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Influence of Connector Groups on the Interactions of Substituents with Carbon-Centered Radicals

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Supporting Information

(Tables S1–S4. A total of 52 pages)

Full Details For References 15, 16 and 17

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Table S1. Calculated Bond Dissociation Energies (BDEs), Radical Stabilization Energies (RSEs, RSE_ws), Radical Connector Energies (RCEs), and Molecule Connector Energies (MCEs) for Species Related to CH_3WX and $^{\bullet}CH_2WX$ at the ROB2-PLYP/6-311+G(3df,2p)/UB3-LYP/6-31G(d) level (0 K, kJ mol^{-1})

#	X	W	BDE (CH_3WX)	RSE ($^{\bullet}CH_2WX$)	RSE_W ($^{\bullet}CH_2WX$)	RCE ($^{\bullet}CH_2WX$)	MCE (CH_3WX)
1	CF_3	NIL	430.2	–3.6	–3.6	0.0	0.0
2	CF_3	–CH=CH–	362.2	64.4	–3.8	9.6	9.9
3	CF_3	–C≡C–	377.3	49.3	–4.8	–14.3	–13.0
4	CF_3	–*p*-C_6H_4–	371.8	54.8	–1.3	9.4	7.1
5	CF_3	–*o*-C_6H_4–	373.5	53.1	–3.0	2.0	1.5
6	CF_3	–*m*-C_6H_4–	372.2	54.4	–1.7	8.2	6.3
7	CF_3	–CH_2–	416.6	10.0	–7.0	9.2	12.6
8	H	NIL	426.6	0.0	0.0	0.0	0.0
9	H	–CH=CH–	358.4	68.2	0.0	0.0	0.0
10	H	–C≡C–	372.5	54.1	0.0	0.0	0.0
11	H	–*p*-C_6H_4–	370.5	56.1	0.0	0.0	0.0
12	H	–*o*-C_6H_4–	370.5	56.1	0.0	0.0	0.0
13	H	–*m*-C_6H_4–	370.5	56.1	0.0	0.0	0.0
14	H	–CH_2–	409.6	17.0	0.0	0.0	0.0
15	CH_3	NIL	409.6	17.0	17.0	0.0	0.0
16	CH_3	–CH=CH–	355.9	70.7	2.6	8.3	22.7
17	CH_3	–C≡C–	368.5	58.1	3.9	20.4	33.4
18	CH_3	–*p*-C_6H_4–	368.7	57.9	1.8	7.8	23.0
19	CH_3	–*o*-C_6H_4–	369.9	56.7	0.6	5.3	21.7
20	CH_3	–*m*-C_6H_4–	370.0	56.6	0.5	7.3	23.7
21	CH_3	–CH_2–	412.8	13.8	–3.2	–9.6	10.6
22	CHO	NIL	390.3	36.3	36.3	0.0	0.0
23	CHO	–CH=CH–	350.5	76.2	8.0	7.9	36.2
24	CHO	–C≡C–	368.3	58.3	4.2	–16.1	16.0
25	CHO	–*p*-C_6H_4–	368.4	58.2	2.1	0.1	34.3
26	CHO	–*o*-C_6H_4–	371.6	55.0	–1.1	–14.4	23.0
27	CHO	–*m*-C_6H_4–	371.9	54.7	–1.4	–5.4	32.3
28	CHO	–CH_2–	416.7	9.9	–7.1	–31.5	11.9
29	NH_2	NIL	375.7	50.9	50.9	0.0	0.0
30	NH_2	–CH=CH–	344.4	82.2	14.1	9.7	46.5

#	X	W	BDE (CH_3WX)	RSE ($^{\bullet}CH_2WX$)	RSE_W ($^{\bullet}CH_2WX$)	RCE ($^{\bullet}CH_2WX$)	MCE (CH_3WX)
31	NH_2	–C≡C–	359.5	67.2	13.0	–4.6	33.3
32	NH_2	–*p*-C_6H_4–	364.5	62.1	6.0	5.4	50.3
33	NH_2	–*o*-C_6H_4–	368.9	57.7	1.6	3.5	52.7
34	NH_2	–*m*-C_6H_4–	370.7	55.9	–0.2	1.8	52.8
35	NH_2	–CH_2–	413.5	13.1	-3.9	–36.8	18.0
36	CH=CH_2	NIL	358.4	68.2	68.2	0.0	0.0
37	CH=CH_2	–CH=CH–	336.8	89.8	21.7	–6.9	39.6
38	CH=CH_2	–C≡C–	358.6	68.0	13.9	–15.9	38.3
39	CH=CH_2	–*p*-C_6H_4–	365.7	60.9	4.8	–32.0	31.3
40	CH=CH_2	–*o*-C_6H_4–	370.4	56.3	0.1	–43.0	25.0
41	CH=CH_2	–*m*-C_6H_4–	370.8	55.8	–0.3	–37.5	30.9
42	CH=CH_2	–CH_2–	412.5	14.1	–2.9	–61.3	9.7

Table S2. G3X(MP2)-RAD and ROB2−PLYP/6-311+G(3df,2p) Total Energies of Substituted Methanes (CH_3WX) and Substituted Methyl Radicals ($^{\bullet}CH_2WX$) in Hartrees (0 K)

			G3X(MP2)-RAD		ROB2-PLYP/6-311+G(3df,2p)	
#	X	W	(CH_3WX)	($^{\bullet}CH_2WX$)	(CH_3WX)	($^{\bullet}CH_2WX$)
1	CF_3	NIL	-377.16972	-376.50175	-377.44273	-376.78012
2	CF_3	–CH=CH–	-454.42398	-453.78474	-454.76417	-454.12744
3	CF_3	–C≡C–	-453.18703	-452.53975	-453.53708	-452.89461
4	CF_3	–*p*-C_6H_4–	-607.82195	-607.17666	-608.30568	-607.66533
5	CF_3	–*o*-C_6H_4–	-607.82062	-607.17684	-608.30353	-607.66251
6	CF_3	–*m*-C_6H_4–	-607.82180	-607.17858	-608.30537	-607.66485
7	CF_3	–CH_2–	-416.40428	-415.74196	-416.70634	-416.04891
8	H	NIL	-40.42170	-39.75649	-40.44399	-39.78275
9	H	–CH=CH–	-117.67293	-117.03480	-117.76167	-117.12639
10	H	–C≡C–	-116.44525	-115.80019	-116.54331	-115.90269
11	H	–*p*-C_6H_4–	-271.07059	-270.42793	-271.30424	-270.66437
12	H	–*o*-C_6H_4–	-271.07059	-270.42793	-271.30424	-270.66437
13	H	–*m*-C_6H_4–	-271.07059	-270.42793	-271.30424	-270.66437
14	H	–CH_2–	-79.65086	-78.99118	-79.70279	-79.04802
15	CH_3	NIL	-79.65086	-78.99118	-79.70279	-79.04802
16	CH_3	–CH=CH–	-156.91095	-156.27322	-157.02913	-156.39483
17	CH_3	–C≡C–	-155.68634	-155.04229	-155.81484	-155.17571
18	CH_3	–*p*-C_6H_4–	-310.30969	-309.66750	-310.57179	-309.93262
19	CH_3	–*o*-C_6H_4–	-310.30969	-309.66732	-310.57133	-309.93167
20	CH_3	–*m*-C_6H_4–	-310.30994	-309.66742	-310.57209	-309.93242
21	CH_3	–CH_2–	-118.88478	-118.22385	-118.96562	-118.30964
22	CHO	NIL	-153.60054	-152.94904	-153.71908	-153.07167
23	CHO	–CH=CH–	-230.86486	-230.22850	-231.05054	-230.41831
24	CHO	–C≡C–	-229.62938	-228.98470	-229.82451	-229.18549
25	CHO	–*p*-C_6H_4–	-384.26267	-383.62095	-384.59241	-383.95333
26	CHO	–*o*-C_6H_4–	-384.25925	-383.61598	-384.58810	-383.94781
27	CHO	–*m*-C_6H_4–	-384.26231	-383.61920	-384.59164	-383.95123
28	CHO	–CH_2–	-192.83502	-192.17279	-192.98241	-192.32493
29	NH_2	NIL	-95.68653	-95.03853	-95.74969	-95.10784
30	NH_2	–CH=CH–	-172.95440	-172.31950	-173.08509	-172.45517
31	NH_2	–C≡C–	-171.72074	-171.07927	-171.86167	-171.22601

			G3X(MP2)-RAD		ROB2-PLYP/6-311+G(3df,2p)	
#	X	W	(CH_3WX)	($^{\bullet}CH_2WX$)	(CH_3WX)	($^{\bullet}CH_2WX$)
32	NH_2	–*p*-C_6H_4–	-326.35424	-325.71338	-326.62911	-326.12063
33	NH_2	–*o*-C_6H_4–	-326.35570	-325.71342	-326.63003	-325.99078
34	NH_2	–*m*-C_6H_4–	-326.35506	-325.71226	-326.63006	-325.99013
35	NH_2	–CH_2–	-134.92319	-134.26215	-135.01533	-134.35908
36	$CH=CH_2$	NIL	-117.67293	-117.03480	-117.76167	-117.12639
37	$CH=CH_2$	–CH=CH–	-194.93870	-194.30835	-195.09442	-194.46740
38	$CH=CH_2$	–C≡C–	-193.70958	-193.06998	-193.87560	-193.24025
39	$CH=CH_2$	–*p*-C_6H_4–	-348.33452	-347.69172	-348.63385	-347.99581
40	$CH=CH_2$	–*o*-C_6H_4–	-348.33302	-347.69039	-348.63145	-347.99163
41	$CH=CH_2$	–*m*-C_6H_4–	-348.33456	-347.69180	-348.63370	-347.99373
42	$CH=CH_2$	–CH_2–	-156.90653	-156.24596	-157.02418	-156.36832

Table S3. Optimized UB3-LYP/6-31G(d) Geometries of Substituted Methanes X-W-CH_3 and Substituted Methyl Radicals X-W-$CH_2^{\bullet}$ (Å)

CF_3-CC-CH_3

6	0.000000	0.000000	0.538291
6	0.000000	0.000000	1.745015
6	0.000000	0.000000	3.202355
1	-0.852993	-0.566451	3.593115
1	0.917057	-0.455488	3.593115
1	-0.064064	1.021939	3.593115
6	0.000000	0.000000	-0.919462
9	0.258470	1.229663	-1.413946
9	0.935684	-0.838673	-1.413946
9	-1.194154	-0.390990	-1.413946

CF_3-CH_2-CH_3

6	1.136458	0.258214	0.000000
1	1.454339	0.824126	0.882095
1	1.454339	0.824126	-0.882095
6	1.741335	-1.147860	0.000000
1	1.428721	-1.708355	-0.886205
1	2.833738	-1.089875	0.000000
1	1.428721	-1.708355	0.886205
6	-0.375415	0.249664	0.000000
9	-0.874597	-0.380983	-1.088560
9	-0.874597	-0.380983	1.088560
9	-0.874597	1.506214	0.000000

CF_3-CH=CH-CH_3

6	1.567957	0.310463	-0.000082
6	0.516283	-0.508468	-0.000207
1	1.389661	1.384304	0.000516
1	0.622787	-1.590580	-0.000382
6	-0.898561	-0.031275	-0.000040
6	2.999111	-0.133093	-0.000013
1	3.526591	0.258297	-0.879584
1	3.526008	0.256876	0.880560
1	3.089705	-1.223685	-0.000820
9	-0.999321	1.315551	0.000050
9	-1.570377	-0.486254	1.085462
9	-1.570691	-0.486072	-1.085317

