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Understanding the Mechanism and Reactivity of Pd-Catalyzed C–P Bond Metathesis of Aryl Phosphines: A Computational Study

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1. DFT-computed free energy changes of the Pd-catalyzed C–P bond metathesis catalytic cycle using ωB97X-D functional.

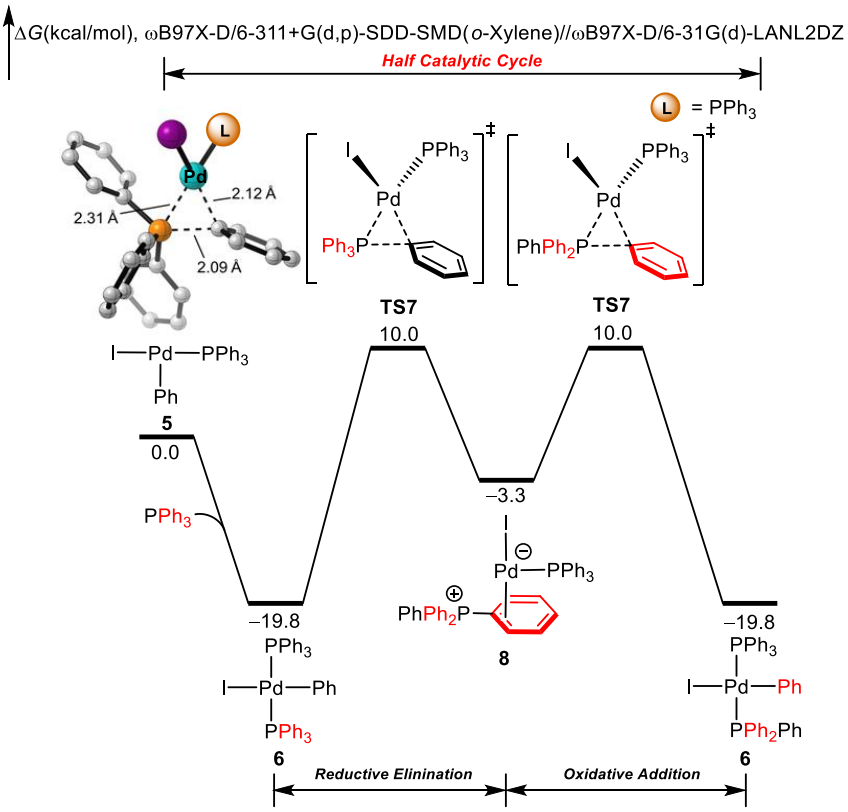


Figure S1. DFT-computed free energy changes of the Pd-catalyzed C–P bond metathesis catalytic cycle using ωB97X-D functional.

2. DFT-computed free energy changes of the Pd-catalyzed C–P bond metathesis catalytic cycle using def2-TZVP basis set for single-point energy calculations.

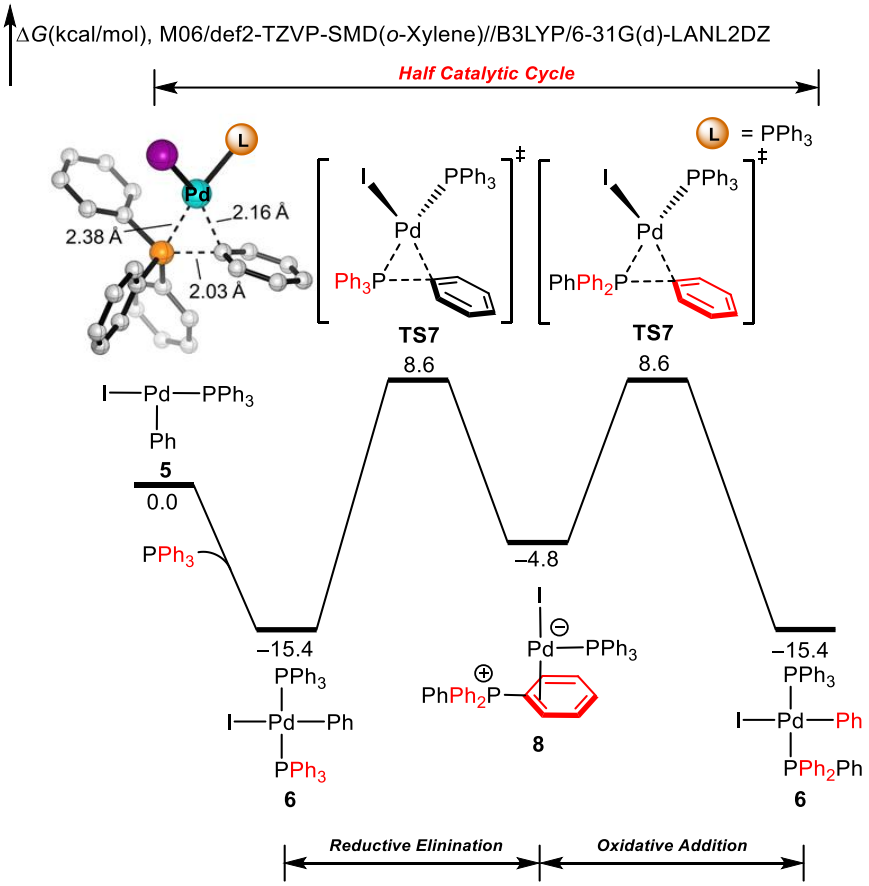


Figure S2. DFT-computed free energy changes of the Pd-catalyzed C–P bond metathesis catalytic cycle using def2-TZVP basis set for single-point energy calculations.

3. DFT-computed free energy changes of Pd-catalyzed C–P bond metathesis of triphenylphosphines without PhI.

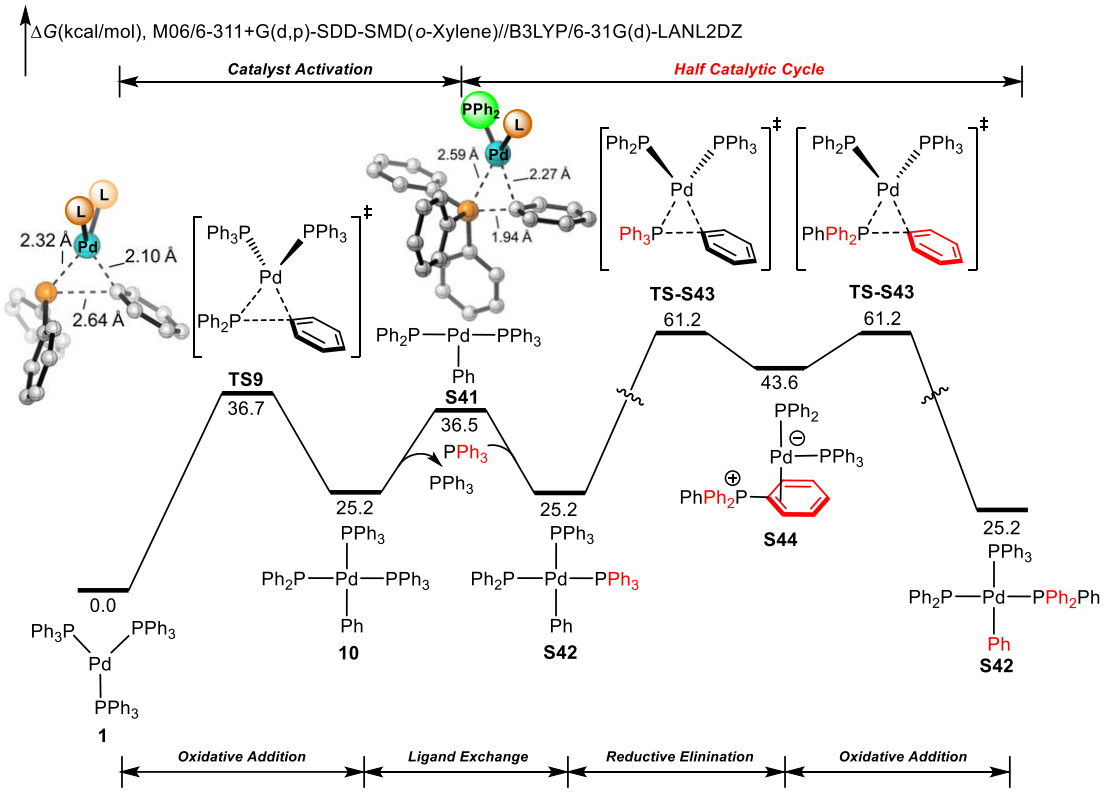


Figure S3. DFT-computed free energy changes of the Pd-catalyzed C–P bond metathesis of triphenylphosphines without PhI.

4. Alternative transition states considered for Pd(0)-catalyzed oxidative addition of tetraphenylphosphonium.

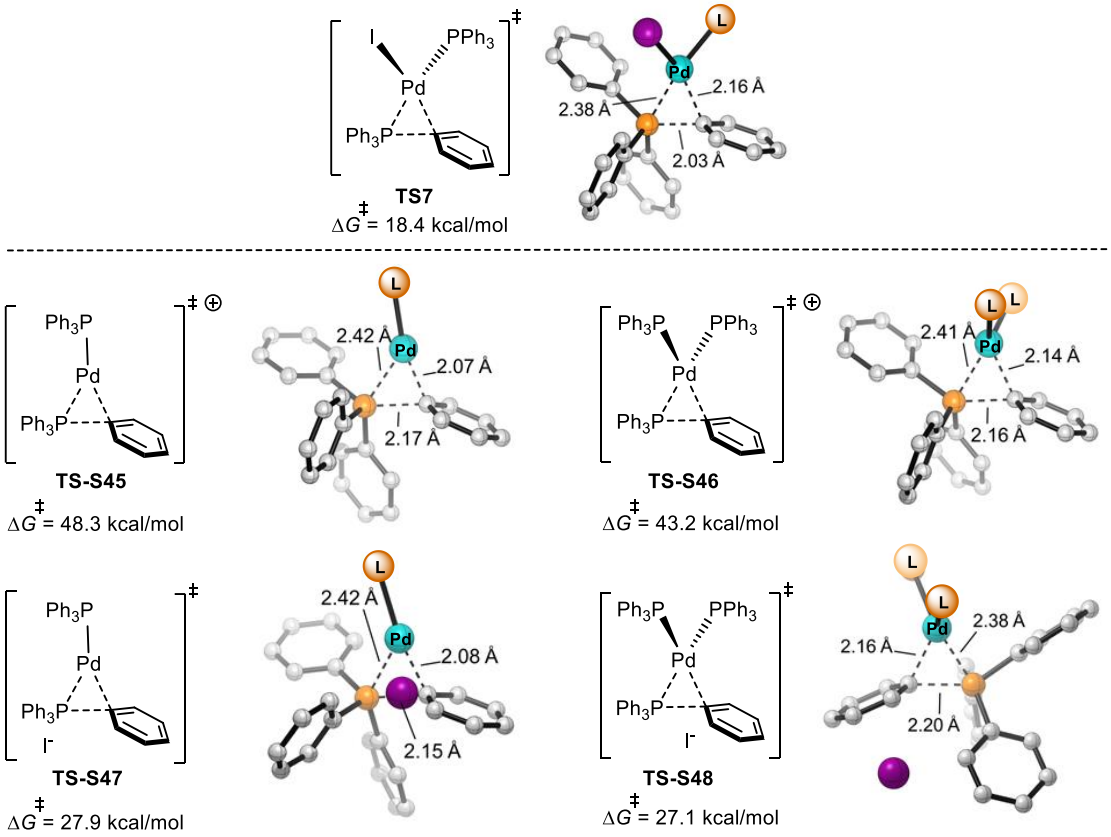


Figure S4. DFT-computed Gibbs free energies of Pd(0)-catalyzed tetraphenylphosphonium oxidative addition transition states.

5. Conformational search of ion complex oxidative addition transition states.

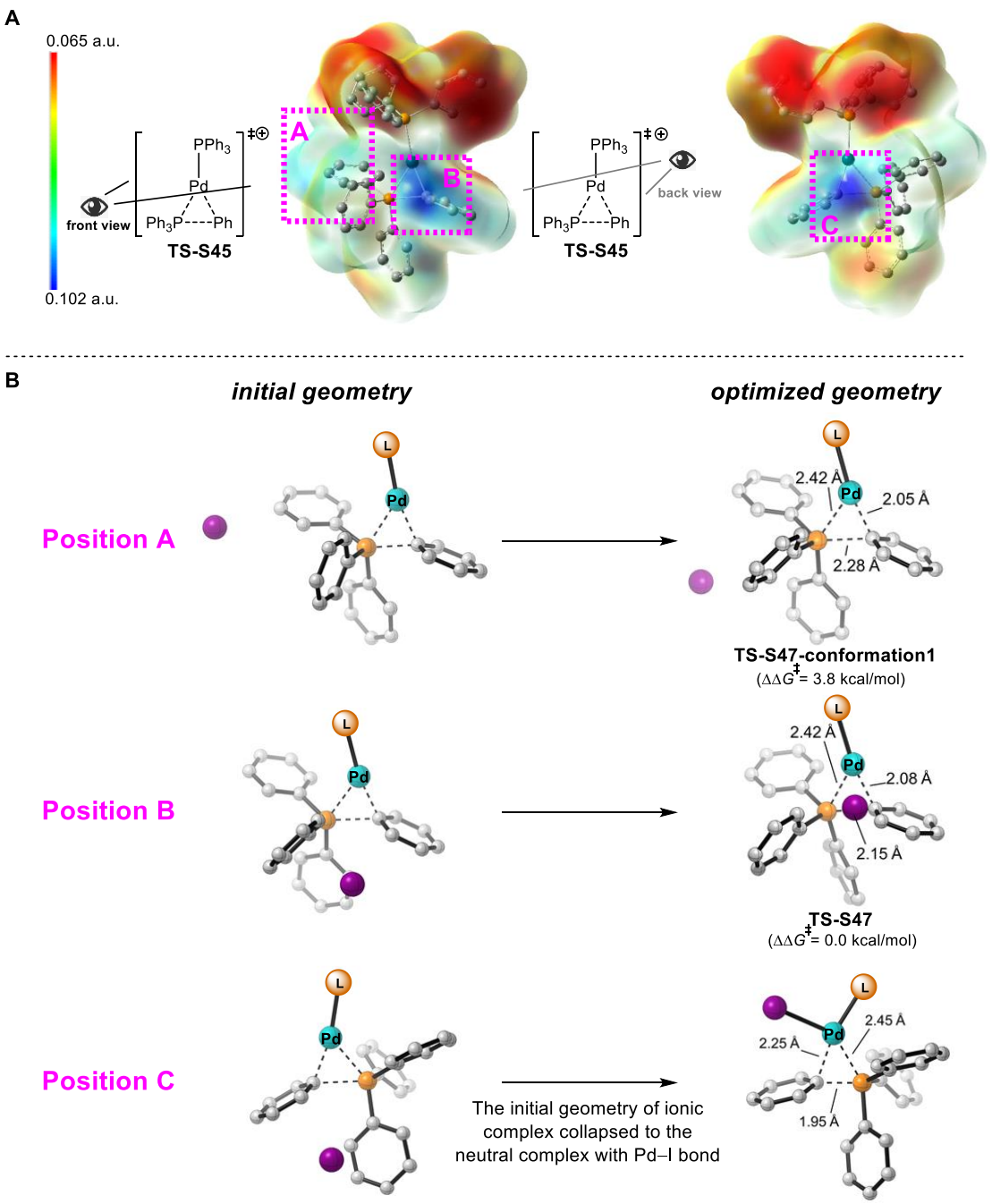


Figure S5. ESP analysis of **TS-S45** (A) and the conformation search of **TS-S47** (B).

The ion complex oxidative addition transition state **TS-S47** has a number of possible conformations. To locate the most favorable conformation, we first computed the electrostatic potential surface of the corresponding cationic transition state **TS-S45** (**Figure S5A**). Since the ionic complexation occurs through electrostatic interactions, the iodide anion was placed in proximity to the positive region of the palladium species in the starting geometry of optimization (**Figure S5B**). These optimizations were converged to two conformations of **TS-S47**.

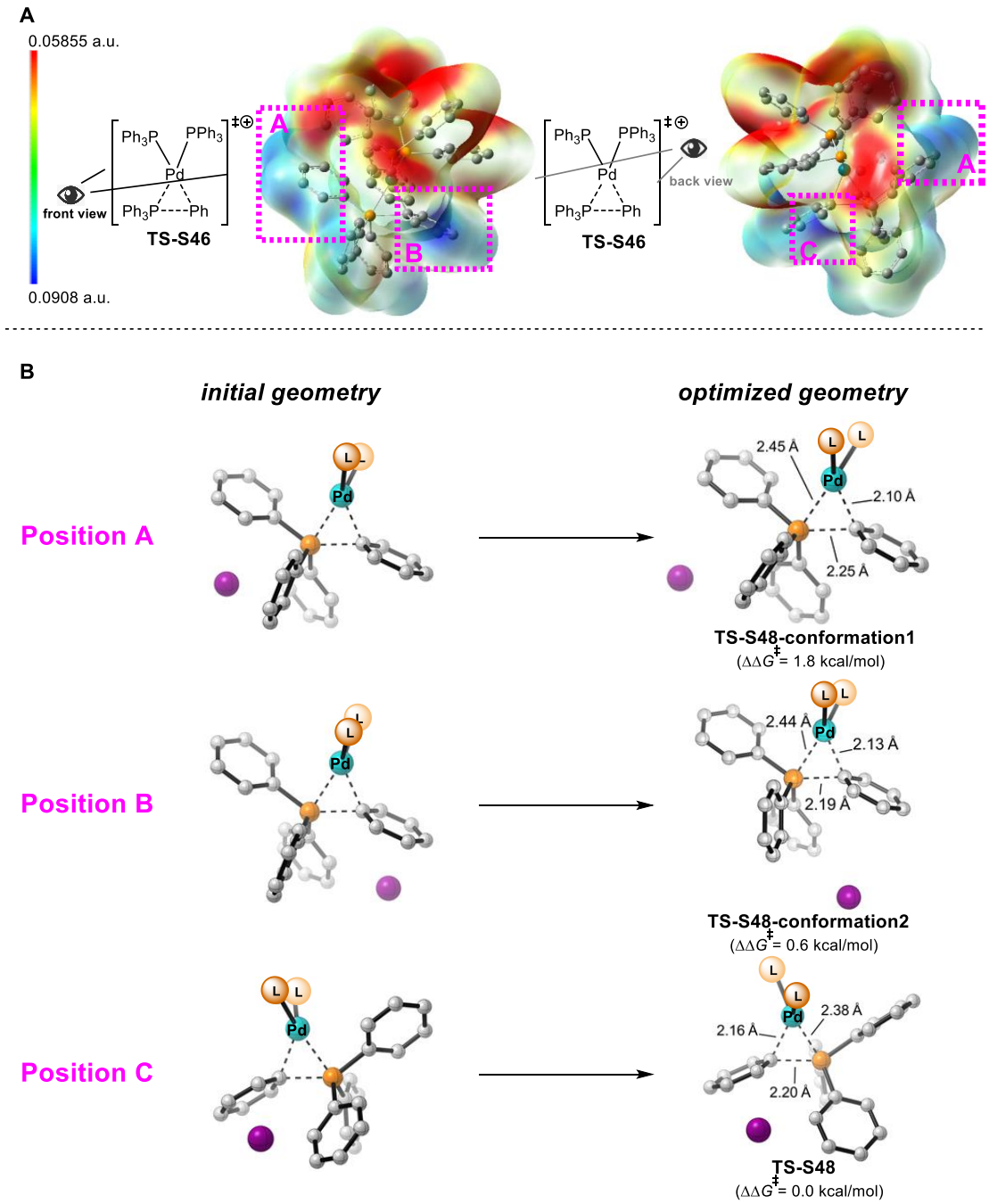


Figure S6. ESP analysis of **TS-S46** (A) and the conformation search of **TS-S48** (B).

The same conformational search process was applied to **TS-S48**, and three conformations were located (**Figure S6**).

6. Key intermediate structures in the IRC of TS7 and TS9.

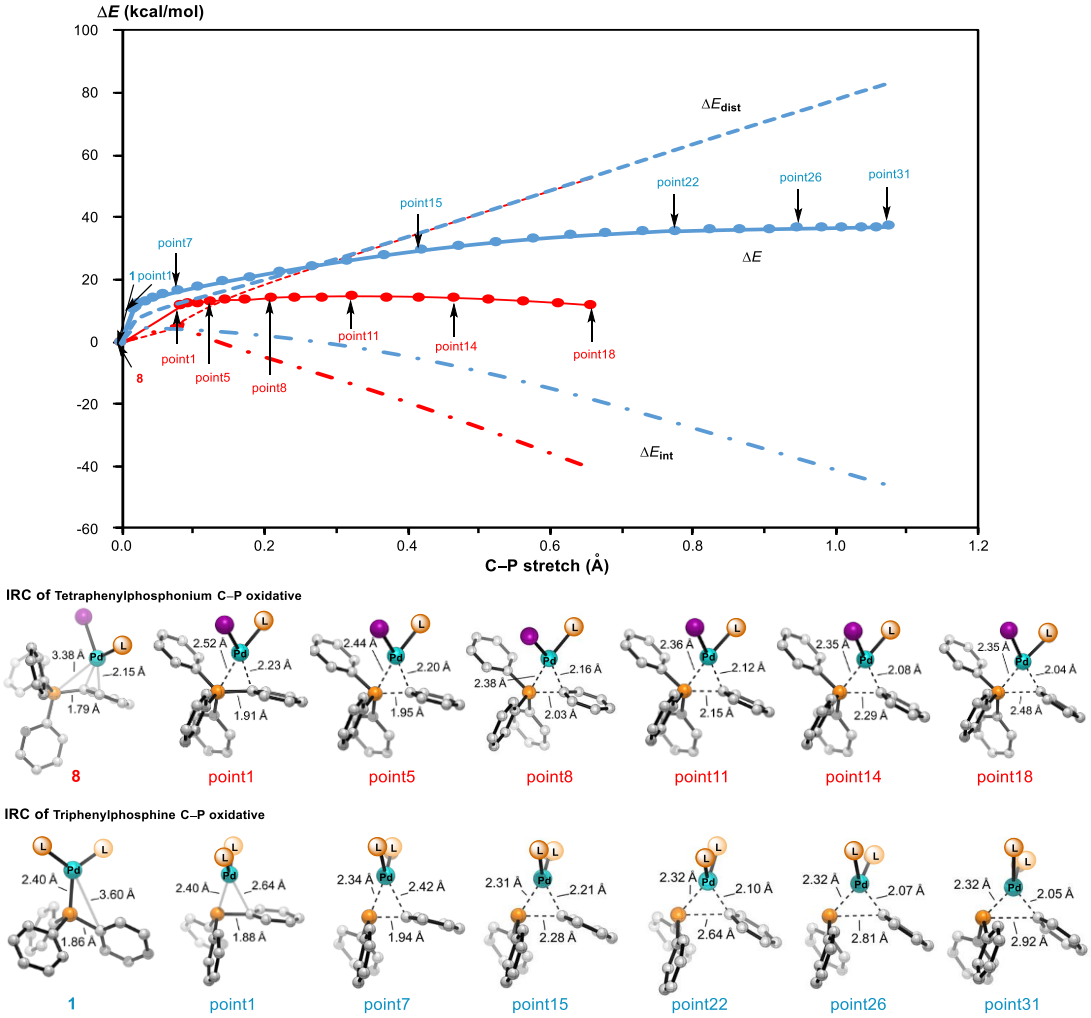


Figure S7. The DFT-computed distortion/interaction analysis of IRC and corresponding structure image.

7. DFT-computed thermodynamics of C–N and C–O bond metathesis.

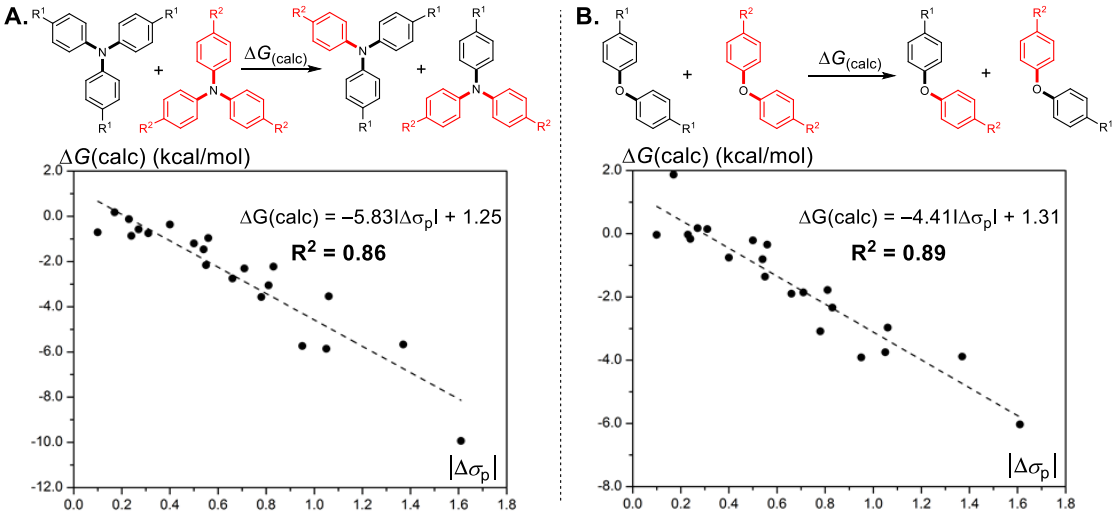
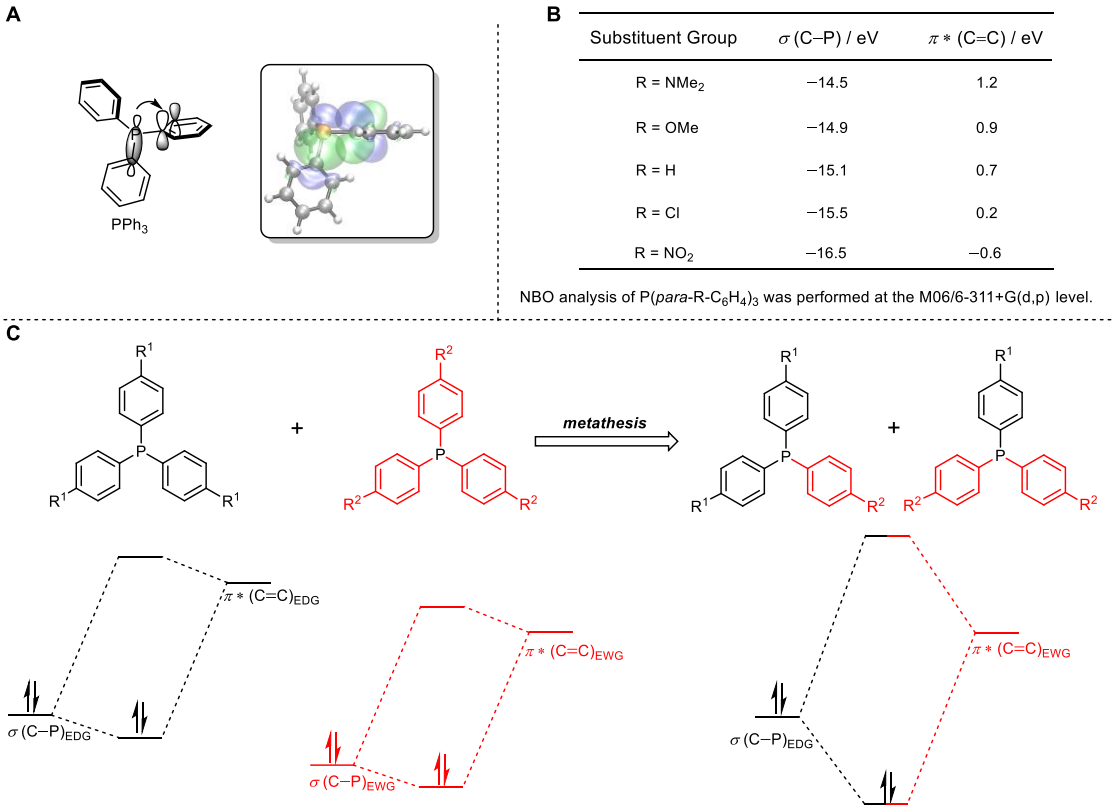


Figure S8. The DFT-computed C–N and C–O metathesis equilibrium with *para*-substituted variants. R^1, R^2 = H, F, Cl, COOMe, CF_3, Ac, CN, NO_2, OMe, Me, NMe_2.

