	Cl	2.555	0.367	4.886
16	H	0.056	7.145	5.404
17	H	-0.755	5.566	5.066
18	H	-2.719	6.241	6.590
19	H	-1.907	7.823	6.936
20	Cl	-2.738	7.697	4.727
21	H	-0.404	5.119	10.005
22	H	0.253	3.456	9.747
23	H	2.210	3.982	11.345
24	H	1.544	5.647	11.607
25	Cl	0.226	3.972	12.631

Tris(2-chloroethoxy)phenylphosphonium ($PhP^{+}(OC_2H_4Cl)_3$).

Total energy (kcal/mol) = −84565.7 (MNDO/d); −1514975.7 (6-31G(d,p)); −1514948.5 (DZVP)

atom	atom	X	Y	Z
1	P	-0.383	0.095	-0.077
2	O	0.884	1.060	-0.333
3	O	-0.366	-1.008	-1.246
4	O	-0.075	-0.683	1.299
5	C	-0.404	-2.422	-1.480
6	C	-0.345	-2.662	-3.016
7	C	0.112	-0.459	2.700
8	C	0.513	-1.808	3.362
9	C	1.436	1.927	-1.330
10	C	2.764	2.519	-0.779
11	H	0.469	-2.897	-0.963
12	H	-1.345	-2.837	-1.038
13	Cl	-0.420	-4.412	-3.328
14	H	-1.204	-2.189	-3.544
15	H	0.604	-2.282	-3.458
16	H	0.909	0.315	2.845
17	H	-0.845	-0.066	3.131
18	Cl	0.734	-1.551	5.108
19	H	-0.277	-2.584	3.233
20	H	1.473	-2.200	2.955
21	H	1.614	1.338	-2.266
22	H	0.695	2.736	-1.559
23	Cl	3.455	3.618	-1.995
24	H	2.602	3.108	0.152
25	H	3.519	1.724	-0.576
26	C	-4.342	2.472	0.107
27	C	-3.182	2.956	0.747
28	C	-1.984	2.230	0.683
29	C	-1.907	0.992	-0.028
30	C	-3.093	0.521	-0.662
31	C	-4.291	1.254	-0.594
32	H	-5.273	3.040	0.158
33	H	-3.216	3.900	1.294
34	H	-1.109	2.642	1.195
35	H	-3.106	-0.421	-1.217
36	H	-5.186	0.872	-1.090

Tris(2-chloroethoxy)phenylphosphoranyl ($PhP^{\bullet}(OC_2H_4Cl)_3$).

Total energy (kcal/mol) = −84705.3 (MNDO/d); −1515048.9 (6-31G(d,p)); −1515026.4 (DZVP)

atom	atom	X	Y	Z
1	P	-0.111	0.156	0.003
2	O	1.024	1.219	-0.589
3	O	-0.225	-1.013	-1.176
4	O	0.074	-0.631	1.469
5	C	-0.499	-2.381	-1.304
6	C	-0.341	-2.782	-2.800
7	C	-0.449	-0.999	2.710
8	C	0.637	-1.758	3.525
9	C	1.371	2.131	-1.592
10	C	2.796	2.688	-1.308
11	H	0.203	-2.983	-0.669
12	H	-1.541	-2.607	-0.950
13	Cl	-0.711	-4.519	-3.000
14	H	-1.041	-2.225	-3.462
15	H	0.700	-2.628	-3.165
16	H	-0.788	-0.091	3.276
17	H	-1.353	-1.651	2.570
18	Cl	-0.023	-2.242	5.116
19	H	0.966	-2.693	3.018
20	H	1.529	-1.124	3.727
21	H	1.345	1.632	-2.597
22	H	0.628	2.972	-1.624
23	Cl	3.252	3.865	-2.575
24	H	2.850	3.226	-0.335
25	H	3.569	1.887	-1.321
26	C	-4.137	2.569	0.202
27	C	-3.034	2.902	1.020
28	C	-1.837	2.156	0.936
29	C	-1.712	1.053	0.036
30	C	-2.833	0.741	-0.782
31	C	-4.032	1.488	-0.699
32	H	-5.061	3.144	0.266
33	H	-3.104	3.738	1.716
34	H	-1.005	2.450	1.582
35	H	-2.802	-0.080	-1.500
36	H	-4.877	1.226	-1.336

Benzyl diethyl phosphite ($BnOP(OEt)_2$).