CF_3-*m*-C_6H_4-CH_3

6	0.306192	0.198030	-0.036331
6	-0.689300	-0.782137	-0.016950
6	-0.034296	1.552126	-0.028358
6	-2.042417	-0.428871	0.008919
1	-0.406137	-1.830735	-0.028230
6	-1.380166	1.914272	0.000616
1	0.742999	2.308392	-0.048323
6	-2.371528	0.933659	0.021356
1	-1.656912	2.964834	0.008091
1	-3.418189	1.228509	0.046790
6	-3.120111	-1.487827	-0.004763
1	-3.449123	-1.704719	-1.029667
1	-2.764583	-2.427885	0.429120
1	-4.003004	-1.166736	0.558107
6	1.753204	-0.212697	-0.002114
9	1.964874	-1.374492	-0.661732
9	2.557464	0.720763	-0.558693
9	2.191604	-0.400826	1.265966

CF_3-*o*-C_6H_4-CH_3

6	-0.058640	-0.250969	-0.006954
6	-0.752861	0.977775	0.001877
6	-0.751387	-1.463990	-0.009366
6	-2.151134	0.930332	0.008097
6	-2.145401	-1.483594	-0.004898
1	-0.194088	-2.393668	-0.014985
6	-2.846049	-0.280026	0.004145
1	-2.674435	-2.432093	-0.007152
1	-3.932741	-0.278292	0.009394
1	-2.704939	1.865819	0.016547
6	-0.047974	2.316097	-0.008908
1	0.713069	2.378408	0.774415
1	0.461035	2.489032	-0.963403
1	-0.765123	3.127338	0.144587
6	1.449101	-0.276857	0.000477
9	1.961047	0.274691	1.129952
9	1.942951	-1.531392	-0.076445
9	1.976368	0.415685	-1.038643

CF_3-*p*-C_6H_4-CH_3

6	2.412375	-0.000013	0.012886
6	1.692494	1.202383	0.001664

6	1.692499	-1.202400	0.001665
6	0.299916	1.208121	-0.024320
1	2.229872	2.147620	0.011990
6	0.299908	-1.208141	-0.024323
1	2.229875	-2.147635	0.011990
6	-0.401336	-0.000016	-0.037957
1	-0.242380	2.148063	-0.037636
1	-0.242382	-2.148087	-0.037642
6	-1.903721	-0.000005	-0.001731
6	3.922758	0.000014	0.008172
1	4.313949	0.000935	-1.017923
1	4.325270	0.886085	0.509969
1	4.325283	-0.886919	0.508420
9	-2.377418	-0.000103	1.267971
9	-2.423989	1.090471	-0.609752
9	-2.424020	-1.090338	-0.609943

CH_3-CC-CH_3

6	0.604601	-0.002282	0.003572
6	-0.604597	-0.000239	0.000980
6	-2.066187	0.000514	-0.001000
1	-2.468015	-0.291385	0.977359
1	-2.465361	0.994640	-0.238086
1	-2.465635	-0.700985	-0.744107
6	2.066185	0.000770	-0.001327
1	2.462956	0.994354	-0.244649
1	2.470870	-0.285130	0.977632
1	2.465173	-0.704074	-0.741499

CH_3-CH_2-CH_3

6	0.000000	0.000000	0.586502
1	0.877607	0.000000	1.247354
1	-0.877607	0.000000	1.247354
6	0.000000	1.277193	-0.259856
1	-0.884678	1.321887	-0.907445
1	0.000000	2.176504	0.367166
1	0.884678	1.321887	-0.907445
6	0.000000	-1.277193	-0.259856
1	0.000000	-2.176504	0.367166
1	-0.884678	-1.321887	-0.907445
1	0.884678	-1.321887	-0.907445

CH_3-CH=CH-CH_3

6	0.538139	-0.395334	-0.000188
6	-0.538139	0.395334	0.000188
1	0.392537	-1.477694	0.000275
1	-0.392537	1.477694	-0.000275
6	-1.963573	-0.079229	0.000005
1	-2.023082	-1.173062	0.001196
1	-2.508334	0.290133	0.879609
1	-2.507423	0.288089	-0.881115
6	1.963573	0.079229	-0.000005
1	2.507423	-0.288089	0.881115
1	2.508334	-0.290133	-0.879609
1	2.023082	1.173062	-0.001196

CH_3-*m*-C_6H_4-CH_3

6	-1.224869	-0.270994	0.012214
6	0.000000	-0.949255	0.000000
6	-1.209617	1.129426	0.016139
6	1.224869	-0.270994	-0.012214
1	0.000000	-2.038309	0.000000
6	0.000000	1.823483	0.000000
1	-2.149331	1.677398	0.029189
6	1.209617	1.129426	-0.016139
1	0.000000	2.910717	0.000000
1	2.149331	1.677398	-0.029189
6	2.531145	-1.031729	0.008302
1	2.907330	-1.150991	1.033391
1	2.418417	-2.035525	-0.414894
1	3.307963	-0.509988	-0.561515
6	-2.531145	-1.031729	-0.008302
1	-2.907330	-1.150990	-1.033391
1	-2.418417	-2.035525	0.414893
1	-3.307963	-0.509988	0.561516

CH_3-*o*-C_6H_4-CH_3

6	-0.477757	-0.705977	-0.000242
6	-0.477743	0.705980	-0.000201
6	0.746145	-1.384160	-0.000029
6	0.746162	1.384146	-0.000103
6	1.960734	-0.696586	0.000064
1	0.744924	-2.472131	0.000019
6	1.960740	0.696558	0.000048
1	2.897458	-1.247827	0.000363
1	2.897469	1.247789	0.000286
1	0.744957	2.472117	-0.000187

6	-1.774941	1.480588	0.000096
1	-2.389632	1.247186	-0.879226
1	-2.387839	1.248983	0.881254
1	-1.589890	2.559142	-0.001091
6	-1.774988	-1.480558	0.000045
1	-2.388668	-1.247771	0.880305
1	-2.388924	-1.248312	-0.880158
1	-1.589969	-2.559113	0.000372

CH_3-*p*-C_6H_4-CH_3

6	-0.000957	1.421810	0.000000
6	0.000957	0.697284	1.198358
6	0.000957	0.697284	-1.198358
6	-0.000957	-0.697284	1.198358
1	0.001335	1.232145	2.146209
6	-0.000957	-0.697284	-1.198358
1	0.001335	1.232145	-2.146209
6	0.000957	-1.421810	0.000000
1	-0.001335	-1.232145	2.146209
1	-0.001335	-1.232145	-2.146209
6	0.034379	-2.932955	0.000000
1	1.066060	-3.310705	0.000000
1	-0.460815	-3.345556	0.886005
1	-0.460815	-3.345556	-0.886005
6	-0.034379	2.932955	0.000000
1	-1.066060	3.310705	0.000000
1	0.460815	3.345556	0.886005
1	0.460815	3.345556	-0.886005

$CHCH_2$-CC-CH_3

6	0.068344	-0.229856	-0.000131
6	-1.133335	-0.063673	-0.000244
6	-2.575165	0.160237	0.000012
1	-2.877600	0.808176	-0.832170
1	-3.125839	-0.783377	-0.095987
1	-2.902807	0.642812	0.929449
6	1.470141	-0.480139	0.000056
6	2.418954	0.468691	0.000049
1	1.770236	-1.528566	0.000184
1	3.471812	0.203569	0.000159
1	2.170567	1.525820	-0.000083

$CHCH_2$-CH_2-CH_3

6	-1.729367	-0.246447	-0.294650
1	-1.931162	-1.168015	0.264778
1	-1.527816	-0.526509	-1.334504
1	-2.640651	0.361991	-0.275245
6	-0.540175	0.520606	0.308220
1	-0.366282	1.444342	-0.258163
1	-0.800613	0.826003	1.332862
6	0.723419	-0.296157	0.340058
6	1.861747	0.017853	-0.279405
1	0.672374	-1.223455	0.914785
1	2.740836	-0.618845	-0.223479
1	1.959569	0.929358	-0.866370

$CHCH_2$-CH=CH-CH_3

6	-0.053013	-0.244912	0.000077
6	1.114539	0.419241	0.000115
1	-0.044910	-1.336283	-0.000656
1	1.092944	1.510572	-0.000018
6	2.471811	-0.217070	0.000003
1	2.404700	-1.310204	-0.000916
1	3.055361	0.088591	-0.879535
1	3.054789	0.087033	0.880514
6	-1.360546	0.395519	-0.000302
6	-2.530436	-0.260131	0.000043
1	-1.362074	1.486298	0.000117
1	-3.480626	0.265281	0.000529
1	-2.574313	-1.347173	0.000346

$CHCH_2$-*m*-C_6H_4-CH_3

6	-0.862266	-0.167393	-0.003343
6	0.322054	-0.922002	-0.011699
6	-0.753606	1.234728	0.003363
6	1.588379	-0.326878	-0.009859
1	0.249227	-2.008414	-0.021017
6	0.497275	1.842297	0.000961
1	-1.648313	1.850169	0.005320
6	1.662130	1.070541	-0.006916
1	0.569372	2.926977	0.000580
1	2.634436	1.558105	-0.012812
6	2.840771	-1.173017	0.013369
1	3.156775	-1.388384	1.042964
1	2.684418	-2.135392	-0.485518
1	3.675667	-0.666540	-0.482632

6	-2.153239	-0.875483	-0.006262
6	-3.379989	-0.339107	0.010458
1	-2.070949	-1.962510	-0.022866
1	-4.264122	-0.969261	0.006590
1	-3.555560	0.733129	0.028965

$CHCH_2$-*o*-C_6H_4-CH_3

6	-0.492488	-0.142234	0.095781
6	0.391642	0.960526	0.005402
6	0.044183	-1.440991	0.118696
6	1.767395	0.718034	-0.077073
6	1.415463	-1.663563	0.033017
1	-0.629581	-2.285969	0.228985
6	2.284688	-0.577057	-0.066917
1	1.803025	-2.678600	0.056557
1	3.358276	-0.734091	-0.128799
1	2.445600	1.565049	-0.153582
6	-0.117803	2.384645	-0.024548
1	-0.822673	2.549562	-0.848211
1	-0.640372	2.654285	0.902703
1	0.710310	3.088984	-0.148670
6	-1.950253	0.071168	0.174775
6	-2.898863	-0.791060	-0.213070
1	-2.270845	1.029190	0.580294
1	-3.952645	-0.554013	-0.099778
1	-2.664887	-1.751202	-0.665871

$CHCH_2$-*p*-C_6H_4-CH_3

6	-1.034137	0.226443	-0.000033
6	-0.181053	1.340495	-0.000061
6	-0.435868	-1.048070	-0.000168
6	1.205794	1.193616	-0.000157
1	-0.612753	2.339071	-0.000079
6	0.945534	-1.190880	-0.000274
1	-1.059349	-1.937636	-0.000287
6	1.797022	-0.073231	-0.000191
1	1.837437	2.079191	-0.000233
1	1.377229	-2.189839	-0.000466
6	3.297407	-0.245303	0.000354
1	3.810854	0.721347	-0.005840
1	3.637212	-0.797843	0.885524
1	3.636648	-0.809078	-0.877860
6	-2.490070	0.437362	0.000046
6	-3.452868	-0.493568	0.000251
1	-2.792866	1.484889	-0.000051