8. Orbital interaction between the C–P σ–bonding orbital and aryl π* orbital in PAr_3.



Substituent Group	σ (C–P) / eV	π * (C=C) / eV
R = NMe_2	−14.5	1.2
R = OMe	−14.9	0.9
R = H	−15.1	0.7
R = Cl	−15.5	0.2
R = NO_2	−16.5	−0.6

NBO analysis of P(*para*-R-C_6H_4)$_3$ was performed at the M06/6-311+G(d,p) level.

Figure S9. Orbital interaction between the C–P σ–bonding orbital and aryl π* orbital in PAr_3. (A) Illustration of the orbital interaction between the filled σ(C–P) orbital and the empty π*(C=C) orbital in PPh_3; (B) Substituent effect on the energy levels of the σ(C–P) orbital and the π*(C=C) orbital in PAr_3; (C) Change of orbital interactions prior and after the metathesis.

9. Tables of energies

Table S1. Energies in Figure 1, Figure 2. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
PPh_3	0.274412	0.291255	0.22806	-1035.918221	-1035.626966	-1035.690161	
PhI	0.0903	0.097134	0.059188	-242.907543	-242.810409	-242.848355	
$IPPh_4$	0.367942	0.392206	0.31077	-1278.855516	-1278.46331	-1278.544746	
1	0.825992	0.880592	0.726625	-3235.785027	-3234.904435	-3235.058402	
2	0.641311	0.686115	0.550065	-2442.746818	-2442.060703	-2442.196753	
TS3	0.640612	0.684969	0.553863	-2442.742091	-2442.057122	-2442.188228	139.67*i*
4	0.642964	0.687046	0.560207	-2442.781602	-2442.094556	-2442.221395	
5	0.366866	0.393644	0.304518	-1406.817846	-1406.424202	-1406.513328	
6	0.64315	0.687247	0.559306	-2442.787473	-2442.100226	-2442.228167	
TS7	0.642605	0.686302	0.559006	-2442.746247	-2442.059945	-2442.187241	93.04*i*
8	0.643517	0.68739	0.559839	-2442.768392	-2442.081002	-2442.208553	
TS9	0.825009	0.87914	0.728395	-3235.728341	-3234.849201	-3234.999946	116.84*i*
10	0.825512	0.879868	0.728351	-3235.746513	-3234.866645	-3235.018162	

Table S2. Energies in Figure 3A. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

	Structures		*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
	Ar=*para*–F–phenyl	pre-int, S1	0.618593	0.665222	0.531126	-2740.510994	-2739.845772	-2739.979868	
		TS, S2	0.617975	0.66419	0.531257	-2740.469202	-2739.805012	-2739.937945	87.27*i*
	Ar=*para*–Cl–phenyl	pre-int, S3	0.614058	0.661936	0.523805	-3821.572902	-382.910967	-3821.049098	
		TS, S4	0.613374	0.660813	0.524235	-3821.531254	-3820.870441	-3821.007019	60.60*i*
	Ar=*para*–COOMe–	pre-int, S5	0.772529	0.830477	0.669314	-3126.266755	-3125.436278	-3125.597441	
	phenyl	TS, S6	0.771539	0.829162	0.668597	-3126.223440	-3125.394278	-3125.554843	53.58*i*
	Ar=*para*–CF_3–phen	pre-int, S7	0.657262	0.712511	0.553658	-3453.886521	-3453.17401	-3453.332863	
	yl	TS, S8	0.656471	0.711228	0.555516	-3453.844662	-3453.133435	-3453.289147	46.90*i*
	Ar=*para*–Ac–pheny	pre-int, S9	0.755454	0.810422	0.656321	-2900.59401	-2899.783589	-2899.93769	
	l	TS, S10	0.754630	0.809242	0.655967	-2900.551047	-2899.741806	-2899.895081	53.40*i*
	Ar=*para*–CN–phen	pre-int, S11	0.638549	0.688239	0.546473	-2719.416324	-2718.728085	-2718.869851	
	yl	TS, S12	0.637766	0.687024	0.546290	-2719.372756	-2718.685733	-2718.826467	30.55*i*
	Ar=*para*–NO_2–phen	pre-int, S13	0.650734	0.702609	0.554267	-3056.196561	-3055.493952	-3055.642294	
	yl	TS, S14	0.650017	0.701444	0.554375	-3056.152114	-3055.45067	-3055.597739	28.80*i*
	Ar=*para*–Me–phen	pre-int, S15	0.725668	0.775474	0.633043	-2560.674131	-2559.898658	-2560.041089	
	yl	TS, S16	0.724952	0.774466	0.631887	-2560.634581	-2559.860116	-2560.002695	106.99*i*
	Ar=*para*–OMe–phe	pre-int, S17	0.741658	0.793594	0.647868	-2786.271535	-2785.477942	-2785.623668	
	nyl	TS, S18	0.740901	0.792495	0.647400	-2786.233093	-2785.440598	-2785.585693	99.31*i*
	Ar=*para*–NMe_2–ph	pre-int, S19	0.863616	0.921100	0.762431	-2844.517334	-2843.596235	-2843.754904	
	enyl	TS, S20	0.862965	0.920272	0.761895	-2844.481065	-2843.560793	-2843.71917	129.90*i*

Table S3. Energies in Figure 3B. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

	Structures		*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
	Ar=*para*–F–phenyl	pre-int, S21	0.634919	0.679879	0.549846	-2542.029304	-2541.349425	-2541.479458	
		TS, S22	0.634398	0.678954	0.548453	-2541.987522	-2541.308568	-2541.439069	80.47*i*
	Ar=*para*–Cl–phenyl	pre-int, S23	0.633518	0.678889	0.547603	-2902.385172	-2901.706283	-2901.837569	
		TS, S24	0.632810	0.677775	0.547534	-2902.34195	-2901.664175	-2901.794416	77.44*i*
	Ar=*para*–COOMe–	pre-int, S25	0.686323	0.735039	0.595924	-2670.617481	-2669.882442	-2670.021557	
	phenyl	TS, S26	0.685595	0.733631	0.595451	-2670.577671	-2669.84404	-2669.98222	63.52*i*
	Ar=*para*–CF_3–phen	pre-int, S27	0.647919	0.695717	0.557694	-2779.825681	-2779.129964	-2779.267987	
	yl	TS, S28	0.647215	0.694594	0.557965	-2779.78042	-2779.085826	-2779.222455	83.39*i*
	Ar=*para*–Ac–pheny	pre-int, S29	0.680694	0.728412	0.591784	-2595.393486	-2594.665074	-2594.801702	
	l	TS, S30	0.680057	0.727239	0.592939	-2595.35032	-2594.623081	-2594.757381	86.70*i*
	Ar=*para*–CN–phen	pre-int, S31	0.641748	0.687704	0.555229	-2535.003278	-2534.315574	-2534.448049	
	yl	TS, S32	0.640744	0.686393	0.553492	-2534.957204	-2534.270811	-2534.403712	95.10*i*
	Ar=*para*–NO_2–phen	pre-int, S33	0.645816	0.692512	0.557732	-2647.264958	-2646.572446	-2646.707226	
	yl	TS, S34	0.644962	0.691226	0.557711	-2647.21905	-2646.527824	-2646.661339	99.91*i*
	Ar=*para*–Me–phen	pre-int, S35	0.670594	0.716645	0.583453	-2482.081826	-2481.365181	-2481.498373	
	yl	TS, S36	0.670173	0.715739	0.584114	-2482.041902	-2481.326163	-2481.457788	82.14*i*
	Ar=*para*–OMe–phe	pre-int, S37	0.675986	0.722684	0.589021	-2557.280074	-2556.55739	-2556.691053	
	nyl	TS, S38	0.675497	0.721686	0.589573	-2557.242674	-2556.520988	-2556.653101	57.58*i*
	Ar=*para*–NMe_2–ph	pre-int, S39	0.716540	0.765045	0.626759	-2576.693342	-2575.928297	-2576.066583	
	enyl	TS, S40	0.715859	0.764107	0.624506	-2576.658915	-2575.894808	-2576.034409	61.65*i*

Table S4. Energies in Figure 4. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*
P(*para*–F–phenyl)$_3$	0.249876	0.269213	0.199932	-1333.641080	-1333.371867	-1333.441148
P(*para*–H–phenyl)(*para*–F–phenyl)$_2$	0.257980	0.276502	0.209138	-1234.400224	-1234.123723	-1234.191087
P(*para*–H–phenyl)$_2$(*para*–F–phenyl)	0.266218	0.283885	0.218769	-1135.159298	-1134.875413	-1134.940529
P(*para*–Cl–phenyl)$_3$	0.245280	0.265878	0.192216	-2414.703712	-2414.437834	-2414.511496
P(*para*–H–phenyl)(*para*–Cl–phenyl)$_2$	0.254967	0.274319	0.204129	-1955.108721	-1954.834403	-1954.904593
P(*para*–H–phenyl)$_2$(*para*–Cl–phenyl)	0.264661	0.282765	0.215994	-1495.513500	-1495.230735	-1495.297506
P(*para*–COOMe–phenyl)$_3$	0.403655	0.434347	0.336606	-1719.398715	-1718.964368	-1719.062109
P(*para*–H–phenyl)(*para*–COOMe–phenyl)$_2$	0.360572	0.386642	0.300390	-1491.572143	-1491.185501	-1491.271753
P(*para*–H–phenyl)$_2$(*para*–COOMe–phenyl)	0.317464	0.338919	0.264265	-1263.745383	-1263.406465	-1263.481119
P(*para*–CF_3–phenyl)$_3$	0.288483	0.316391	0.222122	-2047.018990	-2046.702599	-2046.796868
P(*para*–H–phenyl)(*para*–CF_3–phenyl)$_2$	0.283790	0.308006	0.224114	-1709.985991	-1709.677986	-1709.761878
P(*para*–H–phenyl)$_2$(*para*–CF_3–phenyl)	0.279075	0.299603	0.226057	-1372.952354	-1372.652751	-1372.726297
P(*para*–Ac–phenyl)$_3$	0.386744	0.414398	0.324800	-1493.725420	-1493.311023	-1493.400621
P(*para*–H–phenyl)(*para*–Ac–phenyl)$_2$	0.349308	0.373355	0.292449	-1341.123512	-1340.750157	-1340.831063
P(*para*–H–phenyl)$_2$(*para*–Ac–phenyl)	0.311810	0.332269	0.260060	-1188.521127	-1188.188859	-1188.261068
P(*para*–CN–phenyl)$_3$	0.26981	0.292207	0.215164	-1312.548775	-1312.256568	-1312.333611
P(*para*–H–phenyl)(*para*–CN–phenyl)$_2$	0.271348	0.291899	0.219343	-1220.339610	-1220.047711	-1220.120267
P(*para*–H–phenyl)$_2$(*para*–CN–phenyl)	0.272866	0.291566	0.223636	-1128.129491	-1127.837925	-1127.905855
P(*para*–NO_2–phenyl)$_3$	0.282051	0.306604	0.222760	-1649.328258	-1649.021654	-1649.105498
P(*para*–H–phenyl)(*para*–NO_2–phenyl)$_2$	0.279562	0.301532	0.224633	-1444.859945	-1444.558413	-1444.635312
P(*para*–H–phenyl)$_2$(*para*–NO_2–phenyl)	0.276996	0.296393	0.226462	-1240.389881	-1240.093488	-1240.163419
P(*para*–OMe–phenyl)$_3$	0.372875	0.397499	0.316437	-1379.400062	-1379.002563	-1379.083625

P(*para*–H–phenyl)(*para*–OMe–phenyl)$_2$	0.340034	0.362068	0.28686	-1264.906500	-1264.544432	-1264.61964
P(*para*–H–phenyl)$_2$(*para*–OMe–phenyl)	0.307161	0.326614	0.257285	-1150.412271	-1150.085658	-1150.154987
P(*para*–Me–phenyl)$_3$	0.356816	0.379423	0.300798	-1153.803947	-1153.424524	-1153.503149
P(*para*–H–phenyl)(*para*–Me–phenyl)$_2$	0.329311	0.350002	0.276488	-1114.508806	-1114.158805	-1114.232319
P(*para*–H–phenyl)$_2$(*para*–Me–phenyl)	0.301843	0.320606	0.252321	-1075.213471	-1074.892865	-1074.96115
P(*para*–NMe$_2$–phenyl)$_3$	0.494755	0.524875	0.430862	-1437.643884	-1437.119009	-1437.213022
P(*para*–H–phenyl)(*para*–NMe$_2$–phenyl)$_2$	0.421196	0.446967	0.362807	-1303.736230	-1303.289263	-1303.373423
P(*para*–H–phenyl)$_2$(*para*–NMe$_2$–phenyl)	0.347782	0.369093	0.295443	-1169.827391	-1169.458298	-1169.531948
P(*para*–F–phenyl)(*para*–Cl–phenyl)$_2$	0.246798	0.266976	0.194836	-2054.349568	-2054.082592	-2054.154732
P(*para*–F–phenyl)$_2$(*para*–Cl–phenyl)	0.248320	0.268078	0.197354	-1693.995315	-1693.727237	-1693.797961
P(*para*–F–phenyl)(*para*–COOMe–phenyl)$_2$	0.352375	0.379286	0.290915	-1590.813056	-1590.43377	-1590.522141
P(*para*–F–phenyl)$_2$(*para*–COOMe–phenyl)	0.301100	0.324222	0.245473	-1462.227248	-1461.903026	-1461.981775
P(*para*–F–phenyl)(*para*–CF$_3$–phenyl)$_2$	0.275578	0.300638	0.214496	-1809.226692	-1808.926054	-1809.012196
P(*para*–F–phenyl)$_2$(*para*–CF$_3$–phenyl)	0.262707	0.284904	0.207232	-1571.434130	-1571.149227	-1571.226899
P(*para*–F–phenyl)(*para*–Ac–phenyl)$_2$	0.341122	0.366000	0.283133	-1440.364281	-1439.998282	-1440.081149
P(*para*–F–phenyl)$_2$(*para*–Ac–phenyl)	0.295457	0.317575	0.241394	-1387.002893	-1386.685318	-1386.761499
P(*para*–F–phenyl)(*para*–CN–phenyl)$_2$	0.263152	0.284536	0.209941	-1319.580284	-1319.295748	-1319.370343
P(*para*–F–phenyl)$_2$(*para*–CN–phenyl)	0.256493	0.276857	0.204865	-1326.611010	-1326.334154	-1326.406146
P(*para*–F–phenyl)(*para*–NO$_2$–phenyl)$_2$	0.271361	0.294160	0.215297	-1544.100493	-1543.806334	-1543.885197
P(*para*–F–phenyl)$_2$(*para*–NO$_2$–phenyl)	0.260619	0.281681	0.207624	-1438.871337	-1438.589656	-1438.663713
P(*para*–F–phenyl)(*para*–OMe–phenyl)$_2$	0.331842	0.354713	0.277504	-1364.147366	-1363.792653	-1363.869862
P(*para*–F–phenyl)$_2$(*para*–OMe–phenyl)	0.290851	0.311954	0.238762	-1348.894432	-1348.582478	-1348.65567
P(*para*–F–phenyl)(*para*–Me–phenyl)$_2$	0.321143	0.342671	0.267056	-1213.749978	-1213.407307	-1213.482922

P(*para*–F–phenyl)$_2$(*para*–Me–phenyl)	0.285479	0.305916	0.233460	-1273.695576	-1273.389661	-1273.462117
P(*para*–F–phenyl)(*para*–NMe$_2$–phenyl)$_2$	0.413098	0.439669	0.353771	-1402.977536	-1402.537867	-1402.623765
P(*para*–F–phenyl)$_2$(*para*–NMe$_2$–phenyl)	0.331414	0.354421	0.276453	-1368.309874	-1367.955454	-1368.033422
P(*para*–Cl–phenyl)(*para*–COOMe–phenyl)$_2$	0.350895	0.378207	0.288761	-1951.167153	-1950.788946	-1950.878392
P(*para*–Cl–phenyl)$_2$(*para*–COOMe–phenyl)	0.298077	0.322036	0.240363	-2182.935452	-2182.613416	-2182.695089
P(*para*–Cl–phenyl)(*para*–CF$_3$–phenyl)$_2$	0.27408	0.299548	0.212196	-2169.580675	-2169.281127	-2169.368479
P(*para*–Cl–phenyl)$_2$(*para*–CF$_3$–phenyl)	0.2597	0.282722	0.202311	-2292.142409	-2291.859687	-2291.940098
P(*para*–Cl–phenyl)(*para*–Ac–phenyl)$_2$	0.339618	0.364904	0.280841	-1800.718283	-1800.353379	-1800.437442
P(*para*–Cl–phenyl)$_2$(*para*–Ac–phenyl)	0.292446	0.315389	0.236442	-2107.711154	-2107.395765	-2107.474712
P(*para*–Cl–phenyl)(*para*–CN–phenyl)$_2$	0.261645	0.283437	0.207519	-1679.934210	-1679.650773	-1679.726691
P(*para*–Cl–phenyl)$_2$(*para*–CN–phenyl)	0.253491	0.274671	0.200035	-2047.319246	-2047.044575	-2047.119211
P(*para*–Cl–phenyl)(*para*–NO$_2$–phenyl)$_2$	0.269831	0.293051	0.21265	-1904.454361	-1904.16131	-1904.241711
P(*para*–Cl–phenyl)$_2$(*para*–NO$_2$–phenyl)	0.257572	0.279471	0.202511	-2159.579500	-2159.300029	-2159.376989
P(*para*–Cl–phenyl)(*para*–OMe–phenyl)$_2$	0.330344	0.353632	0.275029	-1724.501988	-1724.148356	-1724.226959
P(*para*–Cl–phenyl)$_2$(*para*–OMe–phenyl)	0.287826	0.309767	0.233671	-2069.603226	-2069.293459	-2069.369555
P(*para*–Cl–phenyl)(*para*–Me–phenyl)$_2$	0.31966	0.341591	0.264729	-1574.104233	-1573.762642	-1573.839504
P(*para*–Cl–phenyl)$_2$(*para*–Me–phenyl)	0.282465	0.303734	0.228471	-1994.404161	-1994.100427	-1994.17569
P(*para*–Cl–phenyl)(*para*–NMe$_2$–phenyl)$_2$	0.411558	0.438582	0.350943	-1763.331925	-1762.893343	-1762.980982
P(*para*–Cl–phenyl)$_2$(*para*–NMe$_2$–phenyl)	0.328359	0.352253	0.271281	-2089.018780	-2088.666527	-2088.747499
P(*para*–COOMe–phenyl)(*para*–CF$_3$–phenyl)$_2$	0.326863	0.355703	0.260342	-1937.812277	-1937.456574	-1937.551935
P(*para*–COOMe–phenyl)$_2$(*para*–CF$_3$–phenyl)	0.36526	0.395026	0.298465	-1828.605603	-1828.210577	-1828.307138
P(*para*–COOMe–phenyl)(*para*–Ac–phenyl)$_2$	0.392385	0.421047	0.32879	-1568.949810	-1568.528763	-1568.62102

P(*para*–COOMe–phenyl)$_2$(*para*–Ac–phenyl)	0.398032	0.427707	0.33277	-1644.174311	-1643.746604	-1643.841541
P(*para*–COOMe–phenyl)(*para*–CN–phenyl)$_2$	0.314424	0.339593	0.255569	-1448.165591	-1447.825998	-1447.910022
P(*para*–COOMe–phenyl)$_2$(*para*–CN–phenyl)	0.359064	0.386986	0.296228	-1583.782393	-1583.395407	-1583.486165
P(*para*–COOMe–phenyl)(*para*–NO_2–phenyl)$_2$	0.32262	0.349215	0.260752	-1672.685683	-1672.336468	-1672.424931
P(*para*–COOMe–phenyl)$_2$(*para*–NO_2–phenyl)	0.363176	0.391804	0.298923	-1696.042582	-1695.650778	-1695.743659
P(*para*–COOMe–phenyl)(*para*–OMe–phenyl)$_2$	0.383161	0.409798	0.323252	-1492.733943	-1492.324145	-1492.410691
P(*para*–COOMe–phenyl)$_2$(*para*–OMe–phenyl)	0.393409	0.422075	0.329922	-1606.066757	-1605.644682	-1605.736835
P(*para*–COOMe–phenyl)(*para*–Me–phenyl)$_2$	0.37243	0.39773	0.312666	-1342.336241	-1341.938511	-1342.023575
P(*para*–COOMe–phenyl)$_2$(*para*–Me–phenyl)	0.388055	0.416048	0.324651	-1530.867727	-1530.451679	-1530.543076
P(*para*–COOMe–phenyl)(*para*–NMe_2–phenyl)$_2$	0.464387	0.494754	0.399491	-1531.564287	-1531.069533	-1531.164796
P(*para*–COOMe–phenyl)$_2$(*para*–NMe_2–phenyl)	0.433975	0.464557	0.367697	-1625.482562	-1625.018005	-1625.114865
P(*para*–CF_3–phenyl)(*para*–Ac–phenyl)$_2$	0.354016	0.381738	0.290713	-1678.156724	-1677.774986	-1677.866011
P(*para*–CF_3–phenyl)$_2$(*para*–Ac–phenyl)	0.32124	0.349058	0.256341	-1862.587763	-1862.238705	-1862.331422
P(*para*–CF_3–phenyl)(*para*–CN–phenyl)$_2$	0.276051	0.30028	0.217539	-1557.372293	-1557.072013	-1557.154754
P(*para*–CF_3–phenyl)$_2$(*para*–CN–phenyl)	0.28228	0.308339	0.220082	-1802.195738	-1801.887399	-1801.975656
P(*para*–CF_3–phenyl)(*para*–NO_2–phenyl)$_2$	0.284221	0.309884	0.222612	-1781.892283	-1781.582399	-1781.669671
P(*para*–CF_3–phenyl)$_2$(*para*–NO_2–phenyl)	0.286377	0.313153	0.22255	-1914.455718	-1914.142565	-1914.233168
P(*para*–CF_3–phenyl)(*para*–OMe–phenyl)$_2$	0.344718	0.37045	0.284806	-1601.941096	-1601.570646	-1601.65629
P(*para*–CF_3–phenyl)$_2$(*para*–OMe–phenyl)	0.316623	0.343436	0.253662	-1824.480735	-1824.137299	-1824.227073
P(*para*–CF_3–phenyl)(*para*–Me–phenyl)$_2$	0.334051	0.358421	0.274575	-1451.543428	-1451.185007	-1451.268853
P(*para*–CF_3–phenyl)$_2$(*para*–Me–phenyl)	0.311259	0.337402	0.248243	-1749.281636	-1748.944234	-1749.033393
P(*para*–CF_3–phenyl)(*para*–NMe_2–phenyl)$_2$	0.425992	0.45544	0.361256	-1640.771681	-1640.316241	-1640.410425

P(*para*–CF_3–phenyl)$_2$(*para*–NMe_2–phenyl)	0.357214	0.385935	0.291492	-1843.896650	-1843.510715	-1843.605158
P(*para*–Ac–phenyl)(*para*–CN–phenyl)$_2$	0.308791	0.332938	0.251735	-1372.941187	-1372.608249	-1372.689452
P(*para*–Ac–phenyl)$_2$(*para*–CN–phenyl)	0.347772	0.373672	0.288317	-1433.333396	-1432.959724	-1433.045079
P(*para*–Ac–phenyl)(*para*–NO_2–phenyl)$_2$	0.316955	0.342543	0.25668	-1597.461202	-1597.118659	-1597.204522
P(*para*–Ac–phenyl)$_2$(*para*–NO_2–phenyl)	0.351869	0.37848	0.290825	-1545.593495	-1545.215015	-1545.30267
P(*para*–Ac–phenyl)(*para*–OMe–phenyl)$_2$	0.377544	0.403173	0.31917	-1417.509589	-1417.106416	-1417.190419
P(*para*–Ac–phenyl)$_2$(*para*–OMe–phenyl)	0.382166	0.408801	0.322069	-1455.618044	-1455.209243	-1455.295975
P(*para*–Ac–phenyl)(*para*–Me–phenyl)$_2$	0.366812	0.391101	0.30868	-1267.111874	-1266.720773	-1266.803194
P(*para*–Ac–phenyl)$_2$(*para*–Me–phenyl)	0.376811	0.402771	0.316887	-1380.419068	-1380.016297	-1380.102181
P(*para*–Ac–phenyl)(*para*–NMe_2–phenyl)$_2$	0.458781	0.48814	0.395517	-1456.340101	-1455.851961	-1455.944584
P(*para*–Ac–phenyl)$_2$(*para*–NMe_2–phenyl)	0.422693	0.451283	0.359575	-1475.033858	-1474.582575	-1474.674283
P(*para*–CN–phenyl)(*para*–NO_2–phenyl)$_2$	0.277965	0.301804	0.220126	-1537.068469	-1536.766665	-1536.848343
P(*para*–CN–phenyl)$_2$(*para*–NO_2–phenyl)	0.273892	0.297007	0.217709	-1424.808650	-1424.511643	-1424.590941
P(*para*–CN–phenyl)(*para*–OMe–phenyl)$_2$	0.338586	0.362457	0.282756	-1357.118467	-1356.75601	-1356.835711
P(*para*–CN–phenyl)$_2$(*para*–OMe–phenyl)	0.30422	0.327353	0.249009	-1334.834417	-1334.507064	-1334.585408
P(*para*–CN–phenyl)(*para*–Me–phenyl)$_2$	0.327876	0.350397	0.272421	-1206.720514	-1206.370117	-1206.448093
P(*para*–CN–phenyl)$_2$(*para*–Me–phenyl)	0.29884	0.321307	0.243661	-1259.635465	-1259.314158	-1259.391804
P(*para*–CN–phenyl)(*para*–NMe_2–phenyl)$_2$	0.419832	0.447447	0.359013	-1395.949009	-1395.501562	-1395.589996
P(*para*–CN–phenyl)$_2$(*para*–NMe_2–phenyl)	0.344788	0.369859	0.286641	-1354.250729	-1353.88087	-1353.964088
P(*para*–NO_2–phenyl)(*para*–OMe–phenyl)$_2$	0.342694	0.367275	0.28547	-1469.378934	-1469.011659	-1469.093464
P(*para*–NO_2–phenyl)$_2$(*para*–OMe–phenyl)	0.312401	0.336964	0.254153	-1559.354967	-1559.018003	-1559.100814
P(*para*–NO_2–phenyl)(*para*–Me–phenyl)$_2$	0.332016	0.355232	0.275251	-1318.981025	-1318.625793	-1318.705774

P(*para*–NO_2–phenyl)$_2$(*para*–Me–phenyl)	0.307047	0.330935	0.248928	-1484.155819	-1483.824884	-1483.906891
P(*para*–NO_2–phenyl)(*para*–NMe_2–phenyl)$_2$	0.42393	0.452275	0.361604	-1508.209751	-1507.757476	-1507.848147
P(*para*–NO_2–phenyl)$_2$(*para*–NMe_2–phenyl)	0.353003	0.379504	0.291956	-1578.771344	-1578.39184	-1578.479388
P(*para*–OMe–phenyl)(*para*–Me–phenyl)$_2$	0.367499	0.391461	0.311061	-1304.201398	-1303.809937	-1303.890337
P(*para*–OMe–phenyl)$_2$(*para*–Me–phenyl)	0.362161	0.38545	0.305844	-1229.002828	-1228.617378	-1228.696984
P(*para*–OMe–phenyl)(*para*–NMe_2–phenyl)$_2$	0.454076	0.482405	0.392441	-1418.229602	-1417.747197	-1417.837161
P(*para*–OMe–phenyl)$_2$(*para*–NMe_2–phenyl)	0.413467	0.439966	0.354384	-1398.814936	-1398.37497	-1398.460552
P(*para*–Me–phenyl)(*para*–NMe_2–phenyl)$_2$	0.448752	0.476399	0.387325	-1343.031092	-1342.554693	-1342.643767
P(*para*–Me–phenyl)$_2$(*para*–NMe_2–phenyl)	0.402708	0.4279	0.343562	-1248.417773	-1247.989873	-1248.074211

Table S5. Energies in Figure S1. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the ωB97X-D/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//ωB97X-D /6-31G(d)-LANL2DZ level of theory.