Total energy (kcal/mol) = −63436.7 (MNDO/d); −625013.0 (6-31G(d,p)); −625045.4 (DZVP)

atom	atom	X	Y	Z
1	C	3.510	10.244	6.241
2	C	4.154	11.237	5.482
3	C	5.531	11.136	5.175
4	C	6.242	10.007	5.646
5	C	5.598	9.015	6.406
6	C	4.230	9.131	6.706
7	H	2.448	10.340	6.468
8	H	3.571	12.089	5.129
9	H	7.304	9.891	5.424
10	H	6.164	8.153	6.761
11	H	3.731	8.361	7.295
12	P	6.696	12.484	1.569
13	O	6.683	14.139	1.759
14	O	8.342	12.182	1.668
15	O	6.086	11.959	2.996
16	C	9.107	11.188	1.041
17	C	10.602	11.371	1.376
18	C	6.235	12.225	4.373
19	C	6.942	15.174	0.846
20	C	6.536	16.533	1.451
21	H	8.778	10.166	1.370
22	H	8.972	11.221	-0.074
23	H	11.186	10.574	0.872
24	H	10.989	12.348	1.024
25	H	10.795	11.297	2.464
26	H	7.319	12.279	4.658
27	H	5.800	13.229	4.622
28	H	8.032	15.199	0.577
29	H	6.380	15.013	-0.114
30	H	6.753	17.335	0.716
31	H	5.454	16.575	1.689
32	H	7.101	16.760	2.377

Benzyldiethoxy(phenyl)phosphonium ($Ph(BnO)P^{+}(OEt)_2$).

Total energy (kcal/mol) = −82607.9 (MNDO/d); −770157.8 (6-31G(d,p)); −770191.1 (DZVP)

atom	atom	X	Y	Z
1	C	4.752	7.135	4.063
2	C	4.554	8.442	3.585
3	C	5.415	9.495	3.978
4	C	6.483	9.198	4.858
5	C	6.681	7.891	5.335
6	C	5.816	6.856	4.939
7	H	4.076	6.336	3.753
8	H	3.718	8.632	2.909
9	H	7.167	9.985	5.184
10	H	7.507	7.682	6.017
11	H	5.968	5.842	5.312
12	P	6.369	12.223	1.218
13	O	5.981	13.661	1.831
14	O	7.979	12.192	1.135
15	O	5.917	11.119	2.282
16	C	9.052	11.277	0.892
17	C	10.390	12.039	0.895
18	C	5.175	10.911	3.502
19	C	6.112	15.062	1.574
20	C	5.485	15.859	2.734
21	H	9.047	10.489	1.688
22	H	8.889	10.770	-0.093
23	H	11.207	11.312	0.711
24	H	10.430	12.809	0.099
25	H	10.583	12.534	1.867
26	H	5.508	11.666	4.258
27	H	4.093	11.105	3.289
28	H	7.196	15.318	1.463
29	H	5.599	15.304	0.609
30	H	5.593	16.940	2.513
31	H	4.405	15.639	2.851
32	H	5.990	15.653	3.698
33	C	3.887	10.966	-1.811
34	C	4.461	11.152	-0.540
35	C	5.625	11.954	-0.371
36	C	6.180	12.569	-1.535
37	C	5.602	12.381	-2.799
38	C	4.453	11.576	-2.943
39	H	2.996	10.344	-1.914
40	H	3.982	10.659	0.310
41	H	7.069	13.204	-1.469
42	H	6.045	12.859	-3.675
43	H	4.007	11.430	-3.929

Benzyldiethoxy(phenyl)phosphoranyl ($Ph(BnO)P^{\bullet}(OEt)_2$).

Total energy (kcal/mol) = −82735.3 (MNDO/d); −770212.0 (6-31G(d,p)); −770250.4 (DZVP)