1	-4.501220	-0.211254	0.000302
1	-3.243757	-1.560028	0.000382

CHO-CC-CH_3

6	-1.538531	0.396250	0.000008
8	-2.358601	-0.502998	-0.000055
1	-1.854628	1.459015	-0.000290
6	-0.109273	0.195078	0.000308
6	1.096275	0.057842	-0.000432
6	2.540919	-0.128774	-0.000373
1	2.849947	-0.766402	-0.837206
1	3.070509	0.826952	-0.084661
1	2.866640	-0.617961	0.925530

CHO-CH_2-CH_3

6	0.785936	-0.234673	0.300240
8	1.821319	-0.038087	-0.295592
1	0.700741	-1.079347	1.024757
6	-0.473312	0.589933	0.150792
1	-0.298308	1.353188	-0.613929
1	-0.643999	1.104602	1.108854
6	-1.695763	-0.282391	-0.178916
1	-1.842474	-1.064450	0.575539
1	-2.605724	0.324786	-0.210750
1	-1.581951	-0.771295	-1.152428

CHO-CH=CH-CH_3

6	-1.406137	0.333573	-0.000077
8	-2.472096	-0.253532	0.000215
1	-1.366738	1.447597	-0.000207
6	-0.092155	-0.324051	-0.000286
6	1.043436	0.391490	-0.000122
1	-0.088842	-1.412446	-0.000307
1	0.962431	1.480814	0.000184
6	2.431335	-0.166176	0.000173
1	2.431778	-1.260187	-0.000133
1	2.989816	0.181840	-0.879155
1	2.989453	0.181620	0.879770

CHO-*m*-C_6H_4-CH_3

6	-2.183725	-0.873422	0.000002
8	-3.264487	-0.315223	0.000010

1	-2.119743	-1.984950	-0.000020
6	-0.874934	-0.182311	0.000001
6	0.306448	-0.935938	-0.000023
6	-0.813585	1.217555	0.000006
6	1.560303	-0.318887	-0.000042
1	0.241291	-2.023054	-0.000030
6	0.427927	1.845404	0.000009
1	-1.740684	1.782240	0.000022
6	1.599770	1.083674	-0.000017
1	0.490802	2.930260	0.000021
1	2.564376	1.587231	-0.000023
6	2.836526	-1.128240	0.000026
1	3.449226	-0.908189	0.882843
1	2.627750	-2.202440	-0.001240
1	3.450504	-0.906333	-0.881427

CHO-*o*-C_6H_4-CH_3

6	1.985225	0.040019	-0.000037
8	2.783332	-0.880816	-0.000118
1	2.351155	1.087116	-0.000113
6	0.512816	-0.131685	0.000043
6	-0.369781	0.973757	-0.000034
6	0.008301	-1.441959	0.000114
6	-1.744580	0.712915	-0.000154
6	-1.361061	-1.678144	0.000088
1	0.722725	-2.259488	0.000191
6	-2.239549	-0.592099	-0.000074
1	-1.743188	-2.695134	0.000259
1	-3.313638	-0.758923	-0.000156
1	-2.440041	1.548873	-0.000345
6	0.115623	2.408857	0.000127
1	0.723971	2.638433	0.882757
1	0.725133	2.638479	-0.881652
1	-0.734732	3.097208	-0.000441

CHO-*p*-C_6H_4-CH_3

6	-2.517017	0.368674	0.001721
8	-3.313357	-0.551561	0.002236
1	-2.870821	1.424467	0.002543
6	-1.047464	0.214630	0.000264
6	-0.223129	1.345281	-0.000773
6	-0.463328	-1.062630	-0.001411
6	1.163530	1.205131	-0.002972
1	-0.671102	2.337071	-0.001081

6	0.917732	-1.195494	-0.003726
1	-1.115067	-1.931186	-0.002044
6	1.755196	-0.064489	-0.003351
1	1.796087	2.089398	-0.004836
1	1.364059	-2.187524	-0.006425
6	3.256039	-0.226528	0.004604
1	3.590546	-0.874380	-0.814460
1	3.765415	0.736475	-0.096712
1	3.598385	-0.689284	0.938994

NH_2-CC-CH_3

7	-2.028547	0.000540	-0.104512
6	-0.621697	-0.001038	-0.020656
6	0.549376	-0.001834	-0.009181
6	2.031933	0.000003	0.014548
1	-2.406334	-0.827803	0.381254
1	-2.404426	0.830096	0.380672
1	2.408608	1.020791	0.044991
1	2.408791	-0.526304	0.889795
1	2.435523	-0.483343	-0.873396

NH_2-CH_2-CH_3

7	1.208144	-0.325799	-0.120413
6	0.050289	0.560717	0.054056
6	-1.248440	-0.238079	-0.027540
1	2.068406	0.219470	-0.085764
1	1.257719	-0.973821	0.665718
1	0.075423	1.298023	-0.758227
1	0.064473	1.135694	0.998720
1	-2.120843	0.419576	0.058805
1	-1.307791	-0.976371	0.782820
1	-1.305491	-0.777806	-0.978269

NH_2-CH=CH-CH_3

7	-1.910433	-0.055262	-0.098725
6	-0.575576	0.365753	0.000118
6	0.510863	-0.417927	0.023681
6	1.922075	0.097094	-0.001152
1	-2.556992	0.505930	0.445471
1	-2.041522	-1.039572	0.112687
1	-0.465778	1.449823	-0.018660
1	0.380587	-1.501720	0.040184
1	1.945605	1.193152	0.003910

1	2.499895	-0.251312	0.866641
1	2.467064	-0.238985	-0.895044

NH_2-*m*-C_6H_4-CH_3

7	2.413870	-1.073463	0.080341
6	1.231926	-0.324968	0.011203
6	-0.017789	-0.965606	-0.003590
6	-1.210881	-0.238371	-0.012457
6	-1.152451	1.161871	-0.015587
6	0.084388	1.806847	-0.001619
6	1.271367	1.078637	0.011745
6	-2.542369	-0.954428	0.006885
1	3.232206	-0.601768	-0.285395
1	2.339554	-2.012694	-0.291541
1	-0.054069	-2.054144	-0.003454
1	-2.071533	1.742160	-0.030840
1	0.127309	2.893309	-0.007986
1	2.231019	1.590929	0.023594
1	-2.470362	-1.953203	-0.437025
1	-2.910435	-1.080497	1.034034
1	-3.305929	-0.393749	-0.543259

NH_2-*o*-C_6H_4-CH_3

7	1.599533	1.534764	-0.073701
6	0.442125	0.745283	-0.004659
6	0.544761	-0.664581	0.001561
6	-0.630982	-1.419079	0.011898
6	-1.892734	-0.821799	0.009933
6	-1.982561	0.569946	-0.002763
6	-0.825981	1.346213	-0.006371
6	1.900638	-1.326658	-0.015317
1	1.458789	2.498344	0.205722
1	2.412590	1.142495	0.385305
1	-0.549958	-2.504223	0.018423
1	-2.789208	-1.434977	0.015722
1	-2.954001	1.057776	-0.004708
1	-0.898226	2.432268	-0.014509
1	2.500070	-0.994887	-0.873524
1	2.485959	-1.101005	0.889507
1	1.805661	-2.415084	-0.071721

NH_2-*p*-C_6H_4-CH_3

7	2.843842	0.000002	-0.067813

6	1.442883	0.000007	-0.005946
6	0.721144	-1.204125	-0.008168
6	-0.671507	-1.195633	-0.011160
6	-1.401016	0.000000	-0.009046
6	-0.671513	1.195629	-0.011162
6	0.721147	1.204131	-0.008173
6	-2.912156	-0.000001	0.023142
1	3.277937	0.833686	0.310243
1	3.277920	-0.833752	0.310108
1	1.257750	-2.150819	-0.017942
1	-1.203050	-2.145286	-0.014437
1	-1.203054	2.145283	-0.014440
1	1.257741	2.150831	-0.017958
1	-3.323960	-0.884490	-0.475702
1	-3.298151	-0.000858	1.052120
1	-3.323917	0.885333	-0.474228

CF_3-CC-CH_2•

6	-0.606241	-0.000183	-0.027999
6	-1.834374	0.000174	-0.010190
6	-3.201029	-0.000059	0.001952
1	-3.758032	-0.931760	0.007183
1	-3.758474	0.931364	0.008271
6	0.850412	0.000008	-0.002524
9	1.319696	-0.005290	1.264564
9	1.355002	-1.086139	-0.624770
9	1.354625	1.091513	-0.615671

CF_3-CH_2-CH_2•

6	-0.903507	0.764903	-0.175287
1	-0.867719	1.196905	-1.189761
1	-0.896839	1.608482	0.523010
6	-2.105156	-0.096613	0.014644
1	-2.999893	0.297690	0.480356
1	-2.133025	-1.095914	-0.404330
6	0.405257	0.015397	0.003685
9	0.548361	-0.461485	1.257606
9	0.491785	-1.037986	-0.840728
9	1.461844	0.820662	-0.246603

CF_3-CH=CH-CH_2•

6	-0.180380	1.692066	0.000000
6	0.568159	0.526951	0.000000
1	-1.263613	1.592869	0.000000
1	1.654090	0.549256	0.000000
6	-0.029325	-0.836123	0.000000
6	0.362844	2.965934	0.000000
1	1.437930	3.122347	0.000000
1	-0.268801	3.847455	0.000000
9	-1.379844	-0.814066	0.000000
9	0.362844	-1.548794	1.085046
9	0.362844	-1.548794	-1.085046

CF_3-*m*-C_6H_4-CH_2•

6	0.253324	0.157622	-0.031943
6	-0.701353	-0.846561	-0.023597
6	-0.126382	1.510072	-0.020316
6	-2.092169	-0.534030	-0.001911
1	-0.392862	-1.886818	-0.038423
6	-1.486105	1.839382	0.002096
1	0.630920	2.286684	-0.035858
6	-2.452580	0.845404	0.011795
1	-1.784969	2.883872	0.008802
1	-3.506598	1.110435	0.028009
6	-3.065294	-1.549564	0.003967
1	-2.784242	-2.597317	-0.007570
1	-4.123840	-1.312430	0.021183
6	1.718902	-0.185750	-0.001162
9	1.958265	-1.455169	-0.395244
9	2.437883	0.630689	-0.805576
9	2.234021	-0.053729	1.244185

CF_3-*o*-C_6H_4-CH_2•

6	-0.039558	-0.222587	-0.000125
6	-0.760988	1.020278	-0.000083
6	-0.716687	-1.435069	-0.000132
6	-2.185351	0.932623	0.000083
6	-2.115500	-1.480059	-0.000051
1	-0.147797	-2.357843	-0.000147
6	-2.845084	-0.284407	0.000073
1	-2.625929	-2.438218	-0.000139
1	-3.931415	-0.309633	0.000160
1	-2.753293	1.859204	0.000223
6	-0.145591	2.284279	-0.000144
1	-0.757928	3.179974	0.000078

1	0.927728	2.413632	-0.000496
6	1.465773	-0.224308	0.000059
9	1.974240	0.409195	1.086035
9	1.978611	-1.473705	-0.000366
9	1.974545	0.409887	-1.085419