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
PhI-FigureS1	0.091503	0.098256	0.060479	-243.044782	-242.9465261	-242.9843031	
PPh_3-FigureS1	0.278542	0.295075	0.232532	-1036.248259	-1035.953184	-1036.015727	
5-FigureS1	0.838258	0.891119	0.746263	-3236.800564	-3235.909446	-3236.054302	
6-FigureS1	0.652449	0.695546	0.571625	-2443.613644	-2442.918099	-2443.04202	
TS7-FigureS1	0.651590	0.694267	0.570734	-2443.565226	-2442.870959	-2442.994492	133.61i
8-FigureS1	0.653355	0.695972	0.574560	-2443.590196	-2442.894225	-2443.015637	

Table S6. Energies in Figure S2. Single-point energies (*E*) calculated using def2-TZVP basis set for all atoms in *o*-Xylene.

Structures	*E*
PhI	-529.313183
PPh_3	-1035.996323
5	-1693.330852
6	-2729.375312
TS7	-2729.336749
8	-2729.359019

Table S7. Energies in Figure S3. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
S41	0.549270	0.586511	0.471636	-2199.784747	-2199.198236	-2199.313111	
S42	0.825512	0.879868	0.728351	-3235.746513	-3234.866645	-3235.018162	
TS-S43	0.825359	0.878968	0.732347	-3235.693231	-3234.814263	-3234.960884	76.57*i*
S44	0.825536	0.879592	0.730250	-3235.719226	-3234.839634	-3234.988976	

Table S8. Energies in Figure S4, Figure S5, Figure S6. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
TS-S45	0.642868	0.684164	0.563322	-2431.151024	-2430.46686	-2430.587702	123.82*i*
TS-S46	0.919575	0.978427	0.819565	-3467.102576	-3466.124149	-3466.283011	135.01*i*
TS-S47	0.642289	0.68606	0.556886	-2442.728961	-2442.042901	-2442.172075	123.57*i*
TS-S48	0.919126	0.980487	0.814015	-3478.674615	-3477.694128	-3477.8606	146.39*i*
TS-S47-conformation1	0.642288	0.686156	0.557232	-2442.723268	-2442.037112	-2442.166036	146.23*i*
TS-S48-conformation1	0.918866	0.980317	0.812742	-3478.670282	-3477.689965	-3477.85754	156.3*i*
TS-S48-conformation2	0.919188	0.980648	0.812745	-3478.672309	-3477.691661	-3477.859564	137.53*i*

Table S9. Energies in Figure S7. Energies(*E*) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD level of theory in solvent *o*–Xylene.

Structures		E_1	E_2	E_3	E_4	E_5
IRC of tetraphenylphosphonium C-P oxidative	Point-1	-1267.276996	-1175.428899	-1267.250401	-1175.398894	-2442.750111
	Point-2	-1267.276996	-1175.428899	-1267.248659	-1175.398550	-2442.749589
	Point-3	-1267.276996	-1175.428899	-1267.246499	-1175.398166	-2442.749018
	Point-4	-1267.276996	-1175.428899	-1267.244099	-1175.397789	-2442.748436
	Point-5	-1267.276996	-1175.428899	-1267.241420	-1175.397416	-2442.747847
	Point-6	-1267.276996	-1175.428899	-1267.238369	-1175.397052	-2442.747257
	Point-7	-1267.276996	-1175.428899	-1267.234842	-1175.396688	-2442.746673
	Point-8	-1267.276996	-1175.428899	-1267.230527	-1175.396308	-2442.746127
	Point-9	-1267.276996	-1175.428899	-1267.226590	-1175.396017	-2442.745774
	Point-10	-1267.276996	-1175.428899	-1267.222216	-1175.395732	-2442.745539
	Point-11	-1267.276996	-1175.428899	-1267.217431	-1175.395461	-2442.745446
	Point-12	-1267.276996	-1175.428899	-1267.212264	-1175.395203	-2442.745525
	Point-13	-1267.276996	-1175.428899	-1267.206849	-1175.394953	-2442.745776
	Point-14	-1267.276996	-1175.428899	-1267.201301	-1175.394718	-2442.746291
	Point-15	-1267.276996	-1175.428899	-1267.195694	-1175.394494	-2442.746936
	Point-16	-1267.276996	-1175.428899	-1267.190188	-1175.394282	-2442.747777
	Point-17	-1267.276996	-1175.428899	-1267.184840	-1175.394085	-2442.748781
	Point-18	-1267.276996	-1175.428899	-1267.179731	-1175.393903	-2442.749921
	Point-19	-1267.276996	-1175.428899	-1267.250401	-1175.398894	-2442.750111
IRC of triphenylphosphonine C-P oxidative	Point-1	-1035.918221	-2199.826392	-1035.910444	-2199.810011	-3235.768148
	Point-2	-1035.918221	-2199.826392	-1035.909898	-2199.809423	-3235.767034
	Point-3	-1035.918221	-2199.826392	-1035.909262	-2199.808766	-3235.765801
	Point-4	-1035.918221	-2199.826392	-1035.908507	-2199.808053	-3235.764436
	Point-5	-1035.918221	-2199.826392	-1035.907575	-2199.807303	-3235.762906
	Point-6	-1035.918221	-2199.826392	-1035.906386	-2199.806535	-3235.761174
	Point-7	-1035.918221	-2199.826392	-1035.904834	-2199.805773	-3235.759207
	Point-8	-1035.918221	-2199.826392	-1035.902801	-2199.805037	-3235.756987
	Point-9	-1035.918221	-2199.826392	-1035.900192	-2199.804376	-3235.754524
	Point-10	-1035.918221	-2199.826392	-1035.896979	-2199.803712	-3235.751850
	Point-11	-1035.918221	-2199.826392	-1035.893199	-2199.803076	-3235.749038
	Point-12	-1035.918221	-2199.826392	-1035.888909	-2199.80246	-3235.746191
	Point-13	-1035.918221	-2199.826392	-1035.884178	-2199.801853	-3235.743395
	Point-14	-1035.918221	-2199.826392	-1035.879099	-2199.801247	-3235.740721
	Point-15	-1035.918221	-2199.826392	-1035.873765	-2199.800637	-3235.738238
	Point-16	-1035.918221	-2199.826392	-1035.868253	-2199.800018	-3235.735996
	Point-17	-1035.918221	-2199.826392	-1035.862639	-2199.799383	-3235.734021
	Point-18	-1035.918221	-2199.826392	-1035.857005	-2199.798731	-3235.732328
	Point-19	-1035.918221	-2199.826392	-1035.851512	-2199.798047	-3235.730942
	Point-20	-1035.918221	-2199.826392	-1035.846102	-2199.797339	-3235.729830
	Point-21	-1035.918221	-2199.826392	-1035.840926	-2199.796594	-3235.728977

Point-22	-1035.918221	-2199.826392	-1035.836021	-2199.795811	-3235.728341
Point-23	-1035.918221	-2199.826392	-1035.831483	-2199.794985	-3235.727874
Point-24	-1035.918221	-2199.826392	-1035.827339	-2199.794119	-3235.727530
Point-25	-1035.918221	-2199.826392	-1035.823595	-2199.793205	-3235.727260
Point-26	-1035.918221	-2199.826392	-1035.820293	-2199.792251	-3235.727026
Point-27	-1035.918221	-2199.826392	-1035.817444	-2199.791275	-3235.726805
Point-28	-1035.918221	-2199.826392	-1035.814779	-2199.790303	-3235.726592
Point-29	-1035.918221	-2199.826392	-1035.812774	-2199.789364	-3235.726441
Point-30	-1035.918221	-2199.826392	-1035.811356	-2199.788487	-3235.726240
Point-31	-1035.918221	-2199.826392	-1035.810086	-2199.787686	-3235.726063

Table S10. Energies in Figure S8. Zero-point correction (*ZPE*), thermal correction to enthalpy (*tcH*), thermal correction to Gibbs free energy (*tc*G), energies(*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the M06/6-311+G(d,p)-SDD-SMD(*o*–Xylene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*
N(*para*–H–phenyl)$_3$	0.279032	0.294773	0.235388	-749.307933	-749.01316	-749.072545
N(*para*–Cl–phenyl)$_3$	0.250031	0.269550	0.199853	-2128.092785	-2127.823236	-2127.892933
N(*para*–H–phenyl)(*para*–Cl–phenyl)$_2$	0.259753	0.278001	0.211873	-1668.498149	-1668.220148	-1668.286276
N(*para*–H–phenyl)$_2$(*para*–Cl–phenyl)	0.269410	0.286400	0.223678	-1208.903090	-1208.616691	-1208.679413
N(*para*–CF$_3$–phenyl)$_3$	0.293380	0.320096	0.231657	-1760.412507	-1760.092412	-1760.180851
N(*para*–H–phenyl)(*para*–CF$_3$–phenyl)$_2$	0.288704	0.311734	0.233190	-1423.378766	-1423.067033	-1423.145577
N(*para*–H–phenyl)$_2$(*para*–CF$_3$–phenyl)	0.283796	0.303225	0.233587	-1086.343746	-1086.040522	-1086.11016
N(*para*–NO$_2$–phenyl)$_3$	0.287044	0.310385	0.231454	-1362.725177	-1362.414792	-1362.493723
N(*para*–H–phenyl) (*para*–NO$_2$–phenyl)$_2$	0.284567	0.305347	0.233088	-1158.255598	-1157.950252	-1158.022511
N(*para*–H–phenyl)$_2$(*para*–NO$_2$–phenyl)	0.281878	0.300147	0.234121	-953.7835682	-953.483421	-953.549447
N(*para*–OMe–phenyl)$_3$	0.377276	0.400904	0.323038	-1092.783956	-1092.383053	-1092.460919
N(*para*–H–phenyl)(*para*–OMe–phenyl)$_2$	0.344469	0.365498	0.293501	-978.292240	-977.926742	-977.998739
N(*para*–H–phenyl)$_2$(*para*–OMe–phenyl)	0.311853	0.330197	0.264764	-863.800412	-863.470215	-863.535648
N(*para*–Me–phenyl)$_3$	0.36166	0.383068	0.309463	-867.191626	-866.808558	-866.882163
N(*para*–H–phenyl)(*para*–Me–phenyl)$_2$	0.334132	0.353646	0.284853	-827.897110	-827.543464	-827.612257
N(*para*–H–phenyl)$_2$(*para*–Me–phenyl)	0.306664	0.324251	0.260500	-788.602668	-788.278417	-788.342168
N(*para*–NMe$_2$–phenyl)$_3$	0.499062	0.527952	0.437704	-1151.02432	-1150.496369	-1150.586617
N(*para*–H–phenyl) (*para*–NMe$_2$–phenyl)$_2$	0.425669	0.450331	0.369858	-1017.120701	-1016.67037	-1016.750843
N(*para*–H–phenyl)$_2$(*para*–NMe$_2$–phenyl)	0.352453	0.372629	0.302977	-883.21484	-882.842211	-882.911863
N(*para*–Cl–phenyl)(*para*–CF$_3$–phenyl)$_2$	0.278983	0.303274	0.221351	-1882.973067	-1882.669794	-1882.751717
N(*para*–Cl–phenyl)$_2$(*para*–CF$_3$–phenyl)	0.264442	0.286384	0.209835	-2005.533093	-2005.246710	-2005.323259
N(*para*–Cl–phenyl)(*para*–NO$_2$–phenyl)$_2$	0.274830	0.296863	0.221192	-1617.849459	-1617.552597	-1617.628268
N(*para*–Cl–phenyl)$_2$(*par*	0.262426	0.283210	0.210369	-1872.972198	-1872.688988	-1872.761829

a–NO_2–phenyl)						
N(*para*–Cl–phenyl)(*para*–OMe–phenyl)$_2$	0.334841	0.357124	0.281962	-1437.887903	-1437.530779	-1437.605941
N(*para*–Cl–phenyl)$_2$(*para*–OMe–phenyl)	0.292433	0.313340	0.240816	-1782.990646	-1782.677306	-1782.749830
N(*para*–Cl–phenyl)(*para*–Me–phenyl)$_2$	0.324426	0.345230	0.272751	-1287.492403	-1287.147174	-1287.219653
N(*para*–Cl–phenyl)$_2$(*para*–Me–phenyl)	0.287361	0.307457	0.236925	-1707.792952	-1707.485496	-1707.556028
N(*para*–Cl–phenyl)(*para*–NMe_2–phenyl)$_2$	0.416072	0.442025	0.358095	-1476.71661	-1476.274585	-1476.358515
N(*para*–Cl–phenyl)$_2$(*para*–NMe_2–phenyl)	0.333094	0.355857	0.278969	-1802.405639	-1802.049783	-1802.126671
N(*para*–CF_3–phenyl)(*para*–NO_2–phenyl)$_2$	0.289232	0.313693	0.231416	-1495.288257	-1494.974565	-1495.056842
N(*para*–CF_3–phenyl)$_2$(*para*–NO_2–phenyl)	0.291318	0.316907	0.231436	-1627.850548	-1627.533641	-1627.619112
N(*para*–CF_3–phenyl)(*para*–OMe–phenyl)$_2$	0.349371	0.374034	0.292492	-1315.329383	-1314.955349	-1315.036891
N(*para*–CF_3–phenyl)$_2$(*para*–OMe–phenyl)	0.321399	0.347084	0.262210	-1537.871956	-1537.524873	-1537.609747
N(*para*–CF_3–phenyl)(*para*–Me–phenyl)$_2$	0.338781	0.362048	0.282452	-1164.933473	-1164.571426	-1164.651022
N(*para*–CF_3–phenyl)$_2$(*para*–Me–phenyl)	0.316282	0.341171	0.258142	-1462.673808	-1462.332637	-1462.415666
N(*para*–CF_3–phenyl)(*para*–NMe_2–phenyl)$_2$	0.430694	0.458996	0.369077	-1354.158684	-1353.699688	-1353.789607
N(*para*–CF_3–phenyl)$_2$(*para*–NMe_2–phenyl)	0.362027	0.389570	0.300294	-1557.287191	-1556.897622	-1556.986898
N(*para*–NO_2–phenyl)(*para*–OMe–phenyl)$_2$	0.347525	0.370998	0.293189	-1182.770188	-1182.399190	-1182.476999
N(*para*–NO_2–phenyl)$_2$(*para*–OMe–phenyl)	0.317381	0.340759	0.262533	-1272.749507	-1272.408749	-1272.486975
N(*para*–NO_2–phenyl)(*para*–Me–phenyl)$_2$	0.336819	0.358981	0.281849	-1032.373777	-1032.014797	-1032.091929
N(*para*–NO_2–phenyl)$_2$(*para*–Me–phenyl)	0.312126	0.334773	0.257948	-1197.55104	-1197.216267	-1197.293092
N(*para*–NO_2–phenyl)(*para*–NMe_2–phenyl)$_2$	0.428845	0.456002	0.369622	-1221.600552	-1221.144550	-1221.230930
N(*para*–NO_2–phenyl)$_2$(*para*–NMe_2–phenyl)	0.357969	0.383279	0.300320	-1292.165565	-1291.782286	-1291.865245
N(*para*–OMe–phenyl)(*para*–Me–phenyl)$_2$	0.366766	0.388998	0.313077	-942.3891218	-942.000124	-942.076045
N(*para*–OMe–phenyl)$_2$(	0.372069	0.394958	0.318566	-1017.586732	-1017.191775	-1017.268167

para–Me–phenyl)						
N(*para*–OMe–phenyl)(*para*–NMe_2–phenyl)$_2$	0.458556	0.485769	0.399465	-1131.611715	-1131.125946	-1131.212250
N(*para*–OMe–phenyl)$_2$(*para*–NMe_2–phenyl)	0.417808	0.443275	0.361128	-1112.197957	-1111.754682	-1111.836829
N(*para*–Me–phenyl)(*para*–NMe_2–phenyl)$_2$	0.453179	0.479762	0.393829	-1056.41472	-1055.934959	-1056.020892
N(*para*–Me–phenyl)$_2$(*para*–NMe_2–phenyl)	0.407429	0.431468	0.351238	-961.803516	-961.372048	-961.452278
O(*para*–H–phenyl)$_2$	0.185731	0.196656	0.148387	-538.253823	-538.057168	-538.105437
O(*para*–H–phenyl)(*para*–Cl–phenyl)	0.176070	0.188231	0.136495	-997.848295	-997.660064	-997.711800
O(*para*–H–phenyl)(*para*–CF_3–phenyl)	0.190537	0.205095	0.146740	-875.289051	-875.083957	-875.142312
O(*para*–H–phenyl)(*para*–NO_2–phenyl)	0.188469	0.201927	0.146525	-742.727471	-742.525545	-742.580947
O(*para*–H–phenyl)(*para*–Me–phenyl)	0.213166	0.225129	0.174460	-577.548355	-577.323227	-577.373896
O(*para*–H–phenyl)(*para*–OMe–phenyl)	0.218503	0.232018	0.177644	-652.745925	-652.513907	-652.568281
O(*para*–H–phenyl)(*para*–NMe_2–phenyl)	0.259194	0.274493	0.215772	-672.16036	-671.885867	-671.944588
O(*para*–Cl–phenyl)$_2$	0.166389	0.179791	0.124425	-1457.442541	-1457.262751	-1457.318117
O(*para*–Cl–phenyl)(*para*–CF_3–phenyl)	0.180869	0.196653	0.135161	-1334.883049	-1334.686396	-1334.747888
O(*para*–Cl–phenyl)(*para*–NO_2–phenyl)	0.178802	0.193459	0.135262	-1202.321176	-1202.127718	-1202.185915
O(*para*–Cl–phenyl)(*para*–Me–phenyl)	0.203595	0.217669	0.160757	-1037.14308	-1036.925412	-1036.982324
O(*para*–Cl–phenyl)(*para*–OMe–phenyl)	0.208867	0.223621	0.165824	-1112.34075	-1112.117130	-1112.174927
O(*para*–Cl–phenyl)(*para*–NMe_2–phenyl)	0.249584	0.266143	0.204127	-1131.755562	-1131.489420	-1131.551436
O(*para*–CF_3–phenyl)$_2$	0.195262	0.213486	0.144795	-1212.322688	-1212.109202	-1212.177893
O(*para*–CF_3–phenyl)(*para*–NO_2–phenyl)	0.193227	0.210302	0.145485	-1079.760333	-1079.550032	-1079.614849
O(*para*–CF_3–phenyl)(*para*–Me–phenyl)	0.218083	0.234547	0.170986	-914.584078	-914.349531	-914.413092
O(*para*–CF_3–phenyl)(*para*–OMe–phenyl)	0.223327	0.240493	0.175590	-989.781654	-989.541161	-989.606064
O(*para*–CF_3–phenyl)(*para*–NMe_2–phenyl)	0.264093	0.283037	0.214464	-1009.196517	-1008.913480	-1008.982053
O(*para*–NO_2–phenyl)$_2$	0.191050	0.207005	0.145677	-947.197219	-946.990214	-947.051542
O(*para*–NO_2–phenyl)(*p*	0.215995	0.231358	0.170876	-782.022431	-781.791074	-781.851556

ara–Me–phenyl)						
O(*para*–NO_2–phenyl)(*para*–OMe–phenyl)	0.221272	0.237304	0.175811	-857.22027	-856.982966	-857.044459
O(*para*–NO_2–phenyl)(*para*–NMe_2–phenyl)	0.262059	0.279878	0.214984	-876.635573	-876.355696	-876.420590
O(*para*–Me–phenyl)$_2$	0.240847	0.255543	0.197401	-616.84273	-616.587187	-616.645329
O(*para*–Me–phenyl)(*para*–OMe–phenyl)	0.246025	0.261459	0.201813	-692.040205	-691.778747	-691.838393
O(*para*–Me–phenyl)(*para*–NMe_2–phenyl)	0.286750	0.303937	0.240381	-711.454569	-711.150633	-711.214189
O(*para*–OMe–phenyl)$_2$	0.251249	0.267400	0.205566	-767.236967	-766.969567	-767.031401
O(*para*–OMe–phenyl)(*para*–NMe_2–phenyl)	0.291934	0.309826	0.245397	-786.651382	-786.341557	-786.405986
O(*para*–NMe_2–phenyl)$_2$	0.332560	0.352073	0.283844	-806.063863	-805.711790	-805.780019

10. Cartesian coordinates for calculated species

PPh_3

0 1

P	0.00071700	0.00041700	-1.20745800
C	-0.40763600	-1.61889500	-0.40348600
C	-1.19799800	1.16367700	-0.40387900
C	1.60751000	0.45620700	-0.40364500
C	0.07680800	-2.77949600	-1.03110500
C	-1.18579200	-1.75939100	0.75598700
C	-2.44315400	1.32791800	-1.03476500
C	-0.93402900	1.90302300	0.75970300
C	2.37067100	1.45575600	-1.03138100
C	2.11789400	-0.14685500	0.75662100
C	-0.19038800	-4.04326000	-0.50432800
H	0.66391500	-2.69043800	-1.94239100
C	-1.46328200	-3.02537000	1.27736400
H	-1.57965700	-0.87730700	1.25168500
C	-3.40568900	2.18875800	-0.50691800
H	-2.65674400	0.77957000	-1.94953100
C	-1.89327200	2.77388200	1.28214400
H	0.02534400	1.80138800	1.25794600
C	3.59788800	1.85740500	-0.50351100
H	2.00083800	1.91879600	-1.94345400
C	3.35211200	0.24721800	1.27908300
H	1.55183500	-0.92990400	1.25215100
C	-0.96433500	-4.16930800	0.65167300
H	0.19610000	-4.92905900	-1.00179500
H	-2.07001100	-3.11638400	2.17488300
C	-3.13157300	2.91641500	0.65344500
H	-4.36435500	2.29945900	-1.00711200
H	-1.67141900	3.34106100	2.18272500
C	4.09302300	1.25162500	0.65366300
H	4.17186800	2.63488900	-1.00106000
H	3.73382700	-0.23199900	2.17718300
H	-1.18229700	-5.15336400	1.05836300
H	-3.87608600	3.59522400	1.06110700

H	5.05352900	1.55594900	1.06118800

PhI

0 1

C	0.00000000	1.21564600	-1.26405700
C	0.00000000	0.00000000	-0.58127100
C	0.00000000	-1.21564600	-1.26405700
C	0.00000000	-1.20716400	-2.66160900
C	0.00000000	0.00000000	-3.36214900
C	0.00000000	1.20716400	-2.66160900
H	0.00000000	2.15526100	-0.72252600
H	0.00000000	-2.15526100	-0.72252600
H	0.00000000	-2.15192000	-3.19871200
H	0.00000000	0.00000000	-4.44840800
H	0.00000000	2.15192000	-3.19871200
I	0.00000000	0.00000000	1.56715800