atom	atom	X	Y	Z
1	C	4.565	7.277	4.171
2	C	4.456	8.569	3.608
3	C	5.368	9.600	3.965
4	C	6.398	9.295	4.899
5	C	6.507	8.003	5.461
6	C	5.591	6.990	5.099
7	H	3.855	6.501	3.886
8	H	3.656	8.762	2.893
9	H	7.119	10.058	5.193
10	H	7.302	7.789	6.175
11	H	5.675	5.994	5.533
12	P	6.672	12.334	1.272
13	O	6.124	13.802	1.859
14	O	8.284	11.998	1.050
15	O	6.140	11.159	2.319
16	C	9.238	11.066	0.628
17	C	10.658	11.665	0.670
18	C	5.235	11.001	3.379
19	C	5.348	14.948	1.684
20	C	5.421	15.872	2.916
21	H	9.200	10.152	1.278
22	H	9.012	10.721	-0.417
23	H	11.387	10.900	0.333
24	H	10.758	12.544	0.002
25	H	10.946	11.978	1.694
26	H	5.424	11.766	4.179
27	H	4.184	11.180	3.025
28	H	5.691	15.515	0.777
29	H	4.276	14.667	1.493
30	H	4.799	16.773	2.735
31	H	5.037	15.375	3.830
32	H	6.456	16.211	3.119
33	C	4.289	10.835	-1.854
34	C	4.878	11.009	-0.577
35	C	5.843	12.026	-0.344
36	C	6.204	12.860	-1.446
37	C	5.617	12.688	-2.720
38	C	4.655	11.674	-2.928
39	H	3.550	10.048	-2.005
40	H	4.565	10.329	0.217
41	H	6.949	13.652	-1.329
42	H	5.909	13.339	-3.544
43	H	4.201	11.541	-3.909

Tris(trimethylsilyl) phosphite ($P(OSiMe_3)_3$).

Total energy (kcal/mol) = −67022.0 (MNDO/d); −1126034.2 (6-31G(d,p)); −1126024.0 (DZVP)

atom	atom	X	Y	Z
1	P	-1.614	-0.245	-1.186
2	O	-0.295	0.671	-0.817
3	O	-1.155	-1.786	-0.827
4	O	-2.714	0.135	-0.019
5	Si	1.071	1.714	-0.682
6	Si	-4.026	0.597	1.000
7	Si	-0.750	-3.457	-0.699
8	C	2.044	1.262	0.874
9	C	2.169	1.504	-2.207
10	C	0.478	3.506	-0.567
11	C	-3.388	0.829	2.764
12	C	-4.764	2.220	0.368
13	C	-5.345	-0.757	0.969
14	C	0.855	-3.783	-1.644
15	C	-0.520	-3.900	1.124
16	C	-2.147	-4.495	-1.440
17	H	2.934	1.922	1.001
18	H	1.418	1.366	1.792
19	H	2.411	0.209	0.836
20	H	3.065	2.166	-2.154
21	H	2.534	0.454	-2.307
22	H	1.621	1.759	-3.145
23	H	1.338	4.211	-0.484
24	H	-0.110	3.801	-1.468
25	H	-0.172	3.666	0.325
26	H	-4.212	1.122	3.457
27	H	-2.935	-0.110	3.161
28	H	-2.608	1.625	2.816
29	H	-5.619	2.550	1.005
30	H	-4.010	3.041	0.369
31	H	-5.147	2.117	-0.676
32	H	-4.943	-1.729	1.339
33	H	-6.214	-0.488	1.615
34	H	-5.736	-0.926	-0.062
35	H	1.145	-4.859	-1.587
36	H	0.756	-3.521	-2.724
37	H	1.702	-3.187	-1.230
38	H	-0.249	-4.976	1.248
39	H	0.291	-3.295	1.593
40	H	-1.453	-3.722	1.710
41	H	-1.918	-5.585	-1.374
42	H	-3.112	-4.323	-0.907
43	H	-2.311	-4.252	-2.516

Tris(trimethylsilyloxy)phenylphosphonium ($PhP^{+}(OSiMe_3)_3$).

Total energy (kcal/mol) = −86198.5 (MNDO/d); −1271194.0 (6-31G(d,p)); −1271184.7 (DZVP)