CF_3-*p*-C_6H_4-CH_2•

6	-0.033472	2.485544	0.000000
6	-0.035412	1.742229	1.218166
6	-0.035412	1.742229	-1.218166
6	-0.035412	0.359081	1.214905
1	-0.039542	2.281253	2.161747
6	-0.035412	0.359081	-1.214905
1	-0.039542	2.281253	-2.161747
6	-0.035766	-0.345013	0.000000
1	-0.042867	-0.188500	2.151762
1	-0.042867	-0.188500	-2.151762
6	0.028859	-1.844831	0.000000
6	-0.034088	3.890698	0.000000
1	-0.033498	4.452537	0.928167
1	-0.033498	4.452537	-0.928167
9	1.307737	-2.294766	0.000000
9	-0.568951	-2.376211	1.090786
9	-0.568951	-2.376211	-1.090786

CH_3-CC-CH_2•

6	0.517324	0.002856	-0.000043
6	-0.713049	0.000598	-0.000141
6	-2.083247	-0.000932	-0.000257
1	-2.645790	-0.930029	0.000961
1	-2.647923	0.926885	0.000965
6	1.974019	-0.000141	0.000069
1	2.376964	1.019914	0.000076
1	2.373169	-0.515504	0.883963
1	2.373306	-0.515547	-0.883737

CH_3-CH_2-CH_2•

6	0.000000	0.577713	0.000000
1	0.100599	1.227423	0.880555
1	0.100599	1.227423	-0.880555
6	1.173628	-0.431473	0.000000
1	1.136508	-1.076657	-0.885058
1	2.138113	0.091319	0.000000

1	1.136508	-1.076657	0.885058
6	-1.342393	-0.075733	0.000000
1	-1.799867	-0.407943	-0.927605
1	-1.799867	-0.407943	0.927605

CH_3-CH=CH-CH_2•

6	0.660239	0.381335	-0.000347
6	-0.475873	-0.417428	-0.000316
1	0.507590	1.462358	0.000030
1	-0.344719	-1.499796	-0.000251
6	-1.879179	0.099635	0.000201
1	-1.906375	1.194853	0.000362
1	-2.440124	-0.250770	-0.879006
1	-2.439578	-0.251109	0.879596
6	1.965908	-0.081740	0.000231
1	2.186630	-1.145971	0.000459
1	2.810002	0.599617	0.000195

CH_3-*m*-C_6H_4-CH_2•

6	1.183454	-0.238282	0.000001
6	0.013856	-0.986134	-0.000012
6	1.086118	1.167903	0.000020
6	-1.277941	-0.378624	0.000000
1	0.072993	-2.072730	-0.000023
6	-0.165285	1.795364	0.000003
1	1.992840	1.768415	0.000049
6	-1.331277	1.045395	-0.000017
1	-0.221932	2.881078	0.000002
1	-2.301019	1.536753	-0.000061
6	-2.449433	-1.156374	0.000017
1	-2.404911	-2.240673	0.000061
1	-3.431241	-0.694149	-0.000019
6	2.539390	-0.906399	-0.000008
1	3.125535	-0.619890	0.882187
1	2.448433	-1.997051	-0.000668
1	3.126009	-0.618850	-0.881548

CH_3-*o*-C_6H_4-CH_2•

6	-0.609131	-0.620215	-0.000010
6	-0.441562	0.809165	-0.000035
6	0.521099	-1.430892	-0.000135
6	0.889925	1.325764	0.000160
6	1.817021	-0.897999	-0.000108

1	0.390827	-2.511004	-0.000159
6	1.994520	0.491825	0.000095
1	2.676796	-1.562122	-0.000317
1	2.995571	0.915074	0.000214
1	1.021974	2.405188	0.000380
6	-1.533381	1.693477	-0.000195
1	-1.372111	2.766762	-0.000198
1	-2.560345	1.349067	-0.000349
6	-1.986990	-1.233752	0.000184
1	-2.566633	-0.930293	0.881726
1	-2.566880	-0.930554	-0.881300
1	-1.928197	-2.326348	0.000274

CH_3-*p*-C_6H_4-CH_2•

6	0.005567	-1.503127	0.000000
6	0.006864	-0.754215	1.214183
6	0.006864	-0.754215	-1.214183
6	0.006864	0.630091	1.205216
1	0.012230	-1.290674	2.160052
6	0.006864	0.630091	-1.205216
1	0.012230	-1.290674	-2.160052
6	0.003559	1.357500	0.000000
1	0.011010	1.170252	2.149815
1	0.011010	1.170252	-2.149815
6	-0.031970	2.865682	0.000000
1	-1.064631	3.242487	0.000000
1	0.461408	3.279375	0.886366
1	0.461408	3.279375	-0.886366
6	0.008242	-2.908272	0.000000
1	0.009105	-3.470803	0.928003
1	0.009105	-3.470803	-0.928003

$CHCH_2$-CC-CH_2•

6	0.000000	0.235573	0.000000
6	1.236609	0.108520	0.000000
6	2.579481	-0.041600	0.000000
1	3.244034	0.818180	0.000000
1	3.037932	-1.026835	0.000000
6	-1.382327	0.416249	0.000000
6	-2.297866	-0.590562	0.000000
1	-1.739972	1.446873	0.000000
1	-3.361226	-0.374129	0.000000
1	-1.996146	-1.633173	0.000000

$CHCH_2$-CH_2-CH_2•

6	-1.758353	-0.353640	-0.220687
1	-2.780356	-0.097995	0.040213
1	-1.595561	-1.215250	-0.860687
6	-0.619518	0.552772	0.128322
1	-0.431861	1.273317	-0.688866
1	-0.896544	1.162724	1.001501
6	0.662613	-0.191237	0.417611
6	1.800271	-0.049223	-0.262836
1	0.617278	-0.902507	1.243163
1	2.692680	-0.616593	-0.012154
1	1.884290	0.644272	-1.097632

$CHCH_2$-CH=CH-CH_2•

6	0.000000	0.000000	0.272750
6	0.000000	1.248941	-0.392236
1	0.000000	0.000000	1.363002
1	0.000000	1.223486	-1.483146
6	0.000000	2.465674	0.227239
1	0.000000	2.548159	1.311350
1	0.000000	3.391904	-0.337972
6	0.000000	-1.248941	-0.392236
6	0.000000	-2.465674	0.227239
1	0.000000	-1.223486	-1.483146
1	0.000000	-3.391904	-0.337972
1	0.000000	-2.548159	1.311350

$CHCH_2$-*m*-C_6H_4-CH_2•

6	0.000000	0.832861	0.000000
6	1.017388	-0.120270	0.000000
6	-1.340410	0.383812	0.000000
6	0.754014	-1.520658	0.000000
1	2.054118	0.210503	0.000000
6	-1.629353	-0.983260	0.000000
1	-2.154247	1.101939	0.000000
6	-0.611877	-1.926792	0.000000
1	-2.666099	-1.310014	0.000000
1	-0.846514	-2.988136	0.000000
6	1.800546	-2.460460	0.000000
1	2.839081	-2.145949	0.000000
1	1.598565	-3.526569	0.000000
6	0.364522	2.259791	0.000000
6	-0.462279	3.312678	0.000000

1	1.437715	2.450629	0.000000
1	-0.073455	4.326339	0.000000
1	-1.544473	3.215044	0.000000

$CHCH_2$-*o*-C_6H_4-CH_2•

6	0.519763	-0.080288	-0.093481
6	-0.415126	1.017990	-0.005697
6	0.021665	-1.388627	-0.099328
6	-1.808780	0.702349	0.053125
6	-1.343674	-1.661497	-0.019632
1	0.722690	-2.211949	-0.202606
6	-2.263170	-0.601762	0.053001
1	-1.692688	-2.690119	-0.034990
1	-3.329299	-0.806590	0.102657
1	-2.516773	1.525414	0.112611
6	-0.018266	2.362708	0.054162
1	-0.764407	3.149082	0.105011
1	1.019748	2.669355	0.078640
6	1.964012	0.168251	-0.206788
6	2.940825	-0.646363	0.218008
1	2.253936	1.101036	-0.687349
1	3.986280	-0.395815	0.064386
1	2.737018	-1.576982	0.741422

$CHCH_2$-*p*-C_6H_4-CH_2•

6	0.000000	0.998006	0.000000
6	1.286083	0.407151	0.000000
6	-1.118065	0.125342	0.000000
6	1.457726	-0.961735	0.000000
1	2.159396	1.055966	0.000000
6	-0.961170	-1.242129	0.000000
1	-2.121278	0.541649	0.000000
6	0.336686	-1.849479	0.000000
1	2.459413	-1.384444	0.000000
1	-1.836444	-1.887336	0.000000
6	0.496339	-3.237115	0.000000
1	1.482437	-3.690347	0.000000
1	-0.360811	-3.902801	0.000000
6	-0.117051	2.451838	0.000000
6	-1.243849	3.186183	0.000000
1	0.835013	2.983267	0.000000
1	-1.201229	4.270814	0.000000
1	-2.236691	2.744845	0.000000

CHO-CC-CH_2•

6	-1.374841	0.593327	0.000000
8	-2.309847	-0.198621	0.000000
1	-1.550933	1.686293	0.000000
6	0.000000	0.202959	0.000000
6	1.195190	-0.120750	0.000000
6	2.502976	-0.481316	0.000000
1	2.796815	-1.527339	0.000000
1	3.292944	0.264692	0.000000

CHO-CH_2-CH_2•

6	0.724251	0.028013	0.412418
8	1.691007	-0.255766	-0.256289
1	0.702850	-0.168617	1.507078
6	-0.573274	0.619200	-0.151444
1	-0.376889	0.909942	-1.188681
1	-0.824695	1.514409	0.434531
6	-1.657630	-0.401449	-0.052536
1	-2.251295	-0.503646	0.849864
1	-1.738113	-1.180544	-0.803107

CHO-CH=CH-CH_2•

6	-1.345133	-0.211131	0.000000
8	-2.358418	0.481849	0.000000
1	-1.417759	-1.321489	0.000000
6	0.000000	0.321452	0.000000
6	1.132481	-0.503463	0.000000
1	0.103151	1.404623	0.000000
1	0.963379	-1.581144	0.000000
6	2.428562	-0.047302	0.000000
1	2.651467	1.016219	0.000000
1	3.271648	-0.730335	0.000000

CHO-*m*-C_6H_4-CH_2•

6	0.334842	2.289685	0.000000
8	-0.482151	3.189992	0.000000
1	1.425938	2.511178	0.000000
6	0.000000	0.846297	0.000000
6	1.024508	-0.093428	0.000000
6	-1.346734	0.432102	0.000000
6	0.748477	-1.491070	0.000000
1	2.060506	0.241315	0.000000

6	-1.644254	-0.932397	0.000000
1	-2.125696	1.187547	0.000000
6	-0.625392	-1.877029	0.000000
1	-2.680302	-1.260224	0.000000
1	-0.867757	-2.936881	0.000000
6	1.783636	-2.443473	0.000000
1	2.825281	-2.140113	0.000000
1	1.568741	-3.506874	0.000000