$IPPh_4$

0 1

P	1.08650500	0.02317000	-0.00096900
C	0.74382200	1.22032100	1.32498100
C	0.48342000	-1.63687600	0.40375800
C	-0.57735500	1.67911900	1.47235500
C	1.75598000	1.69032600	2.17874600
C	1.14626900	-2.76134200	-0.12907100
C	-0.67729500	-1.80544000	1.17553100
C	-0.87666300	2.58614200	2.48918100
H	-1.38731200	1.32403400	0.82931200
C	1.44241900	2.60577200	3.18264100
H	2.78199400	1.35938600	2.05941800
C	0.66107800	-4.03886500	0.13156100
H	2.03568100	-2.64084400	-0.73922600
C	-1.15618500	-3.09435500	1.42330900
H	-1.24139900	-0.95872300	1.54809800
C	0.12725300	3.05066700	3.34070300
H	-1.90343400	2.92035600	2.60438600
H	2.22706500	2.97142600	3.83898500

C	-0.48863000	-4.20509600	0.91328600
H	1.17571500	-4.90345200	-0.27772500
H	-2.06982400	-3.21035800	1.99706900
H	-0.11221400	3.76183400	4.12670900
H	-0.86725800	-5.20404200	1.11157500
C	2.89219200	-0.12250700	-0.23310800
C	3.65959400	-0.74565800	0.76875700
C	3.52624900	0.35529000	-1.38866600
C	5.03991700	-0.86746100	0.62002100
H	3.17883200	-1.14810500	1.65554200
C	4.90922800	0.22556300	-1.53280200
H	2.94506900	0.81770700	-2.17867500
C	5.66667300	-0.38008800	-0.53024400
H	5.62389000	-1.34955400	1.39857400
H	5.39047200	0.59521700	-2.43353600
H	6.74212500	-0.48018900	-0.64618100
C	0.31230000	0.64125000	-1.51485100
C	0.61365900	1.94335300	-1.96143500
C	-0.63488100	-0.13521300	-2.19579500
C	0.00892900	2.43525300	-3.11334400
H	1.30407400	2.57212000	-1.40541800
C	-1.24283200	0.37440100	-3.34586300
H	-0.92732400	-1.10862700	-1.82131900
C	-0.91548600	1.64602100	-3.80880700
H	0.24227600	3.43810400	-3.45898300
H	-1.99787700	-0.21819100	-3.85146200
H	-1.39869800	2.03940600	-4.69866700
I	-3.70862900	-0.09223600	0.04398100

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P	-2.37313300	0.36638800	-0.07417900
C	-3.57172300	-0.96076100	-0.59133700
C	-2.96109400	1.80316100	-1.09215700
C	-3.00272700	0.76446700	1.62857100
C	-3.37945600	-2.25238300	-0.07285900
C	-4.64053900	-0.74853700	-1.47528000

C	-2.35031700	1.99401700	-2.34270300
C	-3.96168000	2.70100100	-0.69094400
C	-2.10193000	1.31362500	2.55631000
C	-4.32653400	0.53190600	2.03715100
C	-4.23934000	-3.29561900	-0.41106500
H	-2.54364600	-2.44465700	0.59366600
C	-5.49550600	-1.79810400	-1.82501500
H	-4.81180900	0.23784800	-1.89364800
C	-2.74267100	3.03853600	-3.17915900
H	-1.55081700	1.32423100	-2.65025800
C	-4.34420500	3.75748600	-1.52211000
H	-4.44468500	2.58016300	0.27380500
C	-2.51619900	1.64083900	3.84910400
H	-1.06739900	1.47045700	2.26149600
C	-4.73964200	0.85481800	3.33137200
H	-5.03610600	0.09014700	1.34390000
C	-5.30094200	-3.07208700	-1.29194300
H	-4.06845400	-4.28703600	-0.00055800
H	-6.31645100	-1.61389400	-2.51379400
C	-3.74039500	3.92620600	-2.76915400
H	-2.25860700	3.16899700	-4.14351000
H	-5.11839300	4.44664800	-1.19347400
C	-3.83707800	1.41283300	4.23961200
H	-1.80302000	2.06516400	4.55111300
H	-5.76790200	0.66714000	3.63040300
H	-5.96631000	-3.88720500	-1.56482200
H	-4.03954600	4.74794700	-3.41462400
H	-4.16011200	1.66107100	5.24737500
Pd	-0.00079500	0.00025900	-0.11524200
P	0.86866400	-2.23778200	-0.07444300
C	2.61526600	-2.61336800	-0.59756800
C	-0.08534300	-3.46850500	-1.08504000
C	0.84560700	-2.97700200	1.63061900
C	3.64038500	-1.80376900	-0.08001400
C	2.96179200	-3.64277800	-1.48578300
C	-0.56276600	-3.03845000	-2.33422000
C	-0.35799000	-4.78375100	-0.67992800

C	-0.07507300	-2.46688300	2.56110900
C	1.70887800	-4.00760300	2.03837900
C	4.97240400	-2.02729900	-0.42328700
H	3.39229900	-0.98563600	0.59001000
C	4.29683200	-3.85884200	-1.84058900
H	2.19109800	-4.28215300	-1.90356100
C	-1.27322100	-3.90366300	-3.16567100
H	-0.38587000	-2.01147800	-2.64472600
C	-1.08382800	-5.64638000	-1.50591400
H	-0.00648200	-5.13903500	0.28383800
C	-0.14632100	-2.98515400	3.85581600
H	-0.72772600	-1.64878900	2.26686400
C	1.64075000	-4.52275400	3.33451000
H	2.44231400	-4.40481200	1.34302400
C	5.30555600	-3.05616800	-1.30837400
H	5.74762600	-1.38579000	-0.01327700
H	4.54457500	-4.66014400	-2.53256600
C	-1.53852300	-5.21124800	-2.75174900
H	-1.63338200	-3.55238900	-4.12909700
H	-1.29000400	-6.66117200	-1.17423700
C	0.71136700	-4.01555500	4.24549100
H	-0.86632900	-2.57613100	4.55993800
H	2.31726500	-5.31979200	3.63286900
H	6.34305900	-3.22524600	-1.58511400
H	-2.10220000	-5.88365200	-3.39325200
H	0.66176700	-4.41625500	5.25471800
P	1.50394800	1.87119300	-0.07453900
C	0.95605700	3.57190800	-0.59658900
C	3.04513600	1.65967600	-1.08745800
C	2.15851100	2.21964000	1.62976600
C	-0.26231400	4.05070400	-0.08631500
C	1.67936500	4.39113400	-1.47668400
C	2.90852500	1.03505800	-2.33823100
C	4.32192700	2.07687300	-0.68247500
C	2.18208700	1.16572300	2.55853000
C	2.61642400	3.48319100	2.03885700
C	-0.73469200	5.31634600	-0.42880400

H	-0.85045700	3.42307200	0.57698800
C	1.19924200	5.65568000	-1.83058400
H	2.62206400	4.04643500	-1.88879600
C	4.01172700	0.85182700	-3.17127900
H	1.92942000	0.67825800	-2.64869500
C	5.43059000	1.87904300	-1.51014100
H	4.45599900	2.55588300	0.28253500
C	2.66872700	1.36235200	3.85252500
H	1.80214100	0.19081700	2.26371900
C	3.09866300	3.68095700	3.33437100
H	2.58990600	4.31815400	1.34507000
C	-0.00519100	6.12370800	-1.30568400
H	-1.68166900	5.66364300	-0.02479000
H	1.77316100	6.27437000	-2.51624500
C	5.27829500	1.27146100	-2.75746300
H	3.88537900	0.36730700	-4.13594400
H	6.41367900	2.20447100	-1.17854400
C	3.12925300	2.62104300	4.24345400
H	2.67835400	0.53308700	4.55518200
H	3.44826400	4.66591600	3.63370200
H	-0.37741300	7.10693100	-1.58191900
H	6.14141900	1.11902400	-3.40024200
H	3.50262500	2.77784000	5.25219900

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Pd	0.24915400	-0.19161600	-0.65162700
P	2.41824500	-0.96654900	-0.04070600
C	2.79867300	-0.98141700	1.77432800
C	1.99977900	-0.20160500	2.62443600
C	3.84577200	-1.73237800	2.33697500
C	2.24984000	-0.15671200	3.99775300
H	1.16968300	0.35928900	2.20496300
C	4.09391600	-1.68926200	3.70970400
H	4.46172700	-2.36314000	1.70280600
C	3.29834100	-0.89876500	4.54302600
H	1.61644600	0.45071700	4.63865300

H	4.90683400	-2.27690900	4.12874600
H	3.49056600	-0.86965400	5.61243500
C	3.75316100	0.10238400	-0.76539700
C	4.98061600	0.36528500	-0.13814800
C	3.50203100	0.68528000	-2.01915000
C	5.93194500	1.18358200	-0.75195500
H	5.19507100	-0.05980500	0.83703800
C	4.45874400	1.48952000	-2.63997400
H	2.53942800	0.51661800	-2.49646300
C	5.67681600	1.74291100	-2.00557100
H	6.87487100	1.38178200	-0.24852200
H	4.24634200	1.92953200	-3.61083500
H	6.41916100	2.37816500	-2.48166000
C	2.97153800	-2.66829900	-0.54090800
C	3.86357700	-2.90101200	-1.59830000
C	2.39275300	-3.77888600	0.10118200
C	4.17084700	-4.20434500	-2.00011500
H	4.32934300	-2.06409500	-2.10910500
C	2.70869100	-5.07852800	-0.29294700
H	1.69716500	-3.62449700	0.92213300
C	3.59815400	-5.29687300	-1.34940200
H	4.86711200	-4.36157700	-2.82009300
H	2.25969100	-5.92223800	0.22525600
H	3.84153900	-6.30953000	-1.65952900
C	-2.08122300	-3.30518100	-0.59526400
C	-3.05477600	-2.29512100	-0.69892200
C	-2.83842800	-1.14880500	-1.44112700
C	-1.59942800	-0.97872500	-2.10419000
C	-0.60495600	-1.97850600	-2.01226900
C	-0.87375500	-3.14522200	-1.25817500
H	-2.27887600	-4.20493600	-0.02291000
H	-3.60054000	-0.38280800	-1.53064600
H	-1.49464100	-0.15417100	-2.80208800
H	0.26006500	-1.95760400	-2.66797600
H	-0.12517400	-3.92993300	-1.20759700
I	-4.94327800	-2.57046900	0.30003300
P	-0.67518500	1.93913300	-0.07827500

C	-2.07190300	2.54452900	-1.13985200
C	-1.81648900	2.73432500	-2.51063800
C	-3.37660100	2.75019000	-0.66899500
C	-2.83130100	3.13065800	-3.38001700
H	-0.81227800	2.57370700	-2.89723700
C	-4.39738000	3.13566100	-1.54431100
H	-3.60131000	2.61079500	0.38358300
C	-4.12936500	3.32912900	-2.89926400
H	-2.61134200	3.27889600	-4.43422800
H	-5.40290300	3.28769800	-1.16028800
H	-4.92364000	3.62933600	-3.57740600
C	0.41704600	3.43786800	-0.03129300
C	-0.06108200	4.74265000	-0.24095500
C	1.78233200	3.25759800	0.23573900
C	0.80537900	5.83551800	-0.17758200
H	-1.11194200	4.90606200	-0.46001300
C	2.64777200	4.35072600	0.30434900
H	2.16899200	2.25345700	0.37603100
C	2.16135800	5.64254000	0.09675700
H	0.41992200	6.83817600	-0.34475300
H	3.70297800	4.18725400	0.50598100
H	2.83511700	6.49434400	0.14160100
C	-1.42305300	1.90804200	1.61789300
C	-1.39777500	2.99595500	2.50414100
C	-2.03211300	0.71138400	2.03536600
C	-1.97131700	2.89025300	3.77358800
H	-0.92556500	3.92725900	2.20789600
C	-2.61715100	0.61213600	3.29826700
H	-2.04279700	-0.14499200	1.36597400
C	-2.58488300	1.70134100	4.17239200
H	-1.93845300	3.74057600	4.45015700
H	-3.09051800	-0.31859600	3.59888500
H	-3.03196300	1.62234500	5.15997200

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P	2.17521400	-0.55070000	-0.12857100

C	2.96703600	-0.84743600	1.51707300
C	3.53263700	0.31141900	-1.05392200
C	2.15236400	-2.22483700	-0.92254000
C	2.14029300	-0.88500000	2.65058400
C	4.35043300	-1.02662500	1.68478400
C	3.90605000	1.59887600	-0.62511600
C	4.16304300	-0.23010700	-2.18318700
C	1.25572900	-2.42253700	-1.98477600
C	2.97400100	-3.29165500	-0.52790900
C	2.67717600	-1.12140300	3.91757800
H	1.07495900	-0.70259300	2.53684000
C	4.88734900	-1.25812100	2.95218600
H	5.01128700	-0.97446000	0.82435600
C	4.89146200	2.31607000	-1.30205000
H	3.42025900	2.04145300	0.24081200
C	5.14423600	0.49569800	-2.86565200
H	3.89273500	-1.22105200	-2.53303100
C	1.19696000	-3.64639100	-2.65183000
H	0.59177500	-1.61286500	-2.27674000
C	2.90471100	-4.52135600	-1.18607100
H	3.66620000	-3.16769000	0.29873000
C	4.05161400	-1.31048100	4.07040200
H	2.02243600	-1.14361600	4.78473000
H	5.95994500	-1.39260000	3.06655000
C	5.51327700	1.76719600	-2.42760500
H	5.16957500	3.30701600	-0.95271900
H	5.62203400	0.05966800	-3.73940300
C	2.02074900	-4.70043000	-2.25172300
H	0.49606600	-3.78114700	-3.47121100
H	3.54417400	-5.33965700	-0.86461400
H	4.47220700	-1.48654600	5.05701500
H	6.27732900	2.32892200	-2.95846200
H	1.96841300	-5.65842600	-2.76244000
Pd	-0.00581600	0.64604300	-0.03126100
P	-2.11623900	-0.56518900	0.11946300
C	-2.00176600	-2.41633800	0.02161200
C	-3.33940100	-0.18349600	-1.21883100

C	-3.09836400	-0.35308900	1.67991900
C	-1.07569000	-3.06285700	0.85757200
C	-2.78036700	-3.19767200	-0.84497600
C	-2.83426500	0.04409500	-2.50948100
C	-4.72640400	-0.11290400	-1.01817600
C	-2.93088400	0.82772600	2.41956400
C	-3.99588000	-1.32403900	2.15615000
C	-0.94293500	-4.44998900	0.84019200
H	-0.44863500	-2.47479400	1.52254800
C	-2.63808500	-4.58821100	-0.87100900
H	-3.50292800	-2.72456400	-1.50188400
C	-3.69297600	0.30606500	-3.57685100
H	-1.75954500	0.03407200	-2.67191900
C	-5.58540500	0.16383600	-2.08475500
H	-5.14098300	-0.27303800	-0.02799300
C	-3.65523500	1.04319100	3.59378800
H	-2.21402400	1.57209600	2.08645600
C	-4.71650200	-1.10976300	3.33235900
H	-4.12693000	-2.25421800	1.61133400
C	-1.72331700	-5.21841000	-0.02791200
H	-0.22027800	-4.92971700	1.49479200
H	-3.24904700	-5.17674000	-1.55104700
C	-5.07253000	0.36719100	-3.36695000
H	-3.28250400	0.47852100	-4.56824500
H	-6.65718100	0.21799200	-1.91106900
C	-4.55055900	0.07562900	4.05240100
H	-3.50892300	1.96309600	4.15373200
H	-5.40500200	-1.87220000	3.68796500
H	-1.61407300	-6.29954100	-0.04884900
H	-5.74262100	0.58055200	-4.19575000
H	-5.10988100	0.23922800	4.96988600
C	-0.46402500	2.66337600	-0.67078300
C	-1.79615400	3.09361600	-0.79372100
C	0.43068600	2.79389700	-1.74682100
C	-2.25052200	3.55271500	-2.02691400
H	-2.46781000	3.04883100	0.05613400
C	-0.05323200	3.24380100	-2.98389800

H	1.48482400	2.57525300	-1.62153300
C	-1.38562500	3.62406600	-3.12732500
H	-3.29093000	3.84983400	-2.13055800
H	0.63529400	3.32562500	-3.82150200
H	-1.74885400	3.99601700	-4.08143200
I	0.53708300	3.04105300	1.50001600

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P	-1.97376200	0.21293700	-0.09536300
C	-2.13403500	2.06410100	0.02199700
C	-3.20052700	-0.34142200	1.17109500
C	-2.77512900	-0.10944300	-1.73661500
C	-1.72937700	2.87357500	-1.05410400
C	-2.63102500	2.69023300	1.17492100
C	-2.72580200	-0.66293100	2.45157800
C	-4.57802400	-0.41172900	0.92149000
C	-2.34455700	-1.20017000	-2.50869000
C	-3.80617700	0.70507200	-2.23974300
C	-1.83723600	4.26234800	-0.98606600
H	-1.34666300	2.42117900	-1.96259300
C	-2.73462000	4.08154300	1.24324300
H	-2.95324000	2.09302100	2.02095200
C	-3.61161200	-1.02068000	3.46832200
H	-1.65788100	-0.65533900	2.64598700
C	-5.46193100	-0.78476800	1.93536300
H	-4.96573900	-0.19140900	-0.06753400
C	-2.93059700	-1.47037300	-3.74767500
H	-1.56691400	-1.85440800	-2.12890100
C	-4.39104100	0.43141400	-3.47653000
H	-4.14799100	1.56420100	-1.67144400
C	-2.34418600	4.87274800	0.16314800
H	-1.52973200	4.86554100	-1.83648300
H	-3.13096800	4.54351000	2.14366800
C	-4.98229000	-1.08382000	3.21166100
H	-3.22767400	-1.27109300	4.45354800
H	-6.52634200	-0.84523200	1.72415400

C	-3.95365900	-0.65690800	-4.23495200
H	-2.58547900	-2.32281300	-4.32648000
H	-5.18764800	1.07124400	-3.84730600
H	-2.43570000	5.95459100	0.21417600
H	-5.67202900	-1.37584800	3.99911600
H	-4.40862100	-0.86800600	-5.19921300
Pd	0.28751400	-1.01050700	0.05533300
P	1.74721900	0.86579500	0.08263500
C	1.86833200	1.74895200	-1.53131600
C	3.53468400	0.64063800	0.51191400
C	1.18835200	2.07760000	1.35774900
C	1.06540300	1.32503200	-2.60007100
C	2.78737300	2.79144600	-1.74535300
C	4.39999500	0.09178100	-0.44940800
C	4.04937600	0.97191900	1.77339800
C	0.78499200	1.54746800	2.59577200
C	1.19918800	3.46814100	1.18846700
C	1.15628800	1.94524100	-3.84879000
H	0.37467100	0.49926100	-2.45279400
C	2.87097500	3.41597800	-2.98961000
H	3.45209800	3.10214700	-0.94486500
C	5.74508500	-0.11810000	-0.15391200
H	4.02190400	-0.18866700	-1.42612200
C	5.39909100	0.76030200	2.06571900
H	3.40627300	1.40170500	2.53309200
C	0.43278200	2.39038500	3.65011800
H	0.75265900	0.46900900	2.73216900
C	0.83283900	4.30939100	2.24108500
H	1.47983900	3.90158300	0.23501400
C	2.05393000	2.99566000	-4.04285800
H	0.53028500	1.60075900	-4.66730100
H	3.58281500	4.22311700	-3.14027500
C	6.25011300	0.21602900	1.10486200
H	6.39673900	-0.55113000	-0.90757200
H	5.78129100	1.02627300	3.04775800
C	0.45903600	3.77550500	3.47489000
H	0.13253800	1.96436000	4.60362900

H	0.83878300	5.38568800	2.09237200
H	2.12785500	3.47755000	-5.01406200
H	7.29932000	0.05027900	1.33438000
H	0.18064200	4.43439600	4.29295700
C	1.94828600	-2.19094600	-0.11256400
C	2.66843600	-2.64752400	0.99555400
C	2.36162300	-2.56522300	-1.39649100
C	3.79214800	-3.46121500	0.82068400
H	2.35305300	-2.38768700	2.00223000
C	3.48675200	-3.38050900	-1.56916200
H	1.80430100	-2.23970200	-2.27169600
C	4.20717100	-3.82869000	-0.46102300
H	4.33930500	-3.81313500	1.69258300
H	3.79131800	-3.66931300	-2.57312500
H	5.07857500	-4.46504500	-0.59396800
I	-1.02701300	-3.39918000	0.39549000

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Pd	-1.16077100	-0.42525500	-0.02435100
P	1.17594900	-0.20473200	-0.01916800
I	-3.70022500	-1.20349700	0.02407400
C	2.00186000	0.88520300	-1.24829500
C	1.82060500	-1.89834400	-0.34482200
C	1.88834600	0.27911700	1.60435200
C	2.81406200	0.36891100	-2.26892200
C	1.77816400	2.27228500	-1.18520300
C	1.13087700	-2.70294600	-1.26877000
C	2.94991000	-2.41901700	0.30629900
C	1.17853000	-0.05999600	2.76802600
C	3.11846700	0.94462100	1.72199000
C	3.39457100	1.22442300	-3.20782900
H	2.99672200	-0.69859100	-2.33409100
C	2.36671700	3.12114100	-2.12154200
H	1.14671000	2.68942000	-0.40751300
C	1.56874400	-3.99950900	-1.54211900
H	0.24938100	-2.31514900	-1.77481100

C	3.38219700	-3.71703700	0.03196100
H	3.48799300	-1.81488000	1.02996200
C	1.69403400	0.25311600	4.02587200
H	0.21848300	-0.56396900	2.68413300
C	3.62876600	1.26052700	2.98270600
H	3.67380400	1.22258000	0.83162800
C	3.17364100	2.60005200	-3.13615000
H	4.02147500	0.81165200	-3.99354000
H	2.18651300	4.19078200	-2.06104300
C	2.69406000	-4.50823700	-0.89095800
H	1.02481600	-4.61170800	-2.25572200
H	4.25625200	-4.11131400	0.54309200
C	2.91915400	0.91530100	4.13459100
H	1.13480700	-0.01298900	4.91842600
H	4.58042100	1.77882500	3.06311000
H	3.62612800	3.26384100	-3.86782900
H	3.03092100	-5.52034200	-1.09752400
H	3.31710900	1.16597600	5.11410500
C	-1.43426600	1.54461000	-0.03339500
C	-1.76702400	2.16583700	-1.23846000
C	-1.32240600	2.27857600	1.14761800
C	-1.98037800	3.54891600	-1.25596900
H	-1.87311200	1.58851100	-2.15075300
C	-1.53731300	3.66276000	1.11444200
H	-1.07174900	1.79356600	2.08517800
C	-1.86282800	4.29956300	-0.08425800
H	-2.24566900	4.03345200	-2.19243700
H	-1.45161200	4.23635100	2.03420800
H	-2.03215800	5.37280800	-0.10383500

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P	-2.42037000	0.02204100	-0.02855400
C	-3.11876200	-0.37127300	-1.69198700
C	-3.28066100	1.60360300	0.40605100
C	-2.34808300	-1.10126900	-2.60957600
C	-4.41488100	0.03058700	-2.06077900

C	-3.18357000	-1.18036800	1.14284600
Pd	-0.00001600	-0.01554600	-0.00072600
C	-3.93776500	1.77402200	1.63317100
C	-3.24581600	2.68089000	-0.49563900
C	-2.86381300	-1.42475800	-3.86598100
H	-1.35455100	-1.43457300	-2.32902500
C	-4.92655700	-0.29578400	-3.31719900
H	-5.02274200	0.60768700	-1.37135500
C	-2.58114800	-1.35708700	2.39787000
C	-4.35657800	-1.88570400	0.84517600
C	0.00001600	2.02508900	-0.00067500
C	-4.54522000	2.99180200	1.95045200
H	-3.98684300	0.95668100	2.34438100
C	-3.85609200	3.89244000	-0.17839800
H	-2.73373300	2.57846200	-1.44611700
C	-4.15162000	-1.02330900	-4.22308100
H	-2.25541700	-1.99410900	-4.56340800
H	-5.93005400	0.02197700	-3.58771000
C	-3.15359800	-2.20479900	3.34515500
H	-1.65196400	-0.84221700	2.62499400
C	-4.91942700	-2.74672400	1.78965000
H	-4.82855200	-1.77695900	-0.12571200
C	-0.14838900	2.74151500	1.19494900
C	0.14839100	2.74130900	-1.19643400
C	-4.50782800	4.05288300	1.04704200
H	-5.05277900	3.10351100	2.90505400
H	-3.81555600	4.71417300	-0.88803600
H	-4.55046700	-1.27433500	-5.20245100
C	-4.32390400	-2.90407600	3.04146700
H	-2.67505000	-2.33352100	4.31217200
H	-5.82329400	-3.29699500	1.54211300
C	-0.14500200	4.14091300	1.19582800
H	-0.27602500	2.21360400	2.13738500
C	0.14494300	4.14070600	-1.19755600
H	0.27600300	2.21323900	-2.13878500
H	-4.98184400	4.99915300	1.29415400
H	-4.76322700	-3.57583300	3.77406800

C	-0.00004900	4.84548600	-0.00092500
H	-0.26298700	4.67819200	2.13453800
H	0.26288200	4.67782800	-2.13636200
H	-0.00008000	5.93268400	-0.00102500
P	2.42040400	0.02213500	0.02860700
C	3.18482000	-1.18032800	-1.14194900
C	3.11742000	-0.37098900	1.69266700
C	3.28082300	1.60373900	-0.40563100
C	2.58325900	-1.35777500	-2.39727400
C	4.35805600	-1.88491100	-0.84335200
C	4.41288800	0.03162700	2.06290300
C	2.34630300	-1.10182200	2.60923500
C	3.24557400	2.68110600	0.49594800
C	3.93831600	1.77412300	-1.63255200
C	3.15677600	-2.20544300	-3.34396300
H	1.65390000	-0.84354100	-2.62509900
C	4.92197000	-2.74588900	-1.78722200
H	4.82938800	-1.77560500	0.12778700
C	4.92347900	-0.29476300	3.31976500
H	5.02109300	0.60929200	1.37426100
C	2.86096600	-1.42535900	3.86606100
H	1.35330300	-1.43575900	2.32754300
C	3.85586100	3.89268200	0.17880900
H	2.73319800	2.57871300	1.44626900
C	4.54576600	2.99192700	-1.94973500
H	3.98769600	0.95673100	-2.34368200
C	4.32729400	-2.90395200	-3.03936000
H	2.67887200	-2.33474000	-4.31122100
H	5.82600500	-3.29556500	-1.53897900
C	4.14811700	-1.02310300	4.22462400
H	5.92648100	0.02359800	3.59140300
H	2.25225700	-1.99537700	4.56266900
C	4.50799100	4.05307900	-1.04642400
H	3.81502200	4.71447000	0.88836500
H	5.05362900	3.10359800	-2.90417900
H	4.76745300	-3.57567400	-3.77149100
H	4.54613200	-1.27415000	5.20432700