atom	atom	X	Y	Z
1	P	-1.808	0.055	-1.271
2	O	-0.514	0.914	-0.928
3	O	-1.414	-1.486	-1.223
4	O	-2.906	0.339	-0.154
5	Si	0.958	1.883	-0.503
6	Si	-4.216	0.753	1.024
7	Si	-0.950	-3.233	-1.306
8	C	1.483	1.329	1.213
9	C	2.254	1.484	-1.802
10	C	0.437	3.687	-0.539
11	C	-3.377	0.978	2.689
12	C	-5.012	2.338	0.405
13	C	-5.414	-0.693	1.024
14	C	0.140	-3.425	-2.824
15	C	-0.031	-3.608	0.289
16	C	-2.547	-4.209	-1.451
17	H	2.393	1.890	1.537
18	H	0.689	1.515	1.974
19	H	1.734	0.243	1.244
20	H	3.199	2.041	-1.586
21	H	2.506	0.397	-1.821
22	H	1.927	1.773	-2.829
23	H	1.301	4.342	-0.269
24	H	0.083	4.004	-1.548
25	H	-0.381	3.900	0.189
26	H	-4.135	1.211	3.475
27	H	-2.835	0.057	3.011
28	H	-2.642	1.817	2.677
29	H	-5.828	2.657	1.099
30	H	-4.280	3.177	0.344
31	H	-5.466	2.211	-0.606
32	H	-4.919	-1.646	1.331
33	H	-6.246	-0.504	1.745
34	H	-5.874	-0.858	0.021
35	H	0.464	-4.489	-2.935
36	H	-0.394	-3.140	-3.761
37	H	1.063	-2.802	-2.757
38	H	0.274	-4.683	0.316
39	H	0.897	-2.997	0.391
40	H	-0.663	-3.418	1.189
41	H	-2.328	-5.304	-1.484
42	H	-3.226	-4.033	-0.583
43	H	-3.112	-3.956	-2.379
44	C	-4.219	0.083	-4.590
45	C	-3.665	-0.197	-3.331
46	C	-2.474	0.451	-2.883
47	C	-1.872	1.390	-3.765
48	C	-2.429	1.669	-5.026
49	C	-3.603	1.019	-5.444
50	H	-5.130	-0.427	-4.907
51	H	-4.177	-0.932	-2.702
52	H	-0.958	1.924	-3.492
53	H	-1.945	2.395	-5.682
54	H	-4.035	1.236	-6.423

Tris(trimethylsilyloxy)phenylphosphoranyl ($PhP^{\bullet}(OSiMe_3)_3$).

Total energy (kcal/mol) = −86320.0 (MNDO/d); −1271240.2 (6-31G(d,p)); −1271237.2 (DZVP)

atom	atom	X	Y	Z	atom	atom	X	Y	Z
1	P	-1.761	0.019	-1.139	40	H	-0.132	-3.555	0.985
2	O	-0.421	0.948	-0.832	41	H	-2.266	-5.411	-1.291
3	O	-1.376	-1.595	-1.211	42	H	-2.996	-4.172	-0.210
4	O	-2.992	0.365	-0.080	43	H	-3.264	-4.086	-1.987
5	Si	0.979	1.883	-0.444	44	C	-4.134	0.059	-4.569
6	Si	-4.301	0.794	0.961	45	C	-3.591	-0.227	-3.295
7	Si	-0.955	-3.260	-1.382	46	C	-2.422	0.439	-2.817
8	C	1.583	1.409	1.286	47	C	-1.822	1.402	-3.676
9	C	2.345	1.531	-1.705	48	C	-2.364	1.690	-4.952
10	C	0.541	3.723	-0.477	49	C	-3.521	1.020	-5.403
11	C	-3.622	1.174	2.684	50	H	-5.028	-0.465	-4.907
12	C	-5.184	2.320	0.275	51	H	-4.100	-0.978	-2.685
13	C	-5.519	-0.650	1.067	52	H	-0.926	1.950	-3.379
14	C	-0.184	-3.549	-3.085	53	H	-1.883	2.433	-5.588
15	C	0.288	-3.725	-0.035	54	H	-3.938	1.241	-6.385
16	C	-2.508	-4.325	-1.202					
17	H	2.489	1.994	1.571					
18	H	0.802	1.604	2.059					
19	H	1.851	0.328	1.344					
20	H	3.270	2.107	-1.468					
21	H	2.619	0.449	-1.719					
22	H	2.033	1.810	-2.739					
23	H	1.423	4.352	-0.210					
24	H	0.194	4.046	-1.486					
25	H	-0.272	3.962	0.250					
26	H	-4.442	1.441	3.392					
27	H	-3.082	0.297	3.114					
28	H	-2.907	2.031	2.663					
29	H	-6.028	2.629	0.936					
30	H	-4.491	3.189	0.190					
31	H	-5.607	2.127	-0.739					
32	H	-5.028	-1.570	1.463					
33	H	-6.372	-0.409	1.744					
34	H	-5.947	-0.901	0.068					
35	H	0.109	-4.617	-3.222					
36	H	-0.894	-3.290	-3.906					
37	H	0.734	-2.930	-3.228					
38	H	0.575	-4.801	-0.103					
39	H	1.224	-3.124	-0.116					