CHO-*o*-C_6H_4-CH_2•

6	0.364532	1.978476	0.000000
8	-0.448324	2.888931	0.000000
1	1.446649	2.213544	0.000000
6	0.000000	0.546146	0.000000
6	0.984972	-0.507429	0.000000
6	-1.362768	0.229169	0.000000
6	0.494593	-1.851790	0.000000
6	-1.802004	-1.091252	0.000000
1	-2.068021	1.054602	0.000000
6	-0.857351	-2.134446	0.000000
1	-2.864599	-1.314997	0.000000
1	-1.191780	-3.168418	0.000000
1	1.219746	-2.661502	0.000000
6	2.372829	-0.297362	0.000000
1	2.828953	0.684021	0.000000
1	3.046830	-1.147782	0.000000

CHO-*p*-C_6H_4-CH_2•

6	-0.157854	2.470564	0.000000
8	-1.228896	3.054475	0.000000
1	0.798701	3.040336	0.000000
6	0.000000	1.007868	0.000000
6	1.286711	0.432810	0.000000
6	-1.134605	0.165910	0.000000
6	1.445922	-0.938570	0.000000
1	2.159314	1.083075	0.000000
6	-0.987561	-1.203140	0.000000
1	-2.116722	0.628920	0.000000
6	0.311104	-1.809586	0.000000
1	2.441069	-1.375700	0.000000
1	-1.862756	-1.848048	0.000000
6	0.463364	-3.200127	0.000000
1	1.446999	-3.658513	0.000000
1	-0.397920	-3.860241	0.000000

NH_2-CC-CH_2•

6	0.560766	-0.001071	0.016436
6	-0.670620	-0.000196	-0.004136
6	-2.039593	0.000293	0.005357
1	-2.599016	0.930170	0.004232
1	-2.599872	-0.929063	0.002809
7	1.907588	0.000313	-0.086218
1	2.370193	0.841411	0.244277
1	2.372256	-0.838865	0.246266

NH_2-CH_2-CH_2•

6	0.025200	0.582179	-0.003773
1	-0.015785	1.238088	0.873593
1	-0.017179	1.228209	-0.888119
6	1.269567	-0.240864	0.000790
1	1.672804	-0.632803	0.930899
1	1.655451	-0.663698	-0.923435
7	-1.231820	-0.219560	0.001080
1	-1.217570	-0.850265	-0.801554
1	-1.223579	-0.830502	0.818958

NH_2-CH=CH-CH_2•

6	0.520769	0.405008	0.009146
6	-0.627854	-0.380054	0.008870
1	0.450335	1.489282	-0.006245
1	-0.480827	-1.462825	0.018842
6	-1.927580	0.092628	0.001006
1	-2.144008	1.157296	-0.018524
1	-2.773422	-0.585213	0.018130
7	1.815202	-0.098038	-0.089269
1	2.535055	0.461875	0.352476
1	1.914442	-1.079640	0.146076

NH_2-*m*-C_6H_4-CH_2•

6	-1.194499	-0.287200	-0.009988
6	0.002179	-1.002628	-0.005229
6	-1.148356	1.123152	-0.004805
6	1.264680	-0.346446	-0.000150
1	-0.022631	-2.090671	-0.011935
6	0.083508	1.785475	0.003863
1	-2.075734	1.690743	-0.015325

6	1.275990	1.079512	0.006379
1	0.099337	2.872428	0.009692
1	2.228522	1.601823	0.013443
6	2.465965	-1.079952	0.004215
1	2.464910	-2.165160	-0.001117
1	3.428412	-0.579157	0.010545
7	-2.428873	-0.947478	-0.079464
1	-2.414193	-1.899184	0.266886
1	-3.203324	-0.429962	0.318345

NH_2-*o*-C_6H_4-CH_2•

6	0.573248	-0.675069	-0.006135
6	0.531163	0.767050	0.000095
6	-0.619795	-1.402558	-0.029881
6	-0.758917	1.379328	0.039533
6	-1.859299	-0.761793	-0.023254
1	-0.572558	-2.489934	-0.043220
6	-1.926874	0.640228	0.023070
1	-2.769629	-1.354557	-0.038217
1	-2.890678	1.141089	0.040919
1	-0.801118	2.465642	0.063458
6	1.693018	1.549842	-0.044176
1	2.679840	1.127818	-0.194694
1	1.625925	2.631963	-0.005494
7	1.805085	-1.329749	-0.035814
1	2.541836	-0.877808	0.492179
1	1.755517	-2.318128	0.180258

NH_2-*p*-C_6H_4-CH_2•

6	-1.378070	0.000096	-0.007682
6	-0.654222	1.211444	-0.006482
6	-0.654166	-1.211412	-0.006467
6	0.727206	1.212255	-0.001296
1	-1.196931	2.154791	-0.013260
6	0.727143	-1.212254	-0.001336
1	-1.197089	-2.154640	-0.013229
6	1.482873	0.000060	0.001929
1	1.260850	2.159622	0.002968
1	1.260906	-2.159553	0.002981
6	2.885581	-0.000063	0.010256
1	3.448636	0.927594	0.012484
1	3.448458	-0.927826	0.012370
7	-2.771797	-0.000074	-0.070855
1	-3.220002	-0.837875	0.279163

1	-3.220315	0.837642	0.278972

Table S4. Optimized UB3-LYP/6-31G(2df,p) Geometries of Substituted Methanes X-W-CH_3 and Substituted Radicals X-W-$CH_2^{\cdot}$.

CF_3-CC-CH_3

6	0.000000	0.000000	0.538971
6	0.000000	0.000000	1.739983
6	0.000000	0.000000	3.192728
1	-0.852313	-0.565741	3.582569
1	0.916102	-0.455254	3.582569
1	-0.063789	1.020995	3.582569
6	0.000000	0.000000	-0.918359
9	0.256543	1.221350	-1.409913
9	0.929449	-0.832848	-1.409913
9	-1.185992	-0.388503	-1.409913

CF_3-CH_2-CH_3

6	1.137376	0.258541	0.000000
1	1.454569	0.823538	0.881763
1	1.454569	0.823538	-0.881763
6	1.734472	-1.150014	0.000000
1	1.417616	-1.707519	-0.885206
1	2.825905	-1.099332	0.000000
1	1.417616	-1.707519	0.885206
6	-0.376773	0.250236	0.000000
9	-0.871879	-0.376047	-1.081374
9	-0.871879	-0.376047	1.081374
9	-0.871879	1.498174	0.000000

CF_3-CH=CH-CH_3

6	1.564087	0.307320	-0.000012
6	0.516036	-0.509034	-0.000022
1	1.383238	1.379405	0.000000
1	0.619334	-1.589977	-0.000039
6	-0.899802	-0.030382	-0.000005
6	2.994753	-0.130711	0.000001
1	3.520048	0.262999	-0.878336
1	3.519923	0.262696	0.878551
1	3.089130	-1.219614	-0.000172
9	-0.997417	1.306849	-0.000040
9	-1.566934	-0.482206	1.078420
9	-1.566996	-0.482273	-1.078355

CF_3-*p*-C_6H_4-CH_3

6	0.305130	0.198290	-0.029850
6	-0.687580	-0.780922	-0.016506
6	-0.034560	1.548383	-0.025242
6	-2.037320	-0.429294	0.007528
1	-0.403149	-1.827530	-0.030011
6	-1.378527	1.909217	0.000913
1	0.742217	2.302753	-0.045115
6	-2.366465	0.930674	0.019782
1	-1.655308	2.958069	0.006431
1	-3.411983	1.224237	0.042390
6	-3.116174	-1.484133	-0.003351
1	-3.557195	-1.588549	-1.001968
1	-2.722428	-2.461910	0.285770
1	-3.929786	-1.228491	0.682505
6	1.753855	-0.212556	-0.002425
9	1.961125	-1.358516	-0.671645
9	2.549831	0.722646	-0.544113
9	2.189874	-0.414856	1.255191

CF_3-*o*-C_6H_4-CH_3

6	-0.060371	-0.250859	0.000014
6	-0.750784	0.976211	0.000019
6	-0.751880	-1.460074	0.000004
6	-2.145921	0.930770	0.000003
6	-2.143273	-1.478182	0.000000
1	-0.194530	-2.387907	0.000000
6	-2.840586	-0.276370	-0.000003
1	-2.672468	-2.424563	-0.000004
1	-3.925593	-0.273498	-0.000013
1	-2.697769	1.865625	-0.000006
6	-0.041956	2.309950	-0.000002
1	0.601301	2.419076	0.877654
1	0.600838	2.419295	-0.877974
1	-0.765380	3.128085	0.000283
6	1.448822	-0.277923	-0.000004
9	1.963717	0.341712	1.080040
9	1.935850	-1.526692	-0.000142
9	1.963688	0.341951	-1.079912

CF_3-*p*-C_6H_4-CH_3

6	-2.407298	0.000013	0.012820
6	-1.689447	-1.199838	0.002341

6	-1.689440	1.199851	0.002341
6	-0.299764	-1.205493	-0.021293
1	-2.226763	-2.143296	0.010693
6	-0.299750	1.205495	-0.021294
1	-2.226748	2.143314	0.010693
6	0.399453	0.000001	-0.030574
1	0.243363	-2.143102	-0.035320
1	0.243382	2.143102	-0.035323
6	1.903686	-0.000003	-0.002330
6	-3.915634	-0.000003	0.007051
1	-4.305385	-0.000903	-1.018293
1	-4.317208	-0.885675	0.507358
1	-4.317225	0.886508	0.505843
9	2.380391	0.000058	1.257021
9	2.415121	-1.083654	-0.608460
9	2.415126	1.083587	-0.608564

CH_3-CC-CH_3

6	0.601774	-0.000235	0.002786
6	-0.601772	0.000226	0.000283
6	-2.058129	-0.000032	-0.000630
1	-2.458337	-0.041619	1.018599
1	-2.457539	0.903564	-0.474683
1	-2.457156	-0.862241	-0.546620
6	2.058128	0.000027	-0.000950
1	2.456018	0.901329	-0.480602
1	2.460683	-0.036023	1.017572
1	2.456325	-0.864922	-0.543196

CH_3-CH_2-CH_3

6	0.000000	0.000000	0.586517
1	0.876326	0.000000	1.246854
1	-0.876326	0.000000	1.246854
6	0.000000	1.276030	-0.259782
1	-0.883354	1.320683	-0.906864
1	0.000000	2.174176	0.366016
1	0.883354	1.320683	-0.906864
6	0.000000	-1.276030	-0.259782
1	0.000000	-2.174176	0.366016
1	-0.883354	-1.320683	-0.906864
1	0.883354	-1.320683	-0.906864

CH_3-CH=CH-CH_3

6	0.565764	0.053310	-0.346521
6	-0.565764	-0.053310	0.346521
1	1.325071	0.756896	-0.003460
1	-1.325071	-0.756896	0.003460
6	-0.901005	0.723474	1.585249
1	-0.091548	1.405329	1.862585
1	-1.813348	1.318039	1.449616
1	-1.089069	0.056857	2.436457
6	0.901005	-0.723474	-1.585249
1	1.089069	-0.056857	-2.436457
1	1.813348	-1.318039	-1.449616
1	0.091548	-1.405329	-1.862585