H	4.98200900	4.99936800	-1.29345900
I	-0.00002800	-2.84475000	-0.00122000

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P	-2.30075700	0.21954000	0.15506800
C	-3.64172500	-0.79493200	-0.60375100
C	-3.20230800	1.77484900	0.66717700
C	-3.32063000	-2.00492200	-1.24136900
C	-4.98809400	-0.39818700	-0.52798200
C	-1.90124400	-0.53821200	1.80976900
Pd	-0.05468800	-0.44189600	-0.29784100
C	-3.57256500	2.01258900	1.99986700
C	-3.62909700	2.68727600	-0.31602600
C	-4.32846600	-2.79591600	-1.79566500
H	-2.28810000	-2.34225600	-1.28419700
C	-5.98885700	-1.19444700	-1.08602100
H	-5.26353800	0.52623900	-0.03477000
C	-1.04166200	0.13712600	2.69801800
C	-2.40078500	-1.79992400	2.16786800
C	-1.20479500	1.07251000	-1.32960700
C	-4.31683500	3.14430100	2.34440400
H	-3.28554900	1.31672300	2.77854700
C	-4.38105400	3.80936800	0.02807300
H	-3.38604100	2.51719900	-1.35868900
C	-5.66255000	-2.39290400	-1.72324000
H	-4.06048900	-3.73040100	-2.28050000
H	-7.02528700	-0.87468400	-1.01935200
C	-0.69712900	-0.43967000	3.92027800
H	-0.65634800	1.11935900	2.44178000
C	-2.05680000	-2.36572800	3.39494000
H	-3.04189800	-2.34806400	1.48747800
C	-0.67345500	2.36991700	-1.16174000
C	-1.44106500	0.59543000	-2.63677200
C	-4.71967700	4.04763000	1.36220700
H	-4.58278100	3.31185700	3.38456900
H	-4.70117400	4.49822400	-0.74888900

H	-6.44486200	-3.01004400	-2.15721800
C	-1.20364600	-1.69247200	4.27154200
H	-0.02858600	0.08916800	4.59392500
H	-2.45132900	-3.34268500	3.65956400
C	-0.33951400	3.14304500	-2.27105700
H	-0.51109500	2.76682600	-0.16564900
C	-1.11979300	1.38658600	-3.74277700
H	-1.87352500	-0.38717300	-2.78528300
H	-5.29929200	4.92670200	1.63078000
H	-0.93208400	-2.14275300	5.22221800
C	-0.56472000	2.65498700	-3.56307300
H	0.10431400	4.12346000	-2.12409300
H	-1.30283300	1.00557000	-4.74392700
H	-0.31426100	3.26620800	-4.42603600
P	2.33104000	0.35994600	0.06610200
C	3.46149100	-0.03694100	-1.34135400
C	3.22183800	-0.30944000	1.54544600
C	2.54353700	2.18890900	0.27615200
C	2.88465400	-0.38631900	-2.57118000
C	4.86102200	-0.00440600	-1.23069700
C	4.20987500	0.40693100	2.24253200
C	2.89957600	-1.60900300	1.96968300
C	2.01536900	2.80084200	1.42858500
C	3.10728000	3.00994100	-0.71120400
C	3.69048500	-0.67878100	-3.67392500
H	1.80346400	-0.44858000	-2.65501600
C	5.66415300	-0.30101800	-2.33169700
H	5.32563900	0.24184200	-0.28049500
C	4.86188600	-0.16503100	3.33655500
H	4.46758500	1.41682900	1.93813400
C	3.55950700	-2.17929700	3.05994400
H	2.13712100	-2.17614300	1.44200200
C	2.06087500	4.18446600	1.59329800
H	1.58054900	2.18508100	2.21230700
C	3.14694100	4.39847900	-0.54943300
H	3.52312300	2.56621600	-1.60992200
C	5.07995300	-0.63586700	-3.55639100

H	3.22973800	-0.95531600	-4.61844800
H	6.74633500	-0.27702400	-2.23188500
C	4.53937700	-1.46037600	3.74687000
H	5.62320500	0.40250800	3.86610900
H	3.30083600	-3.18785300	3.37137300
C	2.62620400	4.99128600	0.60074700
H	1.65688700	4.63371600	2.49712100
H	3.59461400	5.01476200	-1.32519800
H	5.70757400	-0.87253400	-4.41176200
H	5.04881700	-1.90508400	4.59808500
H	2.66172400	6.07010500	0.72681500
I	0.27874800	-3.24828500	-0.64528900

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P	-2.91308000	0.23308400	-0.07318200
C	-3.87273200	-1.31355200	0.03008500
C	-4.10855800	1.61880700	0.05259600
C	-3.21393700	-2.51769400	0.32821000
C	-5.26071400	-1.31524500	-0.19389700
C	-1.71860300	0.32907900	1.26201700
Pd	0.35238900	-0.36731600	0.53942800
C	-4.23276400	2.30267900	1.27166100
C	-4.92520100	1.98717900	-1.03165500
C	-3.93982800	-3.70809800	0.38858800
H	-2.14072000	-2.54374700	0.50309800
C	-5.97477800	-2.51086200	-0.13059500
H	-5.78810900	-0.39183300	-0.40526600
C	-0.70745500	1.37738600	1.19911500
C	-2.12643600	-0.16248800	2.55901800
C	-2.11673300	0.38698900	-1.70545000
C	-5.16266400	3.33587300	1.40309900
H	-3.60528000	2.02947200	2.11394300
C	-5.85247500	3.01969400	-0.89294000
H	-4.83110900	1.47649800	-1.98543200
C	-5.31622100	-3.70831000	0.15960700
H	-3.41445200	-4.63128200	0.61444100

H	-7.04749500	-2.50370800	-0.30249400
C	-0.21301900	1.90650100	2.44272100
H	-0.64611300	2.03248300	0.33234600
C	-1.57531800	0.34320600	3.70883100
H	-2.87094400	-0.95043800	2.61672100
C	-1.94951500	1.64621400	-2.30609600
C	-1.59600300	-0.75736200	-2.33137100
C	-5.97216700	3.69473600	0.32468000
H	-5.24946300	3.86121300	2.34982300
H	-6.47762500	3.29864900	-1.73649400
H	-5.87720600	-4.63768700	0.20966700
C	-0.61452200	1.39636300	3.65144800
H	0.49587700	2.72847600	2.39891500
H	-1.87805800	-0.05956500	4.67141500
C	-1.27082800	1.75533300	-3.52048200
H	-2.34479500	2.53913100	-1.83318100
C	-0.92062200	-0.63777800	-3.54522400
H	-1.68497100	-1.73339200	-1.86749000
H	-6.69302700	4.50085400	0.42968200
H	-0.21324800	1.80467800	4.57527200
C	-0.75688200	0.61443100	-4.14031800
H	-1.14507500	2.73191000	-3.97976000
H	-0.50910300	-1.52614400	-4.01387800
H	-0.22436400	0.70206900	-5.08313700
P	2.53870400	0.42591800	0.02334900
C	3.21033600	0.13249100	-1.67937300
C	3.88309500	-0.22603600	1.11117600
C	2.68358400	2.26430000	0.19935900
C	2.95795200	-1.11675000	-2.27097700
C	3.97125800	1.07640900	-2.38790500
C	5.24721700	-0.04140100	0.83116800
C	3.51470000	-0.94370800	2.25842000
C	3.44291400	2.88575000	1.20165900
C	1.89947400	3.07505800	-0.64364500
C	3.46547100	-1.41392200	-3.53668600
H	2.36449800	-1.85480300	-1.73696400
C	4.46839300	0.77817200	-3.65891700

H	4.17491600	2.04987200	-1.95287000
C	6.22024500	-0.55001000	1.69122500
H	5.55072000	0.49214000	-0.06521800
C	4.49086400	-1.45116800	3.11936000
H	2.46169600	-1.12207500	2.45768600
C	3.42397800	4.27589200	1.35381300
H	4.05489900	2.28510300	1.86661800
C	1.89150600	4.46159200	-0.49956000
H	1.29420700	2.61318800	-1.42057600
C	4.21865200	-0.46802800	-4.23604600
H	3.26731500	-2.38839400	-3.97596100
H	5.05461100	1.52096600	-4.19463400
C	5.84309900	-1.25353700	2.83879000
H	7.27289300	-0.40358500	1.46241400
H	4.19103800	-2.01252800	4.00020100
C	2.65272200	5.06879800	0.50424800
H	4.02053100	4.73677800	2.13717800
H	1.28778400	5.07022900	-1.16847600
H	4.60915400	-0.70031500	-5.22378500
H	6.60302200	-1.65473800	3.50462000
H	2.64235700	6.14923500	0.62137000
I	0.53163200	-3.21356800	0.16859300

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P	0.38364300	2.39234000	0.95543500
C	-0.61570100	3.87491900	0.52341800
C	2.10612300	3.05115500	1.09841700
Pd	0.09477500	0.34868300	-0.11393600
C	-1.95378000	3.68048300	0.12868300
C	-0.18090700	5.19858400	0.72819900
C	2.74659100	3.89465500	0.17153300
C	2.81774900	2.67600900	2.25196000
C	0.79858000	1.69754800	-1.55896800
C	-2.81280700	4.75837100	-0.07860200
H	-2.32763500	2.67196000	-0.01645600
C	-1.04291700	6.27689100	0.52374600

H	0.83419000	5.39267200	1.05695400
C	4.04762500	4.34597700	0.39537700
H	2.22335500	4.19730600	-0.72907300
C	4.12325300	3.12221100	2.47541800
H	2.33566100	2.03460800	2.98618200
C	2.12653400	1.61156400	-2.00370100
C	-0.15912200	2.25811500	-2.41622300
C	-2.36054600	6.06572900	0.11363600
H	-3.83665000	4.57090500	-0.39208700
H	-0.67894400	7.28858900	0.68717600
C	4.74155200	3.96025600	1.54612000
H	4.52329100	4.99722900	-0.33381100
H	4.64962800	2.82351400	3.37867100
C	2.47192300	2.01373800	-3.29821600
H	2.90159500	1.23264400	-1.34772900
C	0.18772200	2.65860600	-3.71228200
H	-1.17906600	2.40395900	-2.07793100
C	1.50339000	2.53293400	-4.16045400
H	3.50494900	1.92212100	-3.62717800
H	-0.57344100	3.08517100	-4.36250200
P	1.74012400	-1.61084600	-0.03337900
C	1.36311800	-2.97800000	-1.22528700
C	1.85221700	-2.44805600	1.61895400
C	3.53612900	-1.28921400	-0.37290100
C	0.83906000	-2.60099800	-2.47337000
C	1.57251800	-4.34085800	-0.96636200
C	2.93674700	-3.26080500	1.99272300
C	0.82237700	-2.23642500	2.54879900
C	4.18454800	-0.31135200	0.40156200
C	4.26495800	-1.94131300	-1.37773900
C	0.54870200	-3.56086300	-3.44361900
H	0.65746100	-1.54930600	-2.68095300
C	1.26906100	-5.30175400	-1.93363200
H	1.96751300	-4.65815700	-0.00638000
C	2.97306100	-3.86503400	3.25006900
H	3.76281800	-3.41018100	1.30353100
C	0.85752700	-2.84237500	3.80710500

H	-0.00406200	-1.57889100	2.29381400
C	5.52648400	-0.00330100	0.18498000
H	3.63436500	0.22704400	1.16780600
C	5.60989400	-1.62781200	-1.59703700
H	3.78781900	-2.69645500	-1.99353000
C	0.76030800	-4.91475200	-3.17477500
H	0.14818500	-3.25069200	-4.40511800
C	1.93126100	-3.66101500	4.15876400
H	3.81940700	-4.49042200	3.52262800
H	0.04959200	-2.66287700	4.51132800
C	6.24501800	-0.66172200	-0.81719300
H	6.00237000	0.76310100	0.79056900
H	6.15859100	-2.14348600	-2.38120000
H	0.52548800	-5.66396700	-3.92628800
H	1.96359100	-4.12912700	5.13913600
H	7.28970900	-0.41777700	-0.99154700
H	1.43351100	-6.35421700	-1.71601500
H	-3.02776600	6.90848600	-0.04756400
H	5.75446000	4.31568300	1.71805900
H	1.77490400	2.85135600	-5.16399000
C	-3.59642100	0.38817700	-0.77617400
C	-3.37608000	0.64407000	-2.14164800
C	-4.74716200	0.91628400	-0.17236200
C	-4.28893100	1.39228000	-2.88424800
H	-2.48053400	0.26164200	-2.62398700
C	-5.65393500	1.67883200	-0.91469300
H	-4.94015400	0.73513100	0.87988500
C	-5.43089600	1.91573300	-2.27151900
H	-4.10275400	1.57487000	-3.93933400
H	-6.53862100	2.08199100	-0.42843800
H	-6.13832700	2.50606600	-2.84775900
C	-2.76310100	-2.33734400	-0.41834100
C	-3.84683400	-2.63514800	-1.25896300
C	-1.96638800	-3.39720000	0.04583600
C	-4.12414200	-3.95544700	-1.62363900
H	-4.48240700	-1.83899900	-1.63110900
C	-2.24979100	-4.71486100	-0.31015900

H	-1.11974000	-3.19495400	0.69442700
C	-3.32933500	-4.99887800	-1.14973000
H	-4.96790900	-4.16436000	-2.27656400
H	-1.61774400	-5.51755500	0.05906700
H	-3.54624400	-6.02524000	-1.43399400
P	-2.32804300	-0.61506000	0.13169000
C	-2.96567300	-0.62179500	1.87508600
C	-2.40467900	0.27553800	2.79814200
C	-3.98523500	-1.48690600	2.30783200
C	-2.85979800	0.31362800	4.11848200
H	-1.60352300	0.94079500	2.48583500
C	-4.43397900	-1.45062200	3.62876900
H	-4.42822400	-2.19323300	1.61256600
C	-3.87326300	-0.54962500	4.53748700
H	-2.41474300	1.01628900	4.81812300
H	-5.22203000	-2.12808200	3.94777300
H	-4.22305200	-0.52395200	5.56632200

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P	0.19378000	-2.17034600	-0.21940500
C	1.83842100	-2.76042200	0.40822200
C	0.12935600	-2.68879300	-1.99161600
C	-0.96587200	-3.39024000	0.57071800
C	2.20811500	-2.37627100	1.70884400
C	2.72132200	-3.57005500	-0.32064200
C	-0.01046200	-1.69841500	-2.97505400
C	0.17499500	-4.03509300	-2.39324000
C	-2.16942400	-3.71884600	-0.07872100
C	-0.71463900	-3.94979900	1.83373900
C	3.40049100	-2.82143300	2.28047000
H	1.56300600	-1.71862100	2.28281000
C	3.92131900	-4.00472800	0.24623200
H	2.48192700	-3.86119600	-1.33698400
C	-0.07281300	-2.03842600	-4.32885800
H	-0.09760100	-0.65881200	-2.66910800
C	0.11728100	-4.37512500	-3.74509500

H	0.23996500	-4.82057000	-1.64626700
C	-3.08818400	-4.58247400	0.52024500
H	-2.39214200	-3.30108300	-1.05229900
C	-1.63545300	-4.81324100	2.42855800
H	0.21035200	-3.73254000	2.35600600
C	4.26051100	-3.64288300	1.55027000
H	3.65875500	-2.51542100	3.29078100
H	4.59178400	-4.63024600	-0.33738800
C	-0.00210400	-3.37708100	-4.71596300
H	-0.18692800	-1.25789000	-5.07639900
H	0.15608300	-5.42052500	-4.03979500
C	-2.82695500	-5.13147400	1.77526600
H	-4.01225300	-4.82079100	0.00048300
H	-1.41491100	-5.24059500	3.40335400
H	5.19220100	-3.98890200	1.98999200
H	-0.05326800	-3.64463800	-5.76809600
H	-3.54396100	-5.80305400	2.23994100
Pd	-0.40052500	0.32611300	-0.04704400
P	1.94486400	1.28870900	0.09159200
C	2.26962600	2.98075000	-0.60536300
C	3.31671900	0.30567100	-0.67267900
C	2.44027000	1.54115400	1.85548400
C	1.70405800	4.09423100	0.03942800
C	3.04129400	3.19340000	-1.75792000
C	3.12421000	-0.14490100	-1.98995900
C	4.53090500	0.01124300	-0.03679100
C	1.63467400	1.00370800	2.86949000
C	3.57262000	2.28995000	2.22036000
C	1.91883500	5.38221500	-0.44870200
H	1.08631700	3.96024200	0.92082700
C	3.24731600	4.48513000	-2.24859400
H	3.49939500	2.35733400	-2.27436100
C	4.12836700	-0.83917100	-2.66508700
H	2.18211900	0.04837600	-2.49398000
C	5.53102600	-0.69521300	-0.70833100
H	4.70092100	0.32733600	0.98635400
C	1.96344700	1.18322000	4.21533800

H	0.73323500	0.46155000	2.59677600
C	3.90448500	2.46571300	3.56384900
H	4.18756200	2.74862100	1.45173800
C	2.69046900	5.58385800	-1.59468900
H	1.46791400	6.22678400	0.06470800
H	3.85275700	4.62745500	-3.14013200
C	5.33833500	-1.11409300	-2.02515400
H	3.95896500	-1.17178900	-3.68569400
H	6.46417200	-0.91681000	-0.19708700
C	3.10239500	1.90966900	4.56413700
H	1.32337600	0.76543000	4.98788400
H	4.78430400	3.04556600	3.83003600
H	2.85405700	6.58866000	-1.97539700
H	6.12131200	-1.65866400	-2.54621600
H	3.35821000	2.05432700	5.61043300
C	-1.14186400	2.23808500	0.13805000
C	-1.46014700	2.76535800	1.39985800
C	-1.25975400	3.08498600	-0.97465500
C	-1.87030600	4.09696300	1.54578700
H	-1.41147400	2.13693200	2.28526000
C	-1.67311400	4.41293900	-0.83397200
H	-1.04034600	2.71008800	-1.97139400
C	-1.97845000	4.92710800	0.42789700
H	-2.11530400	4.47814600	2.53543500
H	-1.75758100	5.04495500	-1.71545100
H	-2.30482400	5.95864300	0.53818000
P	-2.70911600	-0.32922400	-0.33355900
C	-3.67665800	0.86878200	-1.35489300
C	-4.41151100	1.96418700	-0.86791300
C	-3.69309700	0.62935700	-2.74164700
C	-5.14218100	2.77807300	-1.73338500
H	-4.40010500	2.18840300	0.19355900
C	-4.40704200	1.45497600	-3.61156300
H	-3.14758600	-0.22409500	-3.13977300
C	-5.14155600	2.53063100	-3.10861600
H	-5.70264100	3.61945900	-1.33268900
H	-4.40258000	1.24815000	-4.67936400

H	-5.70927000	3.16923300	-3.78085900
C	-3.52031800	-0.25968600	1.32056400
C	-4.92443900	-0.25961500	1.44458300
C	-2.76707000	-0.38963700	2.50240800
C	-5.54052100	-0.36259700	2.69126700
H	-5.54181800	-0.17819900	0.55459400
C	-3.38246700	-0.50729300	3.74957900
H	-1.68198600	-0.39837400	2.43534900
C	-4.77407400	-0.48714800	3.85287400
H	-6.62627500	-0.35090100	2.75431800
H	-2.77120900	-0.60505600	4.64412900
H	-5.25572100	-0.56843500	4.82389600

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P	-2.68544600	0.04200500	-0.03889000
C	-3.38695000	-0.36010100	-1.69835200
C	-3.53190800	1.63353500	0.38383800
C	-3.45168600	-1.14708600	1.14325700
C	-2.62346000	-1.10399800	-2.61074900
C	-4.68096400	0.04780000	-2.06808600
C	-3.49039600	2.70258000	-0.52737100
C	-4.18671100	1.81856900	1.61002500
C	-2.85528600	-1.30821300	2.40332200
C	-4.62087000	-1.85920300	0.84688900
C	-3.14376600	-1.43479500	-3.86331100
H	-1.63233900	-1.44305500	-2.32874600
C	-5.19720100	-0.28594100	-3.32067200
H	-5.28370900	0.63467700	-1.38247000
C	-4.09212600	3.92089900	-0.21999400
H	-2.98070300	2.58800600	-1.47780200
C	-4.78546200	3.04319700	1.91730300
H	-4.24107900	1.00747400	2.32792000
C	-3.42976800	-2.14774700	3.35653400
H	-1.92970100	-0.78674500	2.63059700
C	-5.18578000	-2.71190500	1.79767500
H	-5.08805500	-1.76214100	-0.12750000

C	-4.42922000	-1.02691800	-4.22156200
H	-2.54123100	-2.01512100	-4.55673500
H	-6.19893100	0.03644000	-3.59205000
C	-4.74152300	4.09614400	1.00471700
H	-4.04731700	4.73612600	-0.93680100
H	-5.29159500	3.16658000	2.87116900
C	-4.59618700	-2.85411500	3.05405700
H	-2.95642500	-2.26421600	4.32764100
H	-6.08659200	-3.26763600	1.55144000
H	-4.83172300	-1.28371300	-5.19787300
H	-5.20899500	5.04761600	1.24399700
H	-5.03709700	-3.51945100	3.79146400
Pd	-0.26661500	-0.01591100	-0.00804400
P	2.15488800	0.00187800	0.03046800
C	2.84259000	-0.39284600	1.69584400
C	3.02750700	1.57490300	-0.40214900
C	2.91775700	-1.20616000	-1.13213100
C	2.07105300	-1.13586500	2.60443400
C	4.13168000	0.01737700	2.08167200
C	2.98362900	2.66178600	0.48910100
C	3.69661400	1.73827500	-1.62425800
C	2.30457200	-1.41055700	-2.37852000
C	4.10102800	-1.89754800	-0.83831100
C	2.56933400	-1.46559700	3.86419600
H	1.08324200	-1.47843800	2.31509200
C	4.64105700	-0.30611300	3.33837700
H	4.74358500	0.60321400	1.40367400
C	3.59248100	3.87340900	0.17590000
H	2.46176400	2.57038200	1.43497700
C	4.30689000	2.94996800	-1.95433200
H	3.75428500	0.91731000	-2.33030800
C	2.86845900	-2.26426700	-3.32366900
H	1.36751900	-0.91110400	-2.60541400
C	4.66871700	-2.76859500	-1.76842400
H	4.58428400	-1.77212900	0.12480000
C	3.84756000	-1.04392000	4.21072800
H	1.98253300	-2.04308100	4.57085700

H	5.63300900	0.00676200	3.64742100
C	4.24411300	3.99879200	-1.04704300
H	3.55861700	4.71684000	0.85720100
H	4.82913600	3.08271000	-2.89617300
C	4.04400100	-2.93319600	-2.99878900
H	2.40177000	-2.43398100	-4.28818100
H	5.57794600	-3.31870600	-1.54964500
C	-0.25174500	2.02485500	-0.01613700
C	-0.09276400	2.73526800	-1.21404000
C	-0.39788000	2.74689000	1.17645700
C	-0.08240900	4.13474100	-1.22011700
H	0.03049400	2.20290000	-2.15460200
C	-0.38059800	4.14634900	1.17238100
H	-0.53626200	2.22368700	2.12004400
C	-0.22430700	4.84518100	-0.02634100
H	0.04226000	4.66753700	-2.16047400
H	-0.49757900	4.68814200	2.10854800
I	-0.28376800	-2.84452200	0.00292600
H	-0.21399200	5.93220400	-0.03046800
F	4.33316800	-1.35438500	5.42774900
F	4.59070200	-3.76899500	-3.90283900
F	4.83332800	5.17107700	-1.35651300

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P	-2.06247300	0.18335700	0.06517300
C	-3.38626800	-0.90500500	-0.61229700
C	-3.00278800	1.73601200	0.50568800
C	-3.04634900	-2.13556400	-1.20212200
C	-4.74352200	-0.54635400	-0.52438600
C	-1.62337400	-0.46509700	1.75550300
Pd	0.18697700	-0.44266400	-0.37495500
C	-3.38635200	2.02429600	1.82578200
C	-3.45551100	2.59260300	-0.51688500
C	-4.03413600	-2.98528600	-1.69730500
H	-2.00618000	-2.44809800	-1.25338000
C	-5.73719600	-1.38958800	-1.01759600

H	-5.03872400	0.39101500	-0.06896700
C	-0.78466700	0.28928200	2.59977700
C	-2.05489700	-1.73208600	2.18111600
C	-1.01335300	0.98879200	-1.47365100
C	-4.16237000	3.14467800	2.12747900
H	-3.08501300	1.37328000	2.63689900
C	-4.23926900	3.70784600	-0.23316900
H	-3.20743000	2.38545500	-1.55127600
C	-5.36516600	-2.59666700	-1.60006200
H	-3.77724200	-3.93803800	-2.14833100
H	-6.78719800	-1.12358800	-0.95500200
C	-0.39625800	-0.20255600	3.84434700
H	-0.44448900	1.27337300	2.29281100
C	-1.67680600	-2.22831700	3.42604500
H	-2.67358700	-2.34479700	1.53630100
C	-0.50644000	2.30338800	-1.37898400
C	-1.24566500	0.43677300	-2.75153800
C	-4.57311900	3.97306300	1.09145400
H	-4.45096800	3.37398400	3.14792000
H	-4.59039200	4.36813300	-1.01924800
C	-0.84964200	-1.45770800	4.23617700
H	0.25246400	0.36543400	4.50256700
H	-2.00281600	-3.20567800	3.76545600
C	-0.19684900	3.02285500	-2.53080100
H	-0.34441900	2.75660900	-0.40692700
C	-0.94924300	1.17382200	-3.90083000
H	-1.65480500	-0.56245900	-2.84410400
C	-0.42095500	2.46169600	-3.79302000
H	0.22782900	4.01840700	-2.44033800
H	-1.12997200	0.73578600	-4.87871100
P	2.55998300	0.41875600	-0.06674400
C	3.70397000	-0.05233800	-1.43851600
C	3.44589200	-0.14115100	1.45907800
C	2.74004500	2.26064400	0.02116000
C	3.14015100	-0.47041600	-2.65291200
C	5.10216200	-0.00624300	-1.31668700
C	4.40390300	0.64017400	2.12761500

C	3.15060700	-1.42257000	1.95339900
C	2.20449800	2.94087900	1.13115600
C	3.28227400	3.02173400	-1.02455800
C	3.95749300	-0.81689200	-3.73113200
H	2.06010700	-0.54302500	-2.74317500
C	5.91673900	-0.35707600	-2.39306400
H	5.55652800	0.29317000	-0.37681800
C	5.05073800	0.15061200	3.26399600
H	4.64210400	1.63668800	1.76823800
C	3.80527500	-1.91018700	3.08600700
H	2.41321700	-2.04046800	1.44742700
C	2.22158300	4.33337700	1.19836700
H	1.78824100	2.37262800	1.95960900
C	3.29333200	4.41866000	-0.96064200
H	3.70329500	2.52471100	-1.89244000
C	5.34559900	-0.75989100	-3.60335400
H	3.50713600	-1.14622000	-4.66363100
C	4.75364700	-1.12607700	3.74538600
H	5.78808100	0.76810500	3.77097200
H	3.56697700	-2.90495800	3.45283700
C	2.76496100	5.07988000	0.14808900
H	1.81349900	4.83662400	2.07135000
H	3.72486500	4.98819300	-1.77999700
H	5.98231500	-1.03831500	-4.43914300
I	0.56252300	-3.25563600	-0.57205300
F	-6.32386300	-3.40962600	-2.07860900
F	-5.32118800	5.05476800	1.37261700
H	5.25801600	-1.50610300	4.63013400
H	2.77854600	6.16533900	0.19809100
H	6.99777300	-0.32197500	-2.28503700
F	-0.48291100	-1.93610300	5.43941100
H	-0.18941900	3.03105400	-4.68918300

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P	-2.94497100	0.06587500	-0.05736500
C	-3.63770100	-0.34216700	-1.71864800

C	-3.78021800	1.66645500	0.35112200
C	-3.72419500	-1.11134700	1.12757500
C	-2.87525300	-1.10087900	-2.61969700
C	-4.92547200	0.07467700	-2.10009000
C	-3.72699800	2.72905600	-0.56698900
C	-4.43888900	1.86385400	1.57329400
C	-3.13913800	-1.26537300	2.39385800
C	-4.89257900	-1.82245100	0.82563200
C	-3.39028900	-1.43709500	-3.87294800
H	-1.88949900	-1.44748500	-2.32821700
C	-5.43632600	-0.26445000	-3.35343300
H	-5.52753500	0.67217900	-1.42313200
C	-4.32134400	3.95357400	-0.27007500
H	-3.21450200	2.60432300	-1.51463400
C	-5.03015200	3.09467300	1.86997400
H	-4.50212800	1.05771800	2.29598400
C	-3.72395800	-2.09716500	3.34752900
H	-2.21450300	-0.74435300	2.62616900
C	-5.46788700	-2.66727900	1.77719900
H	-5.35096000	-1.73073600	-0.15342400
C	-4.66935600	-1.01988600	-4.24311100
H	-2.78885800	-2.02897700	-4.55747300
H	-6.43318800	0.06489000	-3.63411000
C	-4.97467700	4.14126500	0.95071000
H	-4.26796100	4.76376500	-0.99195900
H	-5.53956200	3.22790800	2.82072800
C	-4.88950600	-2.80261600	3.03952400
H	-3.25955200	-2.20822200	4.32355100
H	-6.36794500	-3.22235000	1.52688400
H	-5.06777800	-1.28085000	-5.21995800
H	-5.43641300	5.09753500	1.18175000
H	-5.33843500	-3.46194000	3.77744800
Pd	-0.52916100	-0.01270300	-0.01202400
P	1.89211800	-0.01789800	0.03697100
C	2.57573400	-0.40664000	1.70737800
C	2.78144000	1.54503400	-0.40362500
C	2.65706500	-1.23928700	-1.11286500

C	1.80064500	-1.14327600	2.61605500
C	3.86272600	0.00289800	2.09699300
C	2.74051500	2.63916000	0.47701000
C	3.46016400	1.69401900	-1.62120900
C	2.05224200	-1.44761300	-2.36147600
C	3.83495300	-1.93345300	-0.80926200
C	2.29366300	-1.46724700	3.87996400
H	0.81312600	-1.48697000	2.32632500
C	4.36591900	-0.31457500	3.35803300
H	4.48090800	0.58376500	1.42024800
C	3.36070900	3.84381900	0.15763300
H	2.21126400	2.56248100	1.42019400
C	4.08270000	2.89826200	-1.95628900
H	3.51765600	0.86873200	-2.32237700
C	2.61988800	-2.30741500	-3.29928900
H	1.11822400	-0.94705800	-2.59863400
C	4.40576300	-2.81020700	-1.73258400
H	4.31456300	-1.80712100	0.15565800
C	3.57326200	-1.04833200	4.24087800
H	1.69024300	-2.04102100	4.57515400
H	5.35938900	0.00556500	3.65356200
C	4.02804200	3.96393200	-1.06199600
H	3.31947000	4.68332000	0.84296800
H	4.60858200	3.00241500	-2.89942000
C	3.79559300	-2.98408100	-2.97345600
H	2.14745700	-2.46668500	-4.26251500
H	5.31277800	-3.35351400	-1.49009900
C	-0.49842400	2.02827100	-0.02780000
C	-0.32797500	2.73331400	-1.22711900
C	-0.64154800	2.75428300	1.16268100
C	-0.30213500	4.13261700	-1.23655100
H	-0.20821400	2.19741700	-2.16614700
C	-0.60899200	4.15349600	1.15499900
H	-0.78971400	2.23496400	2.10694500
C	-0.44030000	4.84741400	-0.04498100
H	-0.16791000	4.66169400	-2.17757500
H	-0.72380200	4.69897900	2.08924400

I	-0.56059400	-2.83925400	0.01659700
H	-0.41755400	5.93415800	-0.05181800
Cl	4.19835200	-1.44571700	5.83189800
Cl	4.51401400	-4.07791100	-4.14341900
Cl	4.81067900	5.48169900	-1.47314100

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P	-1.83720900	0.16784600	-0.02091300
C	-3.16023900	-0.97663000	-0.60637000
C	-2.79154300	1.73414700	0.34810600
C	-2.81651700	-2.24006200	-1.11567000
C	-4.51828500	-0.62416500	-0.52968000
C	-1.37375700	-0.37574300	1.70237400
Pd	0.41787200	-0.45812200	-0.43811000
C	-3.15890800	2.09015200	1.65516100
C	-3.26484000	2.53284500	-0.70976600
C	-3.80288300	-3.12733400	-1.54559600
H	-1.77448200	-2.54961600	-1.15555700
C	-5.50983000	-1.50543000	-0.95805200
H	-4.81923200	0.33835800	-0.13409900
C	-0.52019600	0.42406800	2.48616300
C	-1.81269400	-1.60511000	2.21725400
C	-0.84984600	0.86703800	-1.61773100
C	-3.94025300	3.21928700	1.90800100
H	-2.84137800	1.48783600	2.49728000
C	-4.05377300	3.65615700	-0.47351900
H	-3.02916600	2.27682700	-1.73623400
C	-5.14304900	-2.75114200	-1.46697600
H	-3.52632000	-4.10228500	-1.93233900
H	-6.55654000	-1.22767500	-0.89639300
C	-0.12061100	0.01067200	3.75584100
H	-0.17613600	1.38395000	2.11374300
C	-1.42432100	-2.02105600	3.48852600
H	-2.44774200	-2.25382100	1.62556800
C	-0.33740600	2.18319700	-1.62721000
C	-1.07257000	0.21188500	-2.84861600

C	-4.37858300	3.99826800	0.83993700
H	-4.20740200	3.48611800	2.92491400
H	-4.41273600	4.26089300	-1.29946400
C	-0.57924800	-1.21129900	4.24765700
H	0.54142600	0.62677500	4.35441300
H	-1.76701900	-2.97183000	3.88202500
C	-0.02105200	2.80682900	-2.83205500
H	-0.17757700	2.71360400	-0.69473800
C	-0.76990000	0.85356700	-4.05153600
H	-1.48095500	-0.79184800	-2.86345800
C	-0.24089900	2.14580100	-4.04530800
H	0.40689600	3.80480400	-2.81984100
H	-0.94563600	0.33784100	-4.99158100
P	2.78599700	0.46521300	-0.24790900
C	3.92186500	-0.12955300	-1.57869600
C	3.69501500	0.07013900	1.31566300
C	2.94004700	2.30822000	-0.34419900
C	3.35713700	-0.76331900	-2.69479800
C	5.31704700	0.01980700	-1.51296200
C	4.65633900	0.92029900	1.88808000
C	3.41464400	-1.15628600	1.94060800
C	2.41643500	3.08719800	0.70505700
C	3.45153200	2.96985700	-1.46999300
C	4.16924100	-1.22380800	-3.73402600
H	2.28267900	-0.91644100	-2.73470500
C	6.12622900	-0.44220900	-2.55038600
H	5.77402000	0.48768200	-0.64582600
C	5.32256300	0.55062400	3.05794700
H	4.88046900	1.87783000	1.42792900
C	4.08803900	-1.52431300	3.10693200
H	2.67376600	-1.82486800	1.51002000
C	2.41544000	4.47965500	0.63550700
H	2.02493200	2.59862800	1.59436300
C	3.44583600	4.36646500	-1.54241900
H	3.86252400	2.39471700	-2.29328100
C	5.55301500	-1.06272800	-3.66419600
H	3.71862000	-1.72154300	-4.58838700

C	5.04076100	-0.67282000	3.66937700
H	6.06240300	1.21986600	3.49004400
H	3.86042300	-2.47742900	3.57646100
C	2.92936000	5.12644800	-0.49290000
H	2.01718700	5.06100300	1.46330400
H	3.85464100	4.85824000	-2.42158400
H	6.18612900	-1.42826100	-4.46856300
I	0.80255400	-3.27007100	-0.40858200
H	5.55967800	-0.95912200	4.58055900
H	2.92985500	6.21168800	-0.54861100
H	7.20492900	-0.32459800	-2.48650100
H	-0.00387800	2.64021300	-4.98346800
Cl	-5.35855200	5.41846700	1.14641600
Cl	-6.38881100	-3.85896000	-2.00988500
Cl	-0.09144500	-1.73266700	5.84941200

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P	-3.32089400	0.26947500	-0.02690200
C	-4.07500500	-0.33105000	-1.60235100
C	-4.02953900	1.97054500	0.14254500
C	-4.16756700	-0.65224200	1.32677000
C	-3.40494000	-1.29751200	-2.36809200
C	-5.32105400	0.14468900	-2.04802300
C	-3.90891100	2.87987300	-0.92204200
C	-4.65124600	2.39580100	1.32530000
C	-3.54632900	-0.71421100	2.58333500
C	-5.42745700	-1.24227300	1.15912600
C	-3.96972100	-1.77800600	-3.55099500
H	-2.45374800	-1.69041900	-2.02508700
C	-5.88160600	-0.33895700	-3.23077400
H	-5.85083500	0.90119000	-1.47834500
C	-4.40216000	4.17750600	-0.80613900
H	-3.42195000	2.57727500	-1.84264300
C	-5.14109800	3.69948500	1.44018000
H	-4.76299200	1.71206500	2.15970800
C	-4.18324900	-1.33431900	3.65778400

H	-2.55396000	-0.29218200	2.71386200
C	-6.05628100	-1.87622000	2.23246700
H	-5.91702900	-1.22044800	0.19104700
C	-5.20659300	-1.30027200	-3.98592900
H	-3.43928900	-2.52933600	-4.12958800
H	-6.84516000	0.03911100	-3.56201300
C	-5.01942500	4.59267300	0.37669500
H	-4.29716000	4.86672400	-1.63938800
H	-5.62294000	4.01035900	2.36344000
C	-5.43936800	-1.91922100	3.48334500
H	-3.68971100	-1.37703000	4.62484400
H	-7.02840300	-2.33964600	2.08705500
H	-5.64326000	-1.67357600	-4.90848300
H	-5.40168200	5.60600000	0.46677000
H	-5.93033900	-2.41451400	4.31673000
Pd	-0.91392300	0.03649300	0.02005900
P	1.49958200	-0.12850500	0.02281900
C	2.23922600	-0.43607100	1.68987200
C	2.47185900	1.33623000	-0.56157800
C	2.12195800	-1.47981700	-1.07083800
C	1.44500000	-0.97068300	2.71510600
C	3.58992600	-0.14381500	1.95694300
C	2.53979100	2.48075200	0.25124800
C	3.10740800	1.35708800	-1.81215000
C	1.44075100	-1.71624900	-2.27520700
C	3.26016800	-2.24025600	-0.76991400
C	1.98686700	-1.21520300	3.97657500
H	0.40784500	-1.21880800	2.51829600
C	4.13054800	-0.38996600	3.21507000
H	4.21966300	0.28551300	1.18454000
C	3.22763500	3.61326800	-0.17065100
H	2.04573800	2.49344500	1.21656700
C	3.79444200	2.49235600	-2.23739200
H	3.07488700	0.48655200	-2.45763500
C	1.89632000	-2.67888400	-3.17150000
H	0.53881200	-1.15528800	-2.50207400
C	3.70955700	-3.21315500	-1.65932100

H	3.79333600	-2.08595300	0.16183300
C	3.33213000	-0.92633700	4.23372200
H	1.36607100	-1.63289100	4.76101500
H	5.17141100	-0.16971300	3.42810000
C	3.86138800	3.62639400	-1.42134000
H	3.27110100	4.49077000	0.46399800
H	4.29130100	2.51243700	-3.20184000
C	3.03540400	-3.43592100	-2.86553700
H	1.36452800	-2.85625100	-4.09929500
H	4.58472900	-3.81308300	-1.43284700
C	-0.74610000	2.04884300	-0.28462900
C	-0.51721400	2.56171100	-1.56879100
C	-0.84256900	2.94512600	0.78848900
C	-0.38859400	3.93991100	-1.77568500
H	-0.42862000	1.89063300	-2.42032500
C	-0.70872400	4.32282100	0.58317500
H	-1.03414700	2.57905000	1.79463400
C	-0.48215100	4.82490200	-0.69985400
H	-0.20930300	4.31826200	-2.77980800
H	-0.78839300	5.00248700	1.42888400
I	-1.11188800	-2.75196000	0.43944100
H	-0.37929600	5.89519600	-0.85980100
C	3.96720200	-1.16482600	5.56346300
C	3.56831800	-4.48960900	-3.77721300
C	4.61364400	4.80928300	-1.92841800
O	5.13097700	-0.92448100	5.81943300
O	5.16098000	4.86317900	-3.01275900
O	4.55740100	-5.15821200	-3.54895000
O	4.62654300	5.83189000	-1.04311000
O	3.10215400	-1.68186400	6.46302100
O	2.82767700	-4.62389300	-4.90033700
C	3.28393100	-5.62980100	-5.81694300
H	2.57949400	-5.60793400	-6.64900900
H	4.29620500	-5.40367400	-6.16286100
H	3.28438000	-6.61264700	-5.33819400
C	3.65263400	-1.94310000	7.76303400
H	4.02499500	-1.01961400	8.21459000

H	2.83131800	-2.35468100	8.35026100
H	4.47454400	-2.66066100	7.69415400
C	5.33871500	7.00216200	-1.47057200
H	5.25170100	7.71364500	-0.64879000
H	6.38804100	6.76380700	-1.66423800
H	4.89493100	7.41085800	-2.38248900

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P	-1.49197800	0.05019000	-0.15201800
C	-2.80374500	-1.24328900	-0.29541200
C	-2.48061500	1.64179700	-0.21197900
C	-2.43630600	-2.59685800	-0.38627200
C	-4.16769400	-0.90368800	-0.29432200
C	-0.92201900	0.05474200	1.62449900
Pd	0.77220500	-0.62493800	-0.48529000
C	-2.76193600	2.38687200	0.94367000
C	-3.04970900	2.06120800	-1.43025300
C	-3.41502800	-3.58363700	-0.48326800
H	-1.38754200	-2.88226400	-0.35897900
C	-5.14272000	-1.89412800	-0.39252200
H	-4.48111000	0.13006400	-0.21603400
C	-0.04010700	1.05848700	2.07312600
C	-1.32819400	-0.94945000	2.51868200
C	-0.61137900	0.25505800	-1.92954700
C	-3.55769000	3.53195600	0.88385900
H	-2.36347900	2.08126400	1.90290700
C	-3.85260100	3.19494200	-1.49020100
H	-2.87546800	1.49443000	-2.33763000
C	-4.77203000	-3.24067400	-0.49169200
H	-3.13436900	-4.62952300	-0.55054100
H	-6.19225600	-1.62260000	-0.39171100
C	0.42033900	1.05888100	3.38690000
H	0.27053200	1.85125200	1.39996900
C	-0.87522300	-0.93732300	3.83305600
H	-1.98505200	-1.74565500	2.18940900
C	-0.15562100	1.51952100	-2.36364000

C	-0.85425000	-0.75170500	-2.88979100
C	-4.10496400	3.94575000	-0.33459100
H	-3.75608100	4.10110800	1.78504900
H	-4.29304600	3.51593500	-2.42837300
C	0.00117900	0.06148900	4.27732400
H	1.10321400	1.83021300	3.72408200
H	-1.18912800	-1.70446900	4.53287700
C	0.08962300	1.75312200	-3.71475500
H	0.01265100	2.31506500	-1.64589800
C	-0.62347500	-0.50002300	-4.24387800
H	-1.22184800	-1.72228700	-2.57788700
C	-0.14780800	0.74635600	-4.65657800
H	0.47450300	2.71899000	-4.02820100
H	-0.81370500	-1.28280900	-4.97295900
P	3.11560400	0.33677400	-0.75644600
C	4.17577400	-0.63356500	-1.91798000
C	4.14525000	0.44373300	0.77912200
C	3.21404300	2.06183300	-1.42333500
C	3.54969300	-1.54428700	-2.78145700
C	5.57315900	-0.50017200	-1.96569700
C	5.09015600	1.45788700	1.00826000
C	3.98148300	-0.56285000	1.74550200
C	2.69348800	3.11308900	-0.64531800
C	3.68442300	2.35880100	-2.71045700
C	4.30324300	-2.29344300	-3.68807900
H	2.47399500	-1.68259000	-2.72461700
C	6.32413900	-1.25115500	-2.86973000
H	6.07730400	0.18278700	-1.28825100
C	5.85497800	1.46381400	2.17653400
H	5.22717100	2.25022700	0.27875900
C	4.75414200	-0.55677300	2.90806900
H	3.25461400	-1.35487700	1.58432300
C	2.65540300	4.41844200	-1.13324700
H	2.33273800	2.90891300	0.36026100
C	3.63990600	3.66698100	-3.20311500
H	4.09343200	1.56882100	-3.33173400
C	5.68975200	-2.14723300	-3.73464100

H	3.80554600	-3.00225100	-4.34432900
C	5.69043700	0.45538000	3.12808200
H	6.58110200	2.25638200	2.33975500
H	4.61779200	-1.34582200	3.64278500
C	3.12712900	4.70050300	-2.41920800
H	2.26002300	5.21650200	-0.50984600
H	4.01533800	3.87553000	-4.20184300
H	6.27737100	-2.73667600	-4.43373800
I	1.27528400	-3.28085700	0.35345000
H	6.28786300	0.45993400	4.03625800
H	3.09752700	5.71708300	-2.80209600
H	7.40539000	-1.14228500	-2.89395600
H	0.03252500	0.93663600	-5.71111100
C	-5.77523700	-4.34206300	-0.60483100
C	0.44540300	0.01933600	5.69967300
C	-4.96430300	5.16046800	-0.46268500
O	-5.46105300	5.53782300	-1.50547900
O	0.07624900	-0.80768600	6.51012100
O	-5.49128700	-5.51861800	-0.70314700
O	1.30954800	1.01572700	6.00010400
O	-5.13130800	5.79953500	0.71484700
O	-7.04663800	-3.88358900	-0.58700900
C	-8.06246400	-4.89366300	-0.69171100
H	-9.01141700	-4.35772200	-0.65916300
H	-7.96127600	-5.44259900	-1.63170500
H	-7.98863600	-5.59887000	0.14032500
C	1.78319600	1.02532600	7.35482100
H	2.46140800	1.87662900	7.42118800
H	0.94952100	1.14083400	8.05286700
H	2.30957900	0.09482700	7.58352700
C	-5.95173500	6.97800400	0.66274500
H	-6.95679300	6.72931200	0.31212300
H	-5.98292300	7.35685400	1.68450100
H	-5.51387400	7.71943800	-0.01076000

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P	-3.38039900	0.02312300	-0.14656400
C	-4.03161600	-1.28910300	-1.26557400
C	-4.15041900	1.56326200	-0.82682200
C	-4.25148000	-0.19029400	1.46507100
C	-5.21958200	-1.98276800	-1.00240400
C	-3.32171900	-1.57305400	-2.44259500
C	-4.62998400	1.62722000	-2.14319700
C	-4.22348200	2.71487600	-0.02467400
C	-3.59221000	-0.81354200	2.53521600
C	-5.57683400	0.24525600	1.64256900
C	-5.69130300	-2.93810800	-1.90508000
H	-5.77377700	-1.79162700	-0.08959600
C	-3.80255800	-2.51630700	-3.34952100
H	-2.38203000	-1.06448600	-2.63980200
C	-5.16984300	2.81434700	-2.64480200
H	-4.59392600	0.75075700	-2.78084000
C	-4.76768600	3.89536800	-0.52610100
H	-3.84732100	2.69481600	0.99233900
C	-4.24473600	-0.99847600	3.75561100
H	-2.57813600	-1.17546300	2.40318700
C	-6.22520500	0.05710700	2.86347300
H	-6.10057700	0.74073600	0.83140200
C	-4.98854100	-3.20344500	-3.08062700
H	-6.60828600	-3.47754900	-1.68388300
H	-3.24229100	-2.72708900	-4.25632000
C	-5.24226200	3.94987100	-1.83896700
H	-5.53979100	2.84383800	-3.66625800
H	-4.81409000	4.77536200	0.10934100
C	-5.55983200	-0.56349600	3.92316800
H	-3.72162500	-1.48596600	4.57365900
H	-7.24944000	0.39889700	2.98610000
H	-5.35705600	-3.94874000	-3.78021600
H	-5.66496600	4.87173600	-2.22943600
H	-6.06527900	-0.70615600	4.87457700
Pd	-0.97402400	-0.04851700	0.00616400
P	1.45011000	-0.01106400	0.01627900
C	2.14447700	-0.03683300	1.72955700

C	2.29952800	1.44214400	-0.76393600
C	2.26507900	-1.42775200	-0.84658000
C	3.39249500	0.52721600	2.04420300
C	1.40816100	-0.66512600	2.74543400
C	2.27587500	2.69647800	-0.12783800
C	2.92678300	1.33524000	-2.01287400
C	1.66203200	-1.94708600	-2.00043100
C	3.48851400	-1.96220000	-0.41852000
C	3.88989700	0.46723000	3.34427700
H	3.97935700	1.02127800	1.27722400
C	1.90642600	-0.72652500	4.04652800
H	0.45402400	-1.12752800	2.51244800
C	2.87319600	3.80336000	-0.71982500
H	1.77846900	2.81713400	0.82757500
C	3.51867600	2.44841800	-2.61349000
H	2.96612800	0.38185200	-2.52721600
C	2.27593800	-2.96725800	-2.72505500
H	0.69827500	-1.56809000	-2.32402300
C	4.09806000	-2.99057700	-1.13366200
H	3.96913600	-1.58581000	0.47792400
C	3.14523300	-0.15809500	4.34783500
H	4.85770400	0.89985000	3.57665000
H	1.33401800	-1.22287600	4.82287200
C	3.49552800	3.68227300	-1.96694500
H	2.84598300	4.76479100	-0.21651400
H	4.00328000	2.35027400	-3.57858000
C	3.49464200	-3.49071200	-2.29050500
H	1.80185500	-3.36244700	-3.61657000
H	5.04499100	-3.39982800	-0.79564400
C	-0.95871000	1.99375700	0.01642200
C	-0.94749300	2.76501800	-1.15213600
C	-0.95127700	2.64876900	1.25735000
C	-0.92525700	4.16183500	-1.08424200
H	-0.95981500	2.28398800	-2.12690700
C	-0.92911400	4.04817900	1.32557900
H	-0.96138600	2.07401100	2.18107700
C	-0.91457800	4.80828500	0.15394400

H	-0.91614900	4.74433000	-2.00256500
H	-0.92374100	4.53962300	2.29632200
I	-1.00364400	-2.84090600	0.41108500
H	-0.89763600	5.89399000	0.20520200
C	3.66319800	-0.16382500	5.76248400
C	4.15442600	-4.62532900	-3.02914000
C	4.11577900	4.90315500	-2.59116300
F	3.35454900	0.98698700	6.40404600
F	3.14192300	-1.17477600	6.48831100
F	5.00856700	-0.28394500	5.79950200
F	5.48540600	-4.41908300	-3.16079500
F	3.64541600	-4.79042900	-4.26847300
F	4.00541300	-5.79781100	-2.37476700
F	3.18516900	5.84998800	-2.85188000
F	5.02453100	5.47163800	-1.76563200
F	4.74317100	4.62440800	-3.75279600

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P	-1.50502500	0.11724700	-0.12871300
C	-2.78232600	-1.16155700	-0.51406100
C	-2.55400900	1.65282600	0.13443700
C	-2.38154400	-2.44304500	-0.92546700
C	-4.15346700	-0.88614300	-0.37778400
C	-0.90808700	-0.18302500	1.61305300
Pd	0.76390700	-0.46454000	-0.60680800
C	-2.87553100	2.11913800	1.41769000
C	-3.13127900	2.30089000	-0.97297900
C	-3.33365900	-3.42181800	-1.20787600
H	-1.32505100	-2.68926900	-0.99426800
C	-5.10230000	-1.86653300	-0.66135700
H	-4.49286600	0.08787100	-0.04783300
C	-0.04391800	0.74447500	2.22528100
C	-1.25775300	-1.35316700	2.30494800
C	-0.64281300	0.71657600	-1.80399800
C	-3.71917200	3.21771200	1.59191800
H	-2.47381500	1.62899700	2.29575400