CH_3-*p*-C_6H_4-CH_3

6	0.000000	1.222049	-0.270211
6	0.000000	0.000000	-0.946921
6	-0.004080	1.207057	1.126991
6	0.000000	-1.222049	-0.270211
1	0.000000	0.000000	-2.034378
6	0.000000	0.000000	1.819309
1	-0.007825	2.145510	1.673750
6	0.004080	-1.207057	1.126991
1	0.000000	0.000000	2.904805
1	0.007825	-2.145510	1.673750
6	-0.031784	-2.526416	-1.029733
1	-1.059153	-2.892537	-1.149174
1	0.392046	-2.416842	-2.032108
1	0.529261	-3.307093	-0.507125
6	0.031784	2.526416	-1.029733
1	1.059153	2.892537	-1.149174
1	-0.392046	2.416842	-2.032108
1	-0.529261	3.307093	-0.507125

CH_3-*o*-C_6H_4-CH_3

6	0.476174	0.704346	-0.000042
6	0.476175	-0.704346	-0.000053
6	-0.744772	1.380963	-0.000006
6	-0.744772	-1.380963	-0.000026
6	-1.956706	0.695011	0.000022
1	-0.743113	2.467292	-0.000002
6	-1.956706	-0.695011	0.000017
1	-2.891834	1.245332	0.000054
1	-2.891833	-1.245332	0.000041
1	-0.743113	-2.467292	-0.000052

6	1.771705	-1.477707	0.000023
1	2.385375	-1.243628	-0.878307
1	2.384468	-1.244858	0.879336
1	1.586691	-2.554849	-0.000797
6	1.771705	1.477707	0.000008
1	2.384958	1.244110	0.878769
1	2.384885	1.244375	-0.878873
1	1.586691	2.554850	0.000173

CH_3-*p*-C_6H_4-CH_3

6	-0.000857	1.418363	0.000000
6	0.000857	0.695664	1.195710
6	0.000857	0.695664	-1.195710
6	-0.000857	-0.695664	1.195710
1	0.000961	1.230001	2.141781
6	-0.000857	-0.695664	-1.195710
1	0.000961	1.230001	-2.141781
6	0.000857	-1.418363	0.000000
1	-0.000961	-1.230001	2.141781
1	-0.000961	-1.230001	-2.141781
6	0.033494	-2.927261	0.000000
1	1.063675	-3.305054	0.000000
1	-0.460841	-3.338137	0.885372
1	-0.460841	-3.338137	-0.885372
6	-0.033494	2.927261	0.000000
1	-1.063675	3.305054	0.000000
1	0.460841	3.338137	0.885372
1	0.460841	3.338137	-0.885372

$CHCH_2$-CC-CH_3

6	0.067045	-0.227535	0.000038
6	-1.129083	-0.062474	0.000122
6	-2.566341	0.159137	-0.000181
1	-2.868728	0.804521	-0.832735
1	-3.115799	-0.783946	-0.093968
1	-2.893715	0.643136	0.927150
6	1.463091	-0.476685	-0.000022
6	2.413211	0.464719	-0.000015
1	1.758234	-1.525044	-0.000089
1	3.463747	0.197404	-0.000107
1	2.168718	1.520959	0.000090

$CHCH_2$-CH_2-CH_3

6	-1.727758	-0.248276	-0.291471
1	-1.926110	-1.165421	0.273869
1	-1.528544	-0.534984	-1.328729
1	-2.638602	0.358183	-0.273860
6	-0.538354	0.523285	0.303280
1	-0.364988	1.442270	-0.268544
1	-0.797036	0.834970	1.325126
6	0.722368	-0.292928	0.338888
6	1.859271	0.014676	-0.277454
1	0.666003	-1.216125	0.916912
1	2.735853	-0.621846	-0.217655
1	1.960262	0.922407	-0.866572

$CHCH_2$-CH=CH-CH_3

6	-0.052801	-0.243288	-0.000018
6	1.111616	0.417734	0.000024
1	-0.045192	-1.333267	-0.000092
1	1.090223	1.507528	0.000036
6	2.467233	-0.216749	0.000000
1	2.400936	-1.308508	-0.000541
1	3.050202	0.089838	-0.878018
1	3.049757	0.088954	0.878629
6	-1.358352	0.393355	-0.000052
6	-2.525267	-0.259088	0.000011
1	-1.357905	1.482704	-0.000022
1	-3.473895	0.265295	0.000132
1	-2.568706	-1.344332	0.000085

$CHCH_2$-*p*-C_6H_4-CH_3

6	-0.860834	-0.165981	-0.003528
6	0.320640	-0.919215	-0.011344
6	-0.751130	1.233105	0.003003
6	1.584519	-0.326408	-0.009286
1	0.246582	-2.003971	-0.020548
6	0.497306	1.838275	0.000814
1	-1.643818	1.848501	0.004399
6	1.659083	1.067625	-0.006436
1	0.570316	2.921208	0.000273
1	2.630300	1.553578	-0.012261
6	2.834903	-1.171946	0.012818
1	3.150390	-1.387826	1.041127
1	2.677246	-2.132751	-0.485721
1	3.668546	-0.665021	-0.481816
6	-2.149419	-0.871962	-0.006451

6	-3.373346	-0.339683	0.010682
1	-2.064674	-1.957513	-0.023573
1	-4.255544	-0.969571	0.006688
1	-3.549674	0.730509	0.029798

$CHCH_2$-*o*-C_6H_4-CH_3

6	-0.491169	-0.142954	0.094356
6	0.390032	0.957926	0.005004
6	0.046189	-1.438174	0.117265
6	1.762930	0.717684	-0.077023
6	1.414611	-1.658931	0.033417
1	-0.626154	-2.282428	0.226732
6	2.280686	-0.573777	-0.066400
1	1.802849	-2.671768	0.057107
1	3.352726	-0.729297	-0.127592
1	2.438719	1.564631	-0.153012
6	-0.120061	2.379768	-0.023786
1	-0.832628	2.541676	-0.839650
1	-0.634416	2.649521	0.906611
1	0.705760	3.083142	-0.156321
6	-1.946032	0.068792	0.172654
6	-2.893362	-0.790259	-0.210701
1	-2.263665	1.027603	0.575125
1	-3.945333	-0.552694	-0.098600
1	-2.660807	-1.750838	-0.659112

$CHCH_2$-*p*-C_6H_4-CH_3

6	-1.032112	0.224727	-0.000032
6	-0.181272	1.336600	-0.000056
6	-0.433849	-1.046567	-0.000162
6	1.202631	1.191293	-0.000146
1	-0.614176	2.332864	-0.000075
6	0.944329	-1.187945	-0.000261
1	-1.055598	-1.935381	-0.000286
6	1.793065	-0.072212	-0.000179
1	1.832994	2.075774	-0.000216
1	1.376932	-2.184718	-0.000446
6	3.291293	-0.243788	0.000331
1	3.803689	0.721827	-0.005794
1	3.629824	-0.796684	0.884170
1	3.629222	-0.807808	-0.876620
6	-2.484891	0.434829	0.000037
6	-3.446801	-0.490951	0.000244
1	-2.784529	1.481926	-0.000070

1	-4.493143	-0.207860	0.000290
1	-3.239575	-1.555850	0.000387

CHO-CC-CH_3

6	-1.532856	0.391944	0.000029
8	-2.353668	-0.497050	-0.000017
1	-1.838968	1.458303	-0.000057
6	-0.107633	0.190018	0.000157
6	1.092503	0.056022	-0.000528
6	2.532654	-0.126752	-0.000329
1	2.842574	-0.761850	-0.837231
1	3.059655	0.829173	-0.082509
1	2.858071	-0.616618	0.923964

CHO-CH_2-CH_3

6	1.441606	-0.502957	0.000108
1	1.249707	-1.121932	-0.880055
1	1.249500	-1.122162	0.880064
1	2.497099	-0.218422	0.000270
6	0.545639	0.732528	0.000164
1	0.738256	1.377441	0.870515
1	0.738467	1.377673	-0.869968
6	-0.932695	0.420732	-0.000057
8	-1.400880	-0.689176	-0.000263
1	-1.593295	1.318991	-0.000014

CHO-CH=CH-CH_3

6	1.405082	0.330244	-0.000015
8	2.466955	-0.249480	0.000019
1	1.356306	1.444549	0.000037
6	0.091571	-0.326289	-0.000023
6	-1.039826	0.387763	-0.000019
1	0.089523	-1.413385	-0.000014
1	-0.955937	1.475622	0.000012
6	-2.427576	-0.163548	0.000016
1	-2.433087	-1.256201	0.000012
1	-2.983962	0.188116	0.877732
1	-2.983992	0.188119	-0.877679

CHO-*p*-C_6H_4-CH_3

6	-2.182175	-0.869807	-0.001058
8	-3.256935	-0.315695	0.001081

1	-2.111639	-1.981628	0.001129
6	-0.873480	-0.180044	-0.000549
6	0.304216	-0.933035	-0.000357
6	-0.810391	1.216800	-0.000335
6	1.556155	-0.319177	0.000011
1	0.236364	-2.018517	-0.000530
6	0.429063	1.841645	0.000024
1	-1.736425	1.780330	-0.000502
6	1.597198	1.080024	0.000192
1	0.493394	2.924760	0.000157
1	2.561212	1.581354	0.000459
6	2.830327	-1.127847	0.000307
1	3.442076	-0.906744	0.881953
1	2.621265	-2.200575	-0.001058
1	3.443752	-0.904783	-0.879667

CHO-*o*-C_6H_4-CH_3

6	1.983223	0.035286	-0.000040
8	2.775093	-0.881593	0.000042
1	2.347307	1.082789	0.000123
6	0.511084	-0.132954	-0.000032
6	-0.366978	0.971168	-0.000011
6	0.004429	-1.439121	-0.000029
6	-1.739727	0.714210	0.000011
6	-1.362007	-1.672197	0.000002
1	0.718431	-2.255143	-0.000050
6	-2.236265	-0.586380	0.000023
1	-1.745833	-2.686512	0.000008
1	-3.309038	-0.750591	0.000042
1	-2.432014	1.550678	0.000014
6	0.120791	2.403085	-0.000006
1	0.729989	2.630570	0.880997
1	0.730435	2.630459	-0.880722
1	-0.727323	3.091914	-0.000261

CHO-*p*-C_6H_4-CH_3

6	-2.513909	0.365684	0.001554
8	-3.306603	-0.548207	0.002019
1	-2.861236	1.424346	0.002462
6	-1.045201	0.212300	0.000307
6	-0.223730	1.340744	-0.000684
6	-0.460730	-1.061693	-0.001246
6	1.160185	1.202878	-0.002750
1	-0.673769	2.329897	-0.001066

6	0.917079	-1.192779	-0.003429
1	-1.112097	-1.928747	-0.001900
6	1.751373	-0.063185	-0.003075
1	1.791258	2.086225	-0.004553
1	1.364598	-2.182524	-0.006005
6	3.250124	-0.224217	0.004133
1	3.583197	-0.870067	-0.815441
1	3.758126	0.738213	-0.094359
1	3.591605	-0.690081	0.935846

NH_2-CC-CH_3

7	1.999540	0.000799	0.089198
6	0.644067	-0.001541	0.007442
6	-0.560463	-0.003108	0.000666
6	-2.017273	-0.000816	-0.008031
1	2.435043	-0.828422	-0.296222
1	2.432173	0.831685	-0.295886
1	-2.402795	1.024274	-0.054016
1	-2.424297	-0.537614	-0.873267
1	-2.434893	-0.462724	0.894538