C	-3.98120100	3.39027600	-0.80310500
H	-2.92864500	1.94952000	-1.97818800
C	-4.69397100	-3.13376500	-1.08219600
H	-3.00941100	-4.41111900	-1.51357300
H	-6.15849300	-1.64645300	-0.54791800
C	0.47101500	0.49694700	3.49547300
H	0.22547200	1.66410100	1.71529600
C	-0.75064500	-1.59111700	3.57881200
H	-1.90539300	-2.09084000	1.84667300
C	-0.19161600	2.04778200	-1.94716000
C	-0.84979900	-0.06279000	-2.96405300
C	-4.26936600	3.85798700	0.48221200
H	-3.95443800	3.56621300	2.59198400
H	-4.42520500	3.87235800	-1.66787100
C	0.12071000	-0.67342400	4.17243100
H	1.14620100	1.20974400	3.95581100
H	-1.02739700	-2.49690100	4.10784600
C	0.08267500	2.56757900	-3.20912300
H	-0.04640900	2.67281900	-1.07271900
C	-0.59229800	0.47603900	-4.22678900
H	-1.21437000	-1.07980100	-2.87921800
C	-0.12270300	1.78493700	-4.35056300
H	0.47001400	3.57798700	-3.29765800
H	-0.75687800	-0.13305300	-5.11125900
P	3.12043200	0.50938000	-0.68137100
C	4.28528500	-0.39622700	-1.79262400
C	3.98389400	0.54049600	0.95591000
C	3.28204200	2.26658400	-1.24659500
C	3.74201800	-1.24855700	-2.76495000
C	5.68049400	-0.25871200	-1.71015300
C	4.96303300	1.49055900	1.29432200
C	3.63661900	-0.44028900	1.89922500
C	2.77121100	3.29399200	-0.43186900
C	3.79259000	2.61093300	-2.50658600
C	4.57567400	-1.93366000	-3.65192300
H	2.66688200	-1.39494300	-2.80657200
C	6.51139700	-0.94740000	-2.59337200

H	6.12103900	0.37833700	-0.94908600
C	5.57924500	1.45824300	2.54653200
H	5.23677600	2.26667600	0.58602300
C	4.25304100	-0.46826300	3.15219700
H	2.88544200	-1.18450000	1.64922200
C	2.78360700	4.62210000	-0.85649900
H	2.37865400	3.05403300	0.55361900
C	3.79837700	3.94147900	-2.93613400
H	4.19414500	1.83992600	-3.15612200
C	5.95994000	-1.78292700	-3.56874900
H	4.14103000	-2.59728000	-4.39446200
C	5.22386900	0.48051900	3.47849600
H	6.33419900	2.20029300	2.79398400
H	3.95525900	-1.22020700	3.87674700
C	3.29717200	4.95166100	-2.11481600
H	2.39711900	5.40091000	-0.20380300
H	4.20510100	4.18599500	-3.91417100
H	6.60961100	-2.32258800	-4.25291900
I	1.27131300	-3.19832100	-0.11315400
H	5.69920500	0.46110200	4.45581500
H	3.30982900	5.98635300	-2.44682400
H	7.58992100	-0.83636900	-2.51651300
H	0.08077100	2.19771100	-5.33482400
C	-5.72282700	-4.17182800	-1.45213100
C	-5.13383400	5.07945900	0.66157600
C	0.72732800	-0.97704600	5.51588700
F	-5.28604200	-5.42290300	-1.20243800
F	-6.02437600	-4.11111200	-2.76919700
F	-6.87768400	-3.99659300	-0.77366300
F	1.85816000	-1.71370700	5.39821800
F	1.06000800	0.14945300	6.18400300
F	-0.11687900	-1.68195100	6.29974600
F	-4.39880000	6.21286100	0.60326300
F	-6.07595200	5.16941200	-0.30152700
F	-5.76526000	5.07625500	1.85423500

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P	-3.11556500	0.09431600	-0.05672200
C	-3.80471400	-0.32858200	-1.71585200
C	-3.93470200	1.70882100	0.32856200
C	-3.91417400	-1.05929100	1.13867900
C	-3.04890400	-1.11550300	-2.59829600
C	-5.08246100	0.10332000	-2.11370500
C	-3.86948800	2.75851700	-0.60350300
C	-4.59299600	1.92898000	1.54705100
C	-3.33532900	-1.20895700	2.40827300
C	-5.09166300	-1.75674700	0.84007500
C	-3.56069400	-1.46384400	-3.84951400
H	-2.07143100	-1.47423300	-2.29355000
C	-5.58984000	-0.24780000	-3.36521800
H	-5.67948200	0.72174600	-1.45126100
C	-4.45231600	3.99263700	-0.32390200
H	-3.35673400	2.61596500	-1.54846900
C	-5.17242200	3.16940000	1.82643700
H	-4.66522900	1.13303200	2.28008700
C	-3.93533600	-2.02242600	3.36832100
H	-2.40361600	-0.69958900	2.63798700
C	-5.68238000	-2.58325500	1.79823300
H	-5.54558000	-1.66837800	-0.14136900
C	-4.82951700	-1.03083500	-4.23646900
H	-2.96471100	-2.07739000	-4.51960300
H	-6.57882900	0.09374800	-3.65880900
C	-5.10552400	4.20296800	0.89324300
H	-4.39017200	4.79247700	-1.05653500
H	-5.68193700	3.32033100	2.77448500
C	-5.11010200	-2.71393100	3.06382800
H	-3.47571000	-2.13041200	4.34697300
H	-6.58964200	-3.12766700	1.55059000
H	-5.22519000	-1.30097200	-5.21193100
H	-5.55845500	5.16660700	1.11068500
H	-5.57099300	-3.35898400	3.80696900
Pd	-0.70061400	-0.00947400	-0.00485400
P	1.72064200	-0.03849000	0.03636500

C	2.41631900	-0.41282000	1.70722100
C	2.61054000	1.51762300	-0.42866900
C	2.47067600	-1.27930200	-1.10614400
C	1.63279400	-1.11007100	2.63746200
C	3.72122200	-0.02768600	2.07046600
C	2.60427300	2.60668700	0.45788600
C	3.24663000	1.66541100	-1.67195400
C	1.85464700	-1.49013700	-2.34829500
C	3.64519800	-1.98267800	-0.80045500
C	2.14261900	-1.42130900	3.89833700
H	0.63279800	-1.43022900	2.36544500
C	4.22389100	-0.33820900	3.32887700
H	4.34240100	0.52287300	1.37144000
C	3.21645600	3.80756500	0.11168100
H	2.11007300	2.52554300	1.41956900
C	3.85544100	2.86883500	-2.01645700
H	3.27527600	0.83901700	-2.37371900
C	2.41020000	-2.37024200	-3.27402100
H	0.92627900	-0.97808000	-2.58313400
C	4.19125600	-2.87056100	-1.72213800
H	4.13131200	-1.84875100	0.16003200
C	3.44108000	-1.03879100	4.25932900
H	1.51493200	-1.96744700	4.59544000
H	5.22845400	-0.04588600	3.61689900
C	3.84878400	3.95553500	-1.13191700
H	3.18946400	4.63083800	0.81826100
H	4.35072900	2.98753700	-2.97470800
C	3.58500800	-3.07339700	-2.96995000
H	1.91089200	-2.51538500	-4.22683500
H	5.09560800	-3.42487100	-1.49350100
C	-0.64897700	2.03087600	-0.05691200
C	-0.47384800	2.71244000	-1.26904100
C	-0.78336500	2.77949100	1.12043900
C	-0.43406400	4.11099600	-1.30378700
H	-0.36143700	2.15908100	-2.19871800
C	-0.73756300	4.17786500	1.08754200
H	-0.93612700	2.27881100	2.07397700

C	-0.56394300	4.84831600	-0.12503600
H	-0.29734100	4.62126900	-2.25481200
H	-0.84693200	4.74112500	2.01186800
I	-0.75544100	-2.83476100	0.07391000
H	-0.53409500	5.93477300	-0.15170500
C	4.04013700	-1.34288700	5.60392400
C	4.22504600	-4.04473300	-3.92028700
C	4.51628800	5.22886400	-1.56242100
O	5.16805700	-0.96251200	5.87639800
O	5.05138100	5.30895900	-2.65767700
O	5.26382400	-4.61138600	-3.61846100
C	4.51128700	6.41593600	-0.61335300
H	3.48630500	6.72165500	-0.37099400
H	5.00965400	6.16783900	0.33158000
H	5.03399000	7.24709000	-1.08970600
C	3.55710100	-4.30963200	-5.25902100
H	3.47311700	-3.38840000	-5.84829900
H	4.15546300	-5.03683100	-5.81042400
H	2.54291400	-4.70330800	-5.12074800
C	3.22074600	-2.13091900	6.61144200
H	2.28815600	-1.60869300	6.85730200
H	2.94783600	-3.11562800	6.21327600
H	3.81245000	-2.25917700	7.51935800

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P	-1.68233700	0.14219000	-0.07790400
C	-2.98296700	-1.06159500	-0.60316400
C	-2.68758200	1.69281100	0.24313700
C	-2.61092300	-2.32105500	-1.10611800
C	-4.34781300	-0.75182000	-0.48325400
C	-1.17190500	-0.31594200	1.65518900
Pd	0.58807600	-0.45444900	-0.49255900
C	-3.02954000	2.10381800	1.53965800
C	-3.21204100	2.41893400	-0.84497200
C	-3.58597200	-3.23807800	-1.48890400
H	-1.56060600	-2.59402300	-1.17119800

C	-5.31742900	-1.67728300	-0.86675900
H	-4.66498200	0.20680200	-0.09144600
C	-0.34120800	0.54959200	2.39814900
C	-1.55802000	-1.54134200	2.21910900
C	-0.73041600	0.81808200	-1.68943500
C	-3.84274900	3.22064600	1.74592200
H	-2.66654500	1.55836300	2.40181000
C	-4.03080500	3.52208000	-0.63804600
H	-2.98828500	2.11491600	-1.86127900
C	-4.94904200	-2.92876000	-1.37847700
H	-3.30258100	-4.21158800	-1.87533200
H	-6.36439600	-1.41000700	-0.76311200
C	0.08323500	0.19259300	3.67210400
H	-0.04268800	1.50751100	1.98298800
C	-1.12841600	-1.88961900	3.49673000
H	-2.17410700	-2.23476700	1.65905100
C	-0.25121300	2.14600900	-1.73499000
C	-0.93666200	0.12356400	-2.90198800
C	-4.35059500	3.94485700	0.66155200
H	-4.07666800	3.51488600	2.76434700
H	-4.43711400	4.07900500	-1.47602900
C	-0.30286900	-1.03200700	4.23839600
H	0.72333700	0.84915100	4.25216900
H	-1.43891100	-2.84531300	3.90653300
C	0.05173000	2.74345900	-2.95596300
H	-0.10561100	2.70565100	-0.81743500
C	-0.64833100	0.73973300	-4.12164400
H	-1.32279900	-0.88896300	-2.89037600
C	-0.15083700	2.04401700	-4.15051300
H	0.45514100	3.75140600	-2.97111000
H	-0.81136700	0.19469900	-5.04729500
P	2.94825400	0.50501000	-0.40447300
C	4.05441500	-0.13726800	-1.73839300
C	3.90719700	0.20178600	1.14998100
C	3.06939300	2.34347400	-0.58934800
C	3.46870400	-0.84220300	-2.79965900
C	5.44754100	0.04222800	-1.72594700

C	4.88193200	1.08799800	1.63913700
C	3.65324400	-0.98534600	1.85619700
C	2.55414600	3.15952000	0.43570200
C	3.54963400	2.96212300	-1.75247200
C	4.25746300	-1.34315400	-3.83814000
H	2.39710200	-1.01868300	-2.79540600
C	6.23354800	-0.46004700	-2.76246600
H	5.92146400	0.56544900	-0.90055100
C	5.58748000	0.79190000	2.80666000
H	5.08482900	2.01758800	1.11601900
C	4.36607100	-1.27981600	3.01990100
H	2.90207500	-1.68080400	1.49152500
C	2.53065800	4.54739300	0.30541600
H	2.18648500	2.70437300	1.35263000
C	3.52117500	4.35406800	-1.88547400
H	3.95379700	2.35736200	-2.55772800
C	5.63902400	-1.15165500	-3.82192300
H	3.79106200	-1.89580700	-4.64919100
C	5.33163700	-0.39318700	3.49943400
H	6.33608700	1.48914600	3.17445100
H	4.15943000	-2.20354000	3.55363100
C	3.01297800	5.15158600	-0.86006900
H	2.14012200	5.15864600	1.11516700
H	3.90562200	4.81282200	-2.79303400
H	6.25423300	-1.54844600	-4.62537900
I	1.02747300	-3.24856200	-0.31984700
H	5.87926800	-0.62146200	4.41007700
H	2.99601900	6.23326700	-0.96290300
H	7.31099200	-0.31820800	-2.73996500
H	0.07442600	2.51829000	-5.10182000
C	-0.14765600	-2.71953700	6.20962200
H	0.23343800	-3.52991600	5.57682400
H	0.30235900	-2.78997300	7.20133500
H	-1.23272700	-2.85546700	6.29521400
C	-5.57868200	5.62890200	2.22145200
H	-6.21803900	6.50970200	2.14318300
H	-6.10434900	4.84872500	2.78529800

H	-4.67413800	5.88591400	2.78583500
C	-7.43505800	-3.64423400	-1.67934700
H	-8.00878200	-4.50105800	-2.03638200
H	-7.70204000	-3.43848300	-0.63566000
H	-7.70443500	-2.75786200	-2.26650300
C	-5.95489700	-3.96028600	-1.81309900
C	0.18843200	-1.36145100	5.61751200
C	-5.23248800	5.15261500	0.82160800
O	-5.65913300	5.73551100	-0.16233300
O	0.84842400	-0.54958800	6.24863700
O	-5.58224000	-5.03060300	-2.26451900

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P	-2.83975300	0.05089200	-0.04011000
C	-3.52838000	-0.34523300	-1.70454600
C	-3.68064900	1.64084100	0.39155600
C	-3.59993100	-1.14923800	1.13259200
C	-2.76345600	-1.09464200	-2.61131200
C	-4.81871500	0.06816600	-2.08111400
C	-3.64767000	2.71201900	-0.51760900
C	-4.32491200	1.82127600	1.62406200
C	-3.01497900	-1.30783600	2.39838500
C	-4.75711100	-1.87411000	0.82012300
C	-3.27819700	-1.42457500	-3.86624700
H	-1.77596700	-1.43908900	-2.32332900
C	-5.32901300	-0.26455900	-3.33636100
H	-5.42336700	0.65707400	-1.39903300
C	-4.24748400	3.92899700	-0.20134900
H	-3.14769900	2.60017900	-1.47353400
C	-4.92130300	3.04478700	1.93993900
H	-4.37377200	1.00783400	2.33966900
C	-3.58896600	-2.15870700	3.34165400
H	-2.09955200	-0.77440200	2.63919500
C	-5.32123200	-2.73778900	1.76137400
H	-5.21538100	-1.77792300	-0.15849800
C	-4.55947600	-1.01015700	-4.23207600

H	-2.67543500	-2.00948600	-4.55549600
H	-6.32766100	0.06190700	-3.61367300
C	-4.88565700	4.10027000	1.02985600
H	-4.21070300	4.74595800	-0.91653700
H	-5.41947500	3.16516100	2.89823600
C	-4.74305300	-2.87831200	3.02319600
H	-3.12557500	-2.27305800	4.31771900
H	-6.21250700	-3.30325000	1.50340000
H	-4.95771300	-1.26611200	-5.21021200
H	-5.35167400	5.05062400	1.27582900
H	-5.18339900	-3.55223600	3.75292200
Pd	-0.42706400	-0.01216100	-0.00477000
P	1.99270600	-0.01222100	0.03511900
C	2.70148000	-0.41463900	1.69624700
C	2.87321800	1.56216800	-0.39290600
C	2.76090000	-1.21921100	-1.13339500
C	1.93072200	-1.14945100	2.61052000
C	3.99584100	-0.00871500	2.06787600
C	2.81928300	2.64312100	0.50432600
C	3.54438800	1.73117700	-1.61305400
C	2.15813400	-1.39144300	-2.38971900
C	3.92619000	-1.93612200	-0.83179400
C	2.43820700	-1.47490100	3.86589600
H	0.93907600	-1.48728200	2.32903300
C	4.51012300	-0.32956600	3.32064300
H	4.60670500	0.56945200	1.38260400
C	3.41922500	3.85735700	0.19496900
H	2.29312500	2.54526600	1.44694100
C	4.14676700	2.94601800	-1.93376300
H	3.60784300	0.91420700	-2.32291100
C	2.71875300	-2.24077800	-3.33688700
H	1.23394400	-0.87040000	-2.62020100
C	4.48642500	-2.80266000	-1.76741900
H	4.39950800	-1.83403100	0.13860900
C	3.73061900	-1.06483900	4.22901700
H	1.83767000	-2.04664400	4.56578400
H	5.50932300	-0.01263300	3.60126400

C	4.08815300	4.01751600	-1.03080200
H	3.36675900	4.68648900	0.89256100
H	4.66645200	3.06553000	-2.87892400
C	3.88934000	-2.95433200	-3.02832700
H	2.24923400	-2.36992400	-4.30643500
H	5.38393200	-3.36285600	-1.52636200
C	-0.41449200	2.02984000	-0.03300500
C	-0.25179700	2.72431200	-1.23941200
C	-0.55040200	2.76434400	1.15287700
C	-0.22384300	4.12369900	-1.25974200
H	-0.14351900	2.18090000	-2.17563800
C	-0.51598100	4.16345800	1.13388000
H	-0.69677600	2.25272000	2.10155800
C	-0.35286600	4.84763700	-0.07259100
H	-0.09737000	4.64558200	-2.20575500
H	-0.62605500	4.71650600	2.06410000
I	-0.40904600	-2.83626600	0.01676300
H	-0.32932300	5.93415100	-0.08817200
C	4.70615400	5.27002700	-1.35601300
C	4.47111600	-3.83544300	-3.99912800
C	4.25428900	-1.39027900	5.52441100
N	5.20712200	6.28633800	-1.61908700
N	4.94673200	-4.54324100	-4.79006400
N	4.67912600	-1.65105900	6.57517400

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P	-1.94000500	0.18641500	-0.01635400
C	-3.27489500	-0.96498400	-0.57798300
C	-2.90925500	1.74656000	0.38175300
C	-2.93333300	-2.22663000	-1.09340300
C	-4.63186200	-0.61064400	-0.48154900
C	-1.43929900	-0.34614000	1.70242900
Pd	0.31630300	-0.45563300	-0.42792600
C	-3.27124800	2.07987300	1.69669700
C	-3.38476500	2.55785300	-0.66565700
C	-3.92461100	-3.11088700	-1.51228900

H	-1.89135500	-2.53375400	-1.14368100
C	-5.62561000	-1.49091000	-0.89955100
H	-4.92699300	0.35074200	-0.08002800
C	-0.57301100	0.46666000	2.46109900
C	-1.86469500	-1.57531100	2.23243900
C	-0.99640500	0.88262300	-1.59121100
C	-4.05352000	3.20176200	1.96609900
H	-2.94703500	1.46551700	2.52737600
C	-4.17357800	3.67431600	-0.40973200
H	-3.14703600	2.31593800	-1.69494200
C	-5.27701800	-2.74652900	-1.42210200
H	-3.64876400	-4.08439500	-1.90423700
H	-6.67090600	-1.21017000	-0.82263300
C	-0.13585300	0.05625000	3.71592900
H	-0.24821800	1.42781800	2.07593000
C	-1.43966000	-1.98272000	3.49132200
H	-2.51152300	-2.22785100	1.65844000
C	-0.44909100	2.18542600	-1.59484400
C	-1.18543900	0.21579300	-2.82268900
C	-4.50601000	4.01008100	0.91335500
H	-4.31664500	3.45068900	2.98899000
H	-4.53372100	4.28917100	-1.22811900
C	-0.56769000	-1.17346500	4.23964200
H	0.54142700	0.67902200	4.29063500
H	-1.77130100	-2.93342500	3.89529400
C	-0.07669200	2.78843500	-2.79410900
H	-0.30835300	2.72267200	-0.66316600
C	-0.82718200	0.83828600	-4.01960300
H	-1.61383500	-0.77933400	-2.84276800
C	-0.27073700	2.11916300	-4.00687600
H	0.37547600	3.77521400	-2.77703900
H	-0.98024600	0.31659200	-4.96005400
P	2.69770600	0.45023100	-0.22685200
C	3.87081700	-0.21588700	-1.48847200
C	3.53969200	0.10902500	1.38579900
C	2.87367500	2.28558900	-0.39587200
C	3.34574400	-0.94963600	-2.56166200

C	5.26043700	-0.02591900	-1.40631000
C	4.48942900	0.97011300	1.96102000
C	3.21922100	-1.08781800	2.04817700
C	2.34563000	3.11538900	0.61143700
C	3.40712700	2.89184900	-1.54247900
C	4.19183100	-1.46934900	-3.54459200
H	2.27693600	-1.13598800	-2.60981000
C	6.10301600	-0.54595900	-2.38782300
H	5.68674900	0.52024400	-0.56984300
C	5.10225300	0.64156500	3.17167300
H	4.74585400	1.90486000	1.47192100
C	3.83907900	-1.41500000	3.25569900
H	2.48934100	-1.76618100	1.61423000
C	2.36060900	4.50351600	0.48095900
H	1.94056000	2.67108300	1.51776800
C	3.41839200	4.28395600	-1.67563600
H	3.82317600	2.27702400	-2.33387800
C	5.56916500	-1.26663200	-3.46039800
H	3.77253300	-2.04450600	-4.36556300
C	4.77880600	-0.55128900	3.82171100
H	5.83315500	1.31920700	3.60562500
H	3.58094300	-2.34494100	3.75490200
C	2.89645400	5.09477600	-0.66752900
H	1.96015300	5.12485700	1.27803100
H	3.84526300	4.73236500	-2.56919900
H	6.22834400	-1.67697800	-4.22091400
I	0.65422300	-3.25791600	-0.33983200
H	5.25494700	-0.80496200	4.76510600
H	2.91115500	6.17643900	-0.76988100
H	7.17675800	-0.39540400	-2.31228700
H	0.01009500	2.59767100	-4.94101100
C	-0.12369800	-1.59515500	5.53556000
C	-5.30876800	5.16773100	1.18363700
C	-6.30252100	-3.65048800	-1.85816300
N	-7.13703100	-4.37855100	-2.21279600
N	0.23366200	-1.93018700	6.59071500
N	-5.95889200	6.10706600	1.40110700

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P	-3.11917800	0.08452800	-0.02693200
C	-3.80566600	-0.33385500	-1.68660600
C	-3.94241300	1.69017500	0.37787600
C	-3.89291900	-1.08963500	1.16256700
C	-3.05074400	-1.12043500	-2.57025800
C	-5.08493000	0.09661200	-2.08122200
C	-3.89742100	2.74635700	-0.54820100
C	-4.58543600	1.89655200	1.60695300
C	-3.31217900	-1.23686700	2.43165200
C	-5.05664800	-1.80705700	0.85706000
C	-3.56411600	-1.46910700	-3.82062200
H	-2.07273900	-1.47929000	-2.26767100
C	-5.59360200	-0.25460600	-3.33216200
H	-5.68226300	0.71266100	-1.41694900
C	-4.48500600	3.97424300	-0.25176200
H	-3.39777000	2.61399100	-1.50166500
C	-5.16906500	3.13109800	1.90301300
H	-4.64315100	1.09484300	2.33499300
C	-3.89660600	-2.06930300	3.38491400
H	-2.39200600	-0.70946300	2.66753700
C	-5.63156800	-2.65199300	1.80867700
H	-5.51171800	-1.71925600	-0.12384500
C	-4.83390900	-1.03644500	-4.20503700
H	-2.96933900	-2.08267000	-4.49162600
H	-6.58351800	0.08563000	-3.62382500
C	-5.12202400	4.17148900	0.97617900
H	-4.43948600	4.77936600	-0.97973600
H	-5.66638400	3.27193900	2.85893300
C	-5.05730800	-2.78132300	3.07351300
H	-3.43623600	-2.17545900	4.36329300
H	-6.52803200	-3.21177700	1.55643600
H	-5.23094900	-1.30665900	-5.17979900
H	-5.57830200	5.13038600	1.20672400
H	-5.50582100	-3.44098100	3.81122900

Pd	-0.70871700	-0.00332000	0.01048200
P	1.70871000	-0.03657000	0.03171200
C	2.44196900	-0.44061600	1.68283800
C	2.60359900	1.52731300	-0.40831100
C	2.44093300	-1.25595300	-1.14834000
C	1.66082000	-1.11575400	2.63359900
C	3.76313900	-0.08285100	2.00994500
C	2.56992000	2.60515300	0.49454100
C	3.25961900	1.69177800	-1.63789900
C	1.82700000	-1.39501500	-2.40443000
C	3.58171600	-2.01494500	-0.85432600
C	2.18419700	-1.43242200	3.88637800
H	0.64833000	-1.41416800	2.38498700
C	4.29764700	-0.39653800	3.25692000
H	4.37992400	0.45156000	1.29519900
C	3.17445900	3.81716700	0.18163000
H	2.05564700	2.50804400	1.44365900
C	3.86801100	2.90285600	-1.96536900
H	3.30659400	0.87607100	-2.35018700
C	2.35188600	-2.25754900	-3.36123500
H	0.92204300	-0.83834500	-2.62778100
C	4.10815900	-2.89609900	-1.79751300
H	4.06116100	-1.93644700	0.11488400
C	3.49472700	-1.06632800	4.17738800
H	1.59422300	-1.95490100	4.62926700
H	5.31280200	-0.12957000	3.52365200
C	3.81555200	3.94794800	-1.04906000
H	3.14969100	4.65541300	0.86641700
H	4.37987300	3.04206500	-2.90963200
C	3.48742500	-2.99800600	-3.03868000
H	1.89194900	-2.37655500	-4.33432600
H	4.98321000	-3.49785700	-1.58526500
C	-0.67347500	2.03727400	-0.06868200
C	-0.50222900	2.69781500	-1.29280500
C	-0.79664500	2.80363200	1.09818500
C	-0.45029700	4.09565300	-1.34863600
H	-0.40714000	2.12933000	-2.21553500