NH_2-CH_2-CH_3

6	-1.215088	-0.360597	0.000000
1	-1.212068	-1.007379	0.885134
1	-1.212068	-1.007379	-0.885134
1	-2.155186	0.202928	0.000000
6	0.000000	0.574574	0.000000
1	-0.042963	1.233033	-0.876170
1	-0.042963	1.233033	0.876170
7	1.311991	-0.079624	0.000000
1	1.385919	-0.690364	0.809781
1	1.385919	-0.690364	-0.809781

NH_2-CH=CH-CH_3

7	-1.906139	-0.056554	-0.096204
6	-0.574476	0.363868	-0.000718
6	0.509179	-0.416005	0.020744
6	1.919014	0.096908	-0.000130
1	-2.554941	0.513938	0.428711
1	-2.042181	-1.035093	0.123014
1	-0.465196	1.446892	-0.016354
1	0.379453	-1.498088	0.036578
1	1.943438	1.191593	0.003656

1	2.493356	-0.251033	0.868533
1	2.466739	-0.240956	-0.890084

NH_2-*p*-C_6H_4-CH_3

7	2.409870	-1.070804	0.081089
6	1.229556	-0.324086	0.010763
6	-0.017308	-0.962893	-0.003783
6	-1.207983	-0.237895	-0.011802
6	-1.150192	1.159113	-0.014090
6	0.083695	1.802775	-0.001797
6	1.267999	1.076198	0.010766
6	-2.537688	-0.953016	0.006100
1	3.225304	-0.599678	-0.283833
1	2.335709	-2.007408	-0.289562
1	-0.053037	-2.049765	-0.005754
1	-2.068069	1.737831	-0.028401
1	0.126236	2.887551	-0.008510
1	2.226232	1.587292	0.019879
1	-2.464517	-1.950618	-0.436866
1	-2.905994	-1.078820	1.031861
1	-3.299443	-0.391929	-0.543383

NH_2-*o*-C_6H_4-CH_3

7	1.596571	1.531644	-0.074551
6	0.441731	0.743621	-0.005140
6	0.542459	-0.662907	0.001228
6	-0.630642	-1.415562	0.010488
6	-1.889312	-0.819181	0.009040
6	-1.978146	0.569559	-0.001811
6	-0.823488	1.342955	-0.005571
6	1.896233	-1.324877	-0.013326
1	1.458916	2.490560	0.211249
1	2.411334	1.135231	0.370889
1	-0.549756	-2.499096	0.016371
1	-2.784489	-1.430821	0.014215
1	-2.947697	1.057143	-0.002611
1	-0.894197	2.427389	-0.011578
1	2.498646	-0.991878	-0.867471
1	2.477386	-1.099862	0.892724
1	1.800854	-2.411815	-0.071385

NH_2-*p*-C_6H_4-CH_3

7	2.838562	-0.000004	-0.069592

6	1.439926	0.000003	-0.005548
6	0.719443	-1.200947	-0.007233
6	-0.670101	-1.192918	-0.010273
6	-1.397685	0.000008	-0.008734
6	-0.670099	1.192923	-0.010273
6	0.719452	1.200950	-0.007236
6	-2.906720	-0.000003	0.021370
1	3.271183	0.831458	0.307339
1	3.271169	-0.831504	0.307273
1	1.255893	-2.145722	-0.014879
1	-1.201338	-2.140862	-0.013194
1	-1.201334	2.140868	-0.013194
1	1.255903	2.145724	-0.014888
1	-3.316699	-0.883942	-0.476959
1	-3.293354	-0.000848	1.048730
1	-3.316660	0.884761	-0.475513

CF_3-CC-CH_2•

6	-0.607393	-0.000274	-0.025471
6	-1.829868	-0.000029	-0.008831
6	-3.191452	-0.000004	0.001873
1	-3.747373	-0.930420	0.006905
1	-3.747364	0.930415	0.006939
6	0.849936	-0.000007	-0.002429
9	1.318683	-0.004348	1.255145
9	1.350223	-1.078921	-0.620542
9	1.349693	1.083479	-0.612902

CF_3-CH_2-CH_2•

6	-0.904295	0.767232	-0.162915
1	-0.869156	1.214944	-1.169721
1	-0.897622	1.599678	0.547305
6	-2.099129	-0.102352	0.015034
1	-3.007168	0.291493	0.450892
1	-2.106214	-1.107070	-0.387874
6	0.406825	0.015487	0.003582
9	0.552917	-0.468139	1.245020
9	0.487523	-1.024370	-0.843520
9	1.455089	0.816816	-0.243146

CF_3-CH=CH-CH_2•

6	-0.177091	1.687853	0.000000
6	0.569362	0.526269	0.000000

1	-1.258648	1.583680	0.000000
1	1.654097	0.545839	0.000000
6	-0.030362	-0.837395	0.000000
6	0.358971	2.960883	0.000000
1	1.432021	3.120677	0.000000
1	-0.275225	3.838528	0.000000
9	-1.371001	-0.811924	0.000000
9	0.358971	-1.544837	1.078237
9	0.358971	-1.544837	-1.078237

CF_3-*p*-C_6H_4-CH_2•

6	0.251685	0.157367	-0.026659
6	-0.699583	-0.844733	-0.022094
6	-0.127138	1.506899	-0.018462
6	-2.088560	-0.534080	-0.001296
1	-0.390050	-1.883160	-0.037323
6	-1.484362	1.834955	0.002146
1	0.629619	2.281708	-0.035485
6	-2.447827	0.843003	0.011883
1	-1.783240	2.877789	0.007241
1	-3.500686	1.106504	0.026909
6	-3.059129	-1.546802	0.003376
1	-2.777533	-2.592765	-0.007954
1	-4.115856	-1.308738	0.019467
6	1.719305	-0.185813	-0.001542
9	1.954173	-1.445396	-0.396164
9	2.428650	0.628702	-0.800547
9	2.233998	-0.057319	1.234827

CF_3-*o*-C_6H_4-CH_2•

6	-0.041017	-0.223486	-0.000005
6	-0.757960	1.018296	0.000000
6	-0.717065	-1.431936	-0.000005
6	-2.180121	0.932363	0.000003
6	-2.113274	-1.475313	-0.000003
1	-0.148137	-2.352924	-0.000008
6	-2.839428	-0.280945	0.000002
1	-2.624251	-2.431222	-0.000004
1	-3.924139	-0.305319	0.000005
1	-2.745255	1.858904	0.000005
6	-0.140206	2.277037	-0.000003
1	-0.750034	3.172701	0.000010
1	0.932090	2.402027	-0.000025
6	1.465937	-0.225441	0.000002

9	1.968365	0.405734	1.078846
9	1.974211	-1.465708	-0.000031
9	1.968372	0.405795	-1.078807

CF_3-*p*-C_6H_4-CH_2•

6	-0.510905	2.428361	0.000000
6	-0.368909	1.699689	1.215850
6	-0.368909	1.699689	-1.215850
6	-0.101049	0.346092	1.212383
1	-0.479142	2.227702	2.157533
6	-0.101049	0.346092	-1.212383
1	-0.479142	2.227702	-2.157533
6	0.038470	-0.342045	0.000000
1	-0.003507	-0.193694	2.146983
1	-0.003507	-0.193694	-2.146983
6	0.383309	-1.804855	0.000000
6	-0.783042	3.803052	0.000000
1	-0.891544	4.352605	0.927372
1	-0.891544	4.352605	-0.927372
9	1.715530	-2.005289	0.000000
9	-0.101049	-2.432338	1.083817
9	-0.101049	-2.432338	-1.083817

CH_3-CC-CH_2•

6	0.514522	0.003080	-0.000160
6	-0.710584	0.000579	-0.000064
6	-2.074903	-0.000958	0.000036
1	-2.635636	-0.929101	0.000152
1	-2.637780	0.925900	0.000162
6	1.966549	-0.000081	0.000068
1	2.370011	1.018516	0.000098
1	2.364804	-0.515490	0.882950
1	2.365095	-0.515548	-0.882647

CH_3-CH_2-CH_2•

6	0.000000	0.576778	0.000000
1	0.101531	1.225476	0.879429
1	0.101531	1.225476	-0.879429
6	1.172885	-0.432406	0.000000
1	1.135086	-1.076861	-0.883810
1	2.135708	0.089922	0.000000
1	1.135086	-1.076861	0.883810
6	-1.340910	-0.074819	0.000000

1	-1.800394	-0.402237	-0.926422
1	-1.800394	-0.402237	0.926422

CH_3-CH=CH-CH_2•

6	0.659141	0.378793	-0.000013
6	-0.474625	-0.416496	-0.000015
1	0.505373	1.458278	-0.000003
1	-0.344775	-1.497618	-0.000023
6	-1.875416	0.100138	0.000009
1	-1.902462	1.193939	0.000038
1	-2.435905	-0.251027	-0.877574
1	-2.435883	-0.251080	0.877585
6	1.962004	-0.080696	0.000004
1	2.182969	-1.143200	0.000042
1	2.804062	0.600276	0.000015

CH_3-*p*-C_6H_4-CH_2•

6	1.180380	-0.238002	-0.000017
6	0.013936	-0.984137	-0.000016
6	1.083336	1.165086	-0.000012
6	-1.275670	-0.378337	0.000001
1	0.072699	-2.069240	-0.000032
6	-0.165287	1.791036	0.000004
1	1.988850	1.764301	-0.000024
6	-1.328391	1.043049	0.000011
1	-0.221511	2.875100	0.000003
1	-2.296987	1.532974	0.000015
6	-2.444354	-1.153612	0.000004
1	-2.399363	-2.236270	-0.000002
1	-3.424004	-0.690650	0.000011
6	2.535163	-0.903860	0.000014
1	3.120052	-0.615638	0.880878
1	2.445046	-1.993177	-0.000554
1	3.120535	-0.614738	-0.880227

CH_3-*o*-C_6H_4-CH_2•

6	0.607759	-0.618576	-0.000001
6	0.440368	0.807934	0.000001
6	-0.519087	-1.427772	0.000009
6	-0.889178	1.322143	-0.000013
6	-1.812604	-0.897014	0.000010
1	-0.388114	-2.506229	0.000010
6	-1.990538	0.489707	-0.000006

1	-2.670495	-1.560661	0.000029
1	-2.990304	0.911443	-0.000018
1	-1.020657	2.400036	-0.000027
6	1.528772	1.690574	0.000016
1	1.365908	2.762056	0.000010
1	2.554083	1.346476	0.000033
6	1.984178	-1.230337	-0.000013
1	2.562947	-0.925681	-0.880174
1	2.562918	-0.925811	0.880214
1	1.925687	-2.321583	-0.000087

CH_3-*p*-C_6H_4-CH_2•

6	0.005458	-1.500385	0.000000
6	0.006528	-0.752359	1.211647
6	0.006528	-0.752359	-1.211647
6	0.006528	0.628423	1.202559
1	0.011806	-1.288782	2.155711
6	0.006528	0.628423	-1.202559
1	0.011806	-1.288782	-2.155711
6	0.003399	1.354104	0.000000
1	0.010680	1.168578	2.145343
1	0.010680	1.168578	-2.145343
6	-0.030510	2.860118	0.000000
1	-1.061774	3.237194	0.000000
1	0.462104	3.272092	0.885934
1	0.462104	3.272092	-0.885934
6	0.008037	-2.901868	0.000000
1	0.008809	-3.462774	0.927096
1	0.008809	-3.462774	-0.927096

$CHCH_2$-CC-CH_2•

6	0.000000	0.232693	0.000000
6	1.231893	0.115524	0.000000
6	2.570261	-0.023993	0.000000
1	3.226837	0.839699	0.000000
1	3.034803	-1.004413	0.000000
6	-1.377958	0.404191	0.000000
6	-2.288942	-0.601299	0.000000
1	-1.737364	1.432807	0.000000
1	-3.351538	-0.389439	0.000000
1	-1.984267	-1.641347	0.000000

$CHCH_2$-CH_2-CH_2•

6	-1.758638	-0.346693	-0.224872
1	-2.781700	-0.063014	-0.007231
1	-1.591285	-1.225612	-0.837079
6	-0.617620	0.546526	0.140992
1	-0.433581	1.287951	-0.656762
1	-0.890440	1.136130	1.028426
6	0.662450	-0.203300	0.407161
6	1.798715	-0.040253	-0.262535
1	0.613167	-0.938351	1.209440
1	2.689684	-0.613111	-0.027957
1	1.884707	0.678326	-1.073311

$CHCH_2$-CH=CH-CH_2•

6	0.000000	0.000000	0.271279
6	0.000000	1.246169	-0.390068
1	0.000000	0.000000	1.360201
1	0.000000	1.219544	-1.479431
6	0.000000	2.460161	0.226007
1	0.000000	2.543433	1.308284
1	0.000000	3.384761	-0.338422
6	0.000000	-1.246169	-0.390068
6	0.000000	-2.460161	0.226007
1	0.000000	-1.219544	-1.479431
1	0.000000	-3.384761	-0.338422
1	0.000000	-2.543433	1.308284

$CHCH_2$-*p*-C_6H_4-CH_2•

6	0.000000	0.831172	0.000000
6	1.014244	-0.120365	0.000000
6	-1.337740	0.383005	0.000000
6	0.751659	-1.518228	0.000000
1	2.049481	0.210141	0.000000
6	-1.626321	-0.980866	0.000000
1	-2.150524	1.099911	0.000000
6	-0.611834	-1.922549	0.000000
1	-2.661670	-1.306808	0.000000
1	-0.846077	-2.982327	0.000000
6	1.794943	-2.456105	0.000000
1	2.831790	-2.141528	0.000000
1	1.591302	-3.520258	0.000000
6	0.364195	2.255070	0.000000
6	-0.456931	3.307030	0.000000
1	1.436816	2.441919	0.000000
1	-0.066966	4.318442	0.000000

1	-1.537440	3.211514	0.000000

$CHCH_2$-*o*-C_6H_4-CH_2•

6	0.518364	-0.081724	-0.093484
6	-0.412646	1.015941	-0.005974
6	0.019090	-1.385951	-0.098760
6	-1.804130	0.702536	0.053031
6	-1.343516	-1.656387	-0.019558
1	0.718220	-2.208998	-0.201433
6	-2.259423	-0.597448	0.052938
1	-1.693623	-2.682775	-0.034606
1	-3.324101	-0.800570	0.102493
1	-2.508884	1.526334	0.112068
6	-0.014599	2.356502	0.054473
1	-0.759328	3.142098	0.105662
1	1.022525	2.660188	0.078704
6	1.959966	0.164585	-0.207123
6	2.934859	-0.645227	0.217910
1	2.247185	1.095311	-0.690071
1	3.978600	-0.395236	0.064191
1	2.731614	-1.573311	0.742278

$CHCH_2$-*p*-C_6H_4-CH_2•

6	0.000000	0.995662	0.000000
6	1.282800	0.404782	0.000000
6	-1.116110	0.124861	0.000000
6	1.453637	-0.960644	0.000000
1	2.154275	1.053456	0.000000
6	-0.960386	-1.239000	0.000000
1	-2.117611	0.541283	0.000000
6	0.334537	-1.846490	0.000000
1	2.453324	-1.384068	0.000000
1	-1.834017	-1.883841	0.000000
6	0.492819	-3.230129	0.000000
1	1.477553	-3.682391	0.000000
1	-0.364077	-3.893451	0.000000
6	-0.115497	2.446309	0.000000
6	-1.236332	3.182341	0.000000
1	0.837407	2.973599	0.000000
1	-1.191164	4.265149	0.000000
1	-2.228505	2.744122	0.000000

CHO-CC-CH_2•

6	-1.374356	0.579749	0.000000
8	-2.302366	-0.209339	0.000000
1	-1.548968	1.673567	0.000000
6	0.000000	0.199869	0.000000
6	1.192143	-0.113084	0.000000
6	2.497310	-0.463298	0.000000
1	2.797034	-1.505970	0.000000
1	3.280277	0.287695	0.000000

CHO-CH_2-CH_2•

6	0.725196	-0.010366	0.408022
8	1.693494	-0.231193	-0.269046
1	0.689390	-0.294732	1.483360
6	-0.570994	0.624004	-0.111595
1	-0.374540	0.983848	-1.125593
1	-0.808945	1.477797	0.536448
6	-1.662185	-0.389820	-0.076439
1	-2.242383	-0.556579	0.823315
1	-1.763580	-1.103700	-0.885094

CHO-CH=CH-CH_2•

6	-1.343489	-0.210543	0.000000
8	-2.354522	0.472774	0.000000
1	-1.405382	-1.321918	0.000000
6	0.000000	0.323045	0.000000
6	1.130752	-0.497567	0.000000
1	0.100894	1.405361	0.000000
1	0.959486	-1.573653	0.000000
6	2.424153	-0.045112	0.000000
1	2.647278	1.016867	0.000000
1	3.265404	-0.727796	0.000000

CHO-*p*-C_6H_4-CH_2•

6	0.335387	2.286402	0.000000
8	-0.475715	3.182766	0.000000
1	1.427610	2.501885	0.000000
6	0.000000	0.844387	0.000000
6	1.021078	-0.093478	0.000000
6	-1.344145	0.431637	0.000000
6	0.745645	-1.488692	0.000000
1	2.055499	0.241073	0.000000
6	-1.641556	-0.929638	0.000000
1	-2.120386	1.187561	0.000000

6	-0.625780	-1.872549	0.000000
1	-2.676284	-1.256279	0.000000
1	-0.867784	-2.930865	0.000000
6	1.777425	-2.439412	0.000000
1	2.817529	-2.136562	0.000000
1	1.561214	-3.500887	0.000000

CHO-*o*-C_6H_4-CH_2•

6	0.362013	1.977068	0.000000
8	-0.446705	2.882032	0.000000
1	1.445050	2.208728	0.000000
6	0.000000	0.545055	0.000000
6	0.982809	-0.506047	0.000000
6	-1.359481	0.227646	0.000000
6	0.493370	-1.848048	0.000000
6	-1.797746	-1.089582	0.000000
1	-2.062592	1.053159	0.000000
6	-0.854885	-2.130356	0.000000
1	-2.858693	-1.313200	0.000000
1	-1.189140	-3.162740	0.000000
1	1.218333	-2.655857	0.000000
6	2.367219	-0.296248	0.000000
1	2.822392	0.683684	0.000000
1	3.038500	-1.146968	0.000000

CHO-*p*-C_6H_4-CH_2•

6	-0.156653	2.466587	0.000000
8	-1.220946	3.048889	0.000000
1	0.802568	3.031224	0.000000
6	0.000000	1.005483	0.000000
6	1.283220	0.430615	0.000000
6	-1.132667	0.165530	0.000000
6	1.441842	-0.937406	0.000000
1	2.153758	1.080976	0.000000
6	-0.986850	-1.199940	0.000000
1	-2.112218	0.630457	0.000000
6	0.308972	-1.806294	0.000000
1	2.434733	-1.375548	0.000000
1	-1.860297	-1.844480	0.000000
6	0.460054	-3.193212	0.000000
1	1.442344	-3.650689	0.000000
1	-0.400820	-3.851231	0.000000

NH_2-CC-CH_2•

6	0.557963	-0.000485	0.016089
6	-0.667632	0.000098	-0.003902
6	-2.031031	0.000081	0.005055
1	-2.589913	0.928121	0.004662
1	-2.589810	-0.928021	0.002767
7	1.899051	0.000053	-0.083836
1	2.364947	0.839098	0.236789
1	2.365620	-0.837735	0.239182

NH_2-CH_2-CH_2•

6	0.024840	0.581861	-0.001761
1	-0.013209	1.236707	0.875759
1	-0.014719	1.231190	-0.883426
6	1.267546	-0.241217	-0.000063
1	1.666218	-0.638952	0.927958
1	1.655256	-0.657602	-0.924602
7	-1.230169	-0.219495	0.001503
1	-1.219756	-0.840515	-0.805168
1	-1.216918	-0.838229	0.809900

NH_2-CH=CH-CH_2•

6	0.520135	0.405209	0.007966
6	-0.626326	-0.376006	0.008479
1	0.452001	1.488504	-0.002861
1	-0.475940	-1.456981	0.018098
6	-1.923782	0.090647	0.001054
1	-2.142744	1.153073	-0.016814
1	-2.766080	-0.588492	0.017253
7	1.809734	-0.099789	-0.086248
1	2.533795	0.461869	0.337648
1	1.910669	-1.078546	0.145418

NH_2-*p*-C_6H_4-CH_2•

6	-1.192164	-0.286634	-0.009662
6	0.001408	-1.000060	-0.004421
6	-1.144833	1.120628	-0.004257
6	1.262466	-0.346595	0.000265
1	-0.023986	-2.086610	-0.008852
6	0.084312	1.781422	0.003878
1	-2.071020	1.687140	-0.012208
6	1.273574	1.076846	0.005593
1	0.100299	2.866844	0.009812

1	2.225143	1.597501	0.012031
6	2.460705	-1.078219	0.003836
1	2.458551	-2.161883	-0.000596
1	3.420968	-0.576620	0.009281
7	-2.424830	-0.944451	-0.080066
1	-2.411776	-1.893278	0.265961
1	-3.197174	-0.426258	0.313642

NH_2-*o*-C_6H_4-CH_2•

6	0.572717	-0.673443	-0.005746
6	0.529881	0.766086	0.000742
6	-0.617259	-1.399203	-0.027710
6	-0.759103	1.375709	0.037127
6	-1.854763	-0.761711	-0.021660
1	-0.568344	-2.484876	-0.039289
6	-1.923234	0.637682	0.021373
1	-2.763139	-1.354258	-0.035348
1	-2.885961	1.136717	0.037906
1	-0.800775	2.460548	0.059768
6	1.687727	1.547503	-0.041715
1	2.674819	1.126487	-0.180362
1	1.619318	2.628055	-0.004476
7	1.801421	-1.326947	-0.038394
1	2.543056	-0.868991	0.471356
1	1.755288	-2.310785	0.184736

NH_2-*p*-C_6H_4-CH_2•

6	-1.375283	0.000005	-0.007123
6	-0.652383	1.208348	-0.005419
6	-0.652377	-1.208347	-0.005424
6	0.725452	1.209758	-0.000806
1	-1.195407	2.149673	-0.010055
6	0.725449	-1.209755	-0.000807
1	-1.195412	-2.149665	-0.010069
6	1.480426	0.000006	0.001785
1	1.259115	2.155378	0.003711
1	1.259126	-2.155367	0.003707
6	2.879102	-0.000005	0.008802
1	3.440210	0.926831	0.010840
1	3.440191	-0.926852	0.010842
7	-2.766071	-0.000011	-0.071960
1	-3.213815	-0.835956	0.274396
1	-3.213827	0.835969	0.274298