C	-0.73870800	4.20103700	1.04346500
H	-0.95196300	2.31909200	2.05958900
C	-0.56479100	4.85145900	-0.18002100
H	-0.31777700	4.59111400	-2.30796900
H	-0.83817100	4.77944800	1.95926500
I	-0.70152300	-2.82555700	0.09536100
H	-0.52159100	5.93656600	-0.22283400
N	4.05258900	-1.39273700	5.50406800
O	5.21898600	-1.07096800	5.72324300
O	3.31537300	-1.96365800	6.30472800
N	4.45413800	5.23050500	-1.38985000
O	5.00063600	5.32020700	-2.48826400
O	4.40053100	6.13189400	-0.55459600
N	4.04724700	-3.92017500	-4.04320000
O	5.04660400	-4.56402800	-3.72907500
O	3.48179600	-3.98305400	-5.13344200

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P	-1.69810300	0.14265200	-0.10407500
C	-3.00676300	-1.08919300	-0.54921400
C	-2.72345000	1.69514000	0.18816800
C	-2.63502200	-2.35437300	-1.03420300
C	-4.37130500	-0.78881100	-0.38613500
C	-1.14708800	-0.22341600	1.64163000
Pd	0.56064700	-0.47439400	-0.50903700
C	-3.05549000	2.13609100	1.47911600
C	-3.26063900	2.38483200	-0.91563400
C	-3.60672500	-3.29836900	-1.36504100
H	-1.58498200	-2.62024900	-1.12369300
C	-5.34769000	-1.72700600	-0.71187800
H	-4.68617600	0.17392400	-0.00379400
C	-0.28500900	0.67557200	2.30362100
C	-1.53717200	-1.40821100	2.28987200
C	-0.79644200	0.77330700	-1.72959700
C	-3.87434800	3.24960300	1.67116300
H	-2.68004900	1.61604400	2.35133700

C	-4.08708000	3.49079600	-0.74021400
H	-3.04175200	2.05560600	-1.92477400
C	-4.94791000	-2.96667400	-1.20287600
H	-3.33030100	-4.27769800	-1.73636100
H	-6.40209800	-1.51098600	-0.59183000
C	0.18336300	0.39399300	3.58313700
H	0.01385500	1.60236100	1.82467100
C	-1.08448400	-1.68791800	3.57459800
H	-2.17572700	-2.12612700	1.78972400
C	-0.29019400	2.08990300	-1.80953500
C	-0.97447000	0.03435200	-2.92068000
C	-4.37424400	3.91236400	0.55610400
H	-4.12714600	3.60111500	2.66398900
H	-4.50576200	4.02533700	-1.58406100
C	-0.22723400	-0.78493800	4.20147600
H	0.85579600	1.06548400	4.10207300
H	-1.37687200	-2.59504800	4.08873200
C	0.05945100	2.63595000	-3.04200200
H	-0.16089500	2.68229300	-0.91023300
C	-0.64282500	0.60109100	-4.15282400
H	-1.37354100	-0.97244300	-2.88430000
C	-0.12250600	1.89552400	-4.21460600
H	0.48368800	3.63440900	-3.08249000
H	-0.78787600	0.02482400	-5.06215600
P	2.93532700	0.46866100	-0.42794600
C	4.10130200	-0.30582500	-1.63101500
C	3.79412600	0.28997400	1.20184700
C	3.09080900	2.28085600	-0.77460800
C	3.56882100	-1.10663800	-2.65149600
C	5.49285500	-0.12683500	-1.55913200
C	4.71957100	1.22510600	1.69476400
C	3.51185000	-0.85442500	1.96662600
C	2.53421900	3.19562700	0.13918800
C	3.64201400	2.78184700	-1.96274700
C	4.40964800	-1.70212700	-3.59487100
H	2.49803200	-1.28441600	-2.68749400
C	6.33037800	-0.72363600	-2.50064200

H	5.92406000	0.47149300	-0.76175200
C	5.34528800	1.02113300	2.92628600
H	4.94714300	2.12038700	1.12432600
C	4.14549000	-1.05720400	3.19383200
H	2.80040900	-1.58882200	1.59840700
C	2.54014900	4.56548300	-0.12036800
H	2.11189400	2.83319100	1.07370700
C	3.64239500	4.15525100	-2.22662500
H	4.07959400	2.10026300	-2.68473500
C	5.78925500	-1.50981000	-3.52219000
H	3.98492500	-2.32783900	-4.37506400
C	5.05988800	-0.11994200	3.67849800
H	6.05615700	1.75560400	3.29619400
H	3.91869500	-1.94852000	3.77243600
C	3.09359100	5.05151300	-1.30925900
H	2.11832500	5.25478000	0.60673000
H	4.08201700	4.52228000	-3.15056900
H	6.44429900	-1.97920200	-4.25145700
I	0.95132700	-3.24529900	-0.19461200
H	5.54485800	-0.27613100	4.63831400
H	3.10092100	6.11886600	-1.51278300
H	7.40573500	-0.58107400	-2.43341500
H	0.13896200	2.32941200	-5.17569100
N	0.25468100	-1.08047000	5.55939600
N	-5.98308600	-3.95924900	-1.55769000
N	-5.24044900	5.09142100	0.75124800
O	-0.14048300	-2.11709900	6.09057300
O	1.02009300	-0.26928900	6.08027700
O	-5.47573200	5.43570900	1.90725700
O	-5.66893500	5.65102500	-0.25571000
O	-5.60264000	-5.04043700	-1.99874100
O	-7.15741100	-3.63585000	-1.38983100

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P	-2.69301800	0.05087400	-0.03845000
C	-3.38877500	-0.35547700	-1.70029800

C	-3.53653600	1.64820400	0.37163700
C	-3.47872000	-1.12651400	1.14375500
C	-2.62452800	-1.11240400	-2.60145200
C	-4.67551900	0.06212300	-2.08402400
C	-3.48200100	2.71425100	-0.54232300
C	-4.19978100	1.84131200	1.59207100
C	-2.88334300	-1.29810100	2.40283000
C	-4.66070600	-1.81826700	0.84964400
C	-3.13741400	-1.44640300	-3.85626700
H	-1.63878200	-1.45851400	-2.30893200
C	-5.18427200	-0.27462200	-3.33895600
H	-5.27833000	0.65943800	-1.40749900
C	-4.07973800	3.93679500	-0.24384500
H	-2.96429500	2.59401100	-1.48765600
C	-4.79449800	3.07003400	1.89064900
H	-4.26329800	1.03305500	2.31242900
C	-3.47144400	-2.12682800	3.35734300
H	-1.94723900	-0.79480900	2.62735300
C	-5.23951400	-2.66031900	1.80153600
H	-5.12747900	-1.71370300	-0.12424200
C	-4.41577100	-1.02874300	-4.22840200
H	-2.53409500	-2.03660200	-4.54068100
H	-6.18051500	0.05568500	-3.62109000
C	-4.73811000	4.11964900	0.97489100
H	-4.02419500	4.74954100	-0.96277100
H	-5.30716200	3.19936100	2.84030600
C	-4.65081700	-2.81225300	3.05727200
H	-2.99797900	-2.25191100	4.32735100
H	-6.15041000	-3.20017500	1.55676200
H	-4.81232000	-1.28788200	-5.20662000
H	-5.20236300	5.07445300	1.20736800
H	-5.10246100	-3.46935100	3.79568300
Pd	-0.27175100	-0.01585500	0.00094000
P	2.14832100	-0.00581100	0.03072500
C	2.83915900	-0.39016200	1.69630500
C	3.02573400	1.55949400	-0.41788500
C	2.89194500	-1.22708300	-1.12963300

C	2.06599200	-1.10066500	2.62653900
C	4.13981300	-0.00537300	2.06440100
C	3.00799000	2.64996600	0.46962200
C	3.68545700	1.71565300	-1.64321400
C	2.29024100	-1.41304500	-2.38326500
C	4.05772600	-1.94346200	-0.83419900
C	2.58169700	-1.41667500	3.88289100
H	1.06818600	-1.42902800	2.35529300
C	4.64659400	-0.32754900	3.32243600
H	4.75962300	0.55376500	1.37061400
C	3.63256000	3.84723800	0.13880300
H	2.49737000	2.56770900	1.42296100
C	4.30660700	2.92418100	-1.96963500
H	3.72860900	0.89400200	-2.35008000
C	2.85250100	-2.27616900	-3.32005600
H	1.36901600	-0.88858200	-2.62126500
C	4.60601600	-2.81898500	-1.77224100
H	4.54007400	-1.83024000	0.13124600
C	3.87654500	-1.03447800	4.25582200
H	1.96496000	-1.97509700	4.58353000
H	5.65762400	-0.02217200	3.58324900
C	4.29287200	4.00916100	-1.08920700
H	3.60055900	4.67473500	0.84414000
H	4.81522500	3.01698400	-2.92673200
C	4.01653300	-3.00132500	-3.02861000
H	2.36917100	-2.40341100	-4.28618700
H	5.50772800	-3.37221300	-1.51887400
C	-0.24449400	2.02431600	-0.01653200
C	-0.08479100	2.73007200	-1.21714100
C	-0.38975700	2.75203000	1.17279200
C	-0.07415300	4.12934300	-1.22926800
H	0.04107900	2.19359900	-2.15491900
C	-0.37218000	4.15127000	1.16287300
H	-0.52593400	2.23276100	2.11885600
C	-0.21615300	4.84506300	-0.03877100
H	0.05170300	4.65775500	-2.17207700
H	-0.48785500	4.69704200	2.09699400

I	-0.30989900	-2.84586900	0.03456800
H	-0.20594700	5.93224300	-0.04730300
C	4.41685900	-1.35088500	5.63034400
H	4.15156900	-0.56459500	6.35003200
H	4.00922800	-2.29219000	6.01417000
H	5.50912300	-1.43016600	5.62393600
C	4.59312800	-3.97641800	-4.02762000
H	5.66335200	-4.13737200	-3.86037100
H	4.09949200	-4.95448500	-3.95225800
H	4.45821900	-3.62463400	-5.05643800
C	4.96045700	5.31800900	-1.43988800
H	5.71133700	5.59790600	-0.69047600
H	5.46110200	5.26464000	-2.41179400
H	4.23148500	6.13712300	-1.48378300

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P	-2.06603000	0.16828200	0.08823600
C	-3.38103200	-0.94589800	-0.55941200
C	-3.01121500	1.72071400	0.50263600
C	-3.03466700	-2.17880900	-1.13771300
C	-4.74100900	-0.61087300	-0.45545200
C	-1.59005000	-0.44751600	1.77690600
Pd	0.18665200	-0.44457800	-0.38493500
C	-3.38102600	2.03592200	1.81847600
C	-3.49098900	2.54932400	-0.52898800
C	-4.02515900	-3.04295600	-1.59982500
H	-1.99146600	-2.47746500	-1.20292300
C	-5.72125900	-1.48553600	-0.92305200
H	-5.04557400	0.32716500	-0.00644000
C	-0.75462700	0.33362200	2.59954100
C	-1.98728000	-1.71293400	2.23061000
C	-1.01672500	0.96026500	-1.48885000
C	-4.17002800	3.15475000	2.09364800
H	-3.06252000	1.40748200	2.64129900
C	-4.28554600	3.65691500	-0.24729000
H	-3.25859600	2.32239700	-1.56328000

C	-5.38411200	-2.71274000	-1.50738400
H	-3.72846500	-3.99446000	-2.03493400
H	-6.76828300	-1.20663100	-0.82842600
C	-0.33662300	-0.14383300	3.83854200
H	-0.44449300	1.32315900	2.27698400
C	-1.56483400	-2.17610100	3.47549100
H	-2.60999800	-2.34643500	1.60936500
C	-0.53808600	2.28667800	-1.42132800
C	-1.28319800	0.39460000	-2.75355500
C	-4.63090200	3.98973600	1.07083000
H	-4.43406300	3.37463100	3.12558300
H	-4.64510900	4.27392500	-1.06774900
C	-0.72714700	-1.41073900	4.29597200
H	0.31148600	0.47405600	4.45588500
H	-1.88377300	-3.16107800	3.80730500
C	-0.28199500	3.00260400	-2.58833900
H	-0.35521300	2.75178400	-0.45866100
C	-1.03980000	1.12769400	-3.91820600
H	-1.67640300	-0.61300300	-2.82378600
C	-0.53456800	2.42656400	-3.83858500
H	0.12231400	4.00859200	-2.51965700
H	-1.24424300	0.67762200	-4.88607600
P	2.54996800	0.44127700	-0.09678200
C	3.70142200	-0.03384700	-1.46185000
C	3.44411200	-0.09644100	1.43389300
C	2.71755600	2.28530200	-0.02915000
C	3.14285800	-0.48345100	-2.66729400
C	5.09885100	0.03959600	-1.34430300
C	4.38901300	0.70194200	2.10069400
C	3.16732700	-1.37981300	1.93405100
C	2.18160100	2.97409900	1.07543100
C	3.24565400	3.03896500	-1.08760700
C	3.96425900	-0.83394000	-3.74124000
H	2.06418600	-0.57768600	-2.75296600
C	5.91760000	-0.31518200	-2.41620700
H	5.54960600	0.36400600	-0.41093500
C	5.04136100	0.22788900	3.24066100

H	4.61299400	1.70013400	1.73686000
C	3.82838300	-1.85241900	3.06944100
H	2.43950200	-2.01084700	1.43013400
C	2.18638900	4.36740700	1.12557200
H	1.77236000	2.41218400	1.91148500
C	3.24371200	4.43648200	-1.04093600
H	3.66503100	2.53544300	-1.95251300
C	5.35131400	-0.74941800	-3.61795700
H	3.51779200	-1.18770100	-4.66665100
C	4.76367600	-1.05115000	3.72722300
H	5.76867600	0.85895400	3.74556700
H	3.60734800	-2.85095500	3.43757600
C	2.71649500	5.10622200	0.06321600
H	1.77750600	4.87722900	1.99441200
H	3.66368700	4.99993700	-1.87049500
H	5.99129400	-1.03067300	-4.45039200
I	0.62180100	-3.26166500	-0.57594200
H	5.27408800	-1.41999000	4.61342900
H	2.71979400	6.19237700	0.09969900
H	6.99811900	-0.25848500	-2.31147800
H	-0.34462300	2.99324200	-4.74629000
C	-6.44652500	-3.64598200	-2.03684200
H	-7.43229600	-3.40966000	-1.62350600
H	-6.52200300	-3.57656700	-3.13012500
H	-6.21644500	-4.68981500	-1.79637300
C	-5.45999500	5.21508400	1.37166400
H	-5.95474900	5.13586800	2.34500500
H	-4.83492600	6.11774400	1.39406900
H	-6.23025600	5.37529000	0.60924100
C	-0.23182500	-1.93765600	5.62122600
H	-0.30579400	-1.17927400	6.40954100
H	-0.79912600	-2.81733600	5.94094500
H	0.82395600	-2.23054200	5.55320100

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P	-2.98062900	0.02977800	-0.05705600

C	-3.68388200	-0.33635800	-1.72496300
C	-3.83966900	1.60677100	0.39754600
C	-3.74591200	-1.18562000	1.09996800
C	-2.90999500	-1.03516100	-2.66366200
C	-4.98593800	0.06052200	-2.07822400
C	-3.79492400	2.69719100	-0.48771100
C	-4.50434500	1.76165700	1.62258200
C	-3.13827200	-1.38053300	2.34981800
C	-4.92270200	-1.88328600	0.79920400
C	-3.42881400	-1.33465100	-3.92485500
H	-1.91101300	-1.36283800	-2.39641600
C	-5.50104700	-0.24228300	-3.33905600
H	-5.59569200	0.61617300	-1.37291900
C	-4.40271900	3.90628000	-0.15672500
H	-3.27710900	2.60648200	-1.43633500
C	-5.10971300	2.97683900	1.95370900
H	-4.56058900	0.93430200	2.32162900
C	-3.70902200	-2.23820700	3.28918100
H	-2.20591300	-0.87217700	2.57855300
C	-5.48400200	-2.75430100	1.73542600
H	-5.39882500	-1.76124100	-0.16810300
C	-4.72309000	-0.94004300	-4.26563800
H	-2.81748400	-1.88008000	-4.63865900
H	-6.50934000	0.07086200	-3.59699200
C	-5.06229200	4.05106800	1.06649300
H	-4.35412300	4.73838800	-0.85369600
H	-5.62323300	3.07633900	2.90651600
C	-4.88320600	-2.92952200	2.98238200
H	-3.22600200	-2.38077300	4.25204200
H	-6.39085700	-3.29849100	1.48520000
H	-5.12449000	-1.17282400	-5.24850800
H	-5.53433100	4.99545900	1.32446900
H	-5.32143600	-3.60901000	3.70853500
Pd	-0.55825400	-0.01400800	-0.01752300
P	1.86178200	0.01772500	0.04316700
C	2.52063500	-0.40985200	1.70775900
C	2.73203200	1.59938300	-0.34792300

C	2.63228300	-1.16507600	-1.13402000
C	1.74993500	-1.19013300	2.59063100
C	3.79134200	0.00544000	2.13164700
C	2.68425700	2.67572700	0.56058900
C	3.41793800	1.78987500	-1.55213700
C	2.06658100	-1.32011900	-2.41289800
C	3.78334000	-1.89508100	-0.82654700
C	2.23359900	-1.53797300	3.84410300
H	0.77286000	-1.54431100	2.27894100
C	4.28871300	-0.33850900	3.39060700
H	4.40813400	0.61644100	1.48031000
C	3.30264300	3.88268700	0.27596800
H	2.15114300	2.57130200	1.49907900
C	4.04012000	3.00547800	-1.85549600
H	3.48401100	0.98337000	-2.27442500
C	2.64739000	-2.15485500	-3.35573500
H	1.15195800	-0.79052700	-2.66425300
C	4.36906000	-2.75419900	-1.76028700
H	4.23427300	-1.81137200	0.15697500
C	3.50631300	-1.11394200	4.25591800
H	1.64207000	-2.14261100	4.52441900
H	5.27453700	0.00557000	3.68221600
C	3.98486500	4.05947300	-0.93876900
H	3.26269600	4.71171800	0.97529200
H	4.56341900	3.10934600	-2.79925600
C	3.80342500	-2.88399000	-3.03358300
H	2.21175000	-2.28118100	-4.34182600
H	5.25419700	-3.31406300	-1.48078700
C	-0.54849400	2.02490200	0.04690100
C	-0.38475800	2.77888700	-1.12366400
C	-0.71196500	2.70470300	1.26205500
C	-0.39089700	4.17760000	-1.08169400
H	-0.24116200	2.28033300	-2.07970800
C	-0.71105900	4.10346600	1.30629200
H	-0.84838600	2.14810500	2.18663500
C	-0.55270500	4.84514400	0.13398400
H	-0.26182600	4.74382300	-2.00186500

H	-0.84051400	4.61131000	2.25980400
I	-0.58012000	-2.84385100	-0.10323100
H	-0.55393200	5.93180400	0.16761300
O	4.55634600	5.28321700	-1.12401000
O	4.29060800	-3.68619900	-4.02108600
O	3.88598300	-1.50204700	5.50436300
C	5.24833000	5.52424000	-2.33842100
H	4.58493000	5.42399500	-3.20763000
H	5.61119900	6.55198400	-2.27802400
H	6.10271000	4.84475900	-2.45830200
C	5.16522200	-1.10750600	5.97506000
H	5.25637300	-0.01460200	6.02786700
H	5.25643700	-1.52582400	6.97903600
H	5.96867700	-1.50621400	5.34184200
C	5.42619400	-4.48827500	-3.73805500
H	5.23191000	-5.18318300	-2.91080700
H	5.62531700	-5.05680600	-4.64834200
H	6.30415400	-3.87475100	-3.49517600

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P	-1.85475000	0.22588300	-0.06024600
C	-3.14843900	-0.92262300	-0.67508700
C	-2.78373900	1.81302500	0.20540000
C	-2.79570600	-2.20376800	-1.12413300
C	-4.51166300	-0.56532500	-0.67807300
C	-1.45634200	-0.27792400	1.68149000
Pd	0.41665400	-0.43549200	-0.40948000
C	-3.17823400	2.23659900	1.48107300
C	-3.22576100	2.57421100	-0.89893600
C	-3.76308500	-3.10551200	-1.56889000
H	-1.75522300	-2.51978900	-1.10662900
C	-5.47923200	-1.45610400	-1.12031300
H	-4.82334300	0.41280000	-0.33093700
C	-0.61599400	0.52340100	2.48480900
C	-1.92128800	-1.48938900	2.20834600
C	-0.75574300	0.87056300	-1.66180900

C	-3.95100900	3.38610500	1.66916200
H	-2.88834000	1.66877200	2.35675800
C	-4.00266800	3.70902000	-0.72784600
H	-2.97079200	2.27041100	-1.90784000
C	-5.11367900	-2.73434100	-1.57251300
H	-3.44567700	-4.08719800	-1.90096100
H	-6.53026900	-1.18469200	-1.12441400
C	-0.26812200	0.12727100	3.76809600
H	-0.24471500	1.47126000	2.10698200
C	-1.57863100	-1.89327200	3.49813400
H	-2.54826800	-2.13915100	1.60893300
C	-0.26598500	2.19435000	-1.69218300
C	-0.99116400	0.20494000	-2.88376300
C	-4.36508400	4.13339200	0.56158600
H	-4.22232100	3.67911900	2.67685600
H	-4.34242400	4.28926900	-1.57996900
C	-0.74327000	-1.08928700	4.28400800
H	0.38072500	0.73732100	4.38834400
H	-1.95621800	-2.83887600	3.86898300
C	0.02669900	2.81104900	-2.90639000
H	-0.10392500	2.73547700	-0.76633100
C	-0.70980800	0.83772400	-4.09743200
H	-1.39380300	-0.80140600	-2.88331000
C	-0.19708400	2.13602700	-4.11155400
H	0.43748400	3.81662000	-2.90864700
H	-0.89188500	0.31055100	-5.03026200
P	2.78161100	0.46572900	-0.19254500
C	3.92644200	-0.14285700	-1.51195200
C	3.69233500	0.08201900	1.37528600
C	2.94924600	2.30730500	-0.30009500
C	3.36959300	-0.81691000	-2.60808600
C	5.31920600	0.03109300	-1.45526100
C	4.65638600	0.93449800	1.93970000
C	3.41121300	-1.13856000	2.01093300
C	2.42598900	3.09452200	0.74327700
C	3.46686700	2.96077500	-1.42785500
C	4.18676500	-1.29291600	-3.63651400

H	2.29773000	-0.98883000	-2.63909500
C	6.13354900	-0.44587000	-2.48183100
H	5.77062200	0.53080500	-0.60302200
C	5.32536400	0.57309100	3.11052100
H	4.88055600	1.88840900	1.47216800
C	4.08785300	-1.49867600	3.17787400
H	2.66734500	-1.80882000	1.58810000
C	2.43355000	4.48650900	0.66683000
H	2.02536800	2.61218600	1.63182700
C	3.46938500	4.35693600	-1.50729100
H	3.87527700	2.37930600	-2.24792300
C	5.56777400	-1.10691400	-3.57606000
H	3.74184900	-1.82150800	-4.47527100
C	5.04380900	-0.64539600	3.73171700
H	6.06725800	1.24478100	3.53553700
H	3.86032100	-2.44844100	3.65459300
C	2.95481800	5.12505000	-0.46287000
H	2.03441100	5.07392200	1.49000400
H	3.88198300	4.84189000	-2.38857000
H	6.20474400	-1.48390200	-4.37222400
I	0.81979300	-3.27397300	-0.30463100
H	5.56537700	-0.92599200	4.64336000
H	2.96099200	6.21006900	-0.52434800
H	7.21037900	-0.30816100	-2.42478800
H	0.02100900	2.62499500	-5.05732000
O	-0.34636200	-1.38948000	5.54964800
O	-5.11557600	5.26430900	0.62256700
O	-6.13511700	-3.52960600	-1.98559100
C	-0.74498200	-2.63503300	6.10432700
H	-0.38013500	-3.47697100	5.50270700
H	-0.29467400	-2.67641600	7.09764200
H	-1.83682700	-2.70305700	6.19853200
C	-5.51747700	5.74280500	1.89866100
H	-6.09669300	6.64784300	1.70858000
H	-6.14690700	5.01164300	2.42204000
H	-4.65143600	5.99021000	2.52589100
C	-5.82793300	-4.83815900	-2.44917400

H	-6.78332500	-5.28770900	-2.72491100
H	-5.17182000	-4.80892700	-3.32823300
H	-5.35433300	-5.44126300	-1.66434300

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P	-3.16170400	0.09051300	-0.06814700
C	-3.86353300	-0.30370500	-1.73173200
C	-3.99389200	1.69556300	0.33923500
C	-3.96812000	-1.07730700	1.11098600
C	-3.10320100	-1.05708800	-2.63909900
C	-5.14782600	0.12372500	-2.11284600
C	-3.91067000	2.76515100	-0.56833000
C	-4.67500400	1.89200300	1.54921200
C	-3.37417800	-1.25933400	2.36931400
C	-5.16047100	-1.75149300	0.81802100
C	-3.61800200	-1.37869500	-3.89646900
H	-2.11904200	-1.40998200	-2.34912300
C	-5.65880400	-0.20084700	-3.37011600
H	-5.74701600	0.71997000	-1.43206200
C	-4.49813600	3.99377300	-0.27454700
H	-3.37818100	2.64215300	-1.50507300
C	-5.25976300	3.12661700	1.84333200
H	-4.75955000	1.08166500	2.26506700
C	-3.97374100	-2.07980100	3.32390700
H	-2.42968800	-0.77135200	2.59239600
C	-5.75098700	-2.58564500	1.76974200
H	-5.62659800	-1.63964000	-0.15542700
C	-4.89435600	-0.95222900	-4.26537200
H	-3.01734600	-1.96625000	-4.58559800
H	-6.65336300	0.13695000	-3.64961300
C	-5.17512900	4.17947500	0.93351700
H	-4.41975700	4.80913400	-0.98843900
H	-5.78663000	3.25820600	2.78496300
C	-5.16362300	-2.74723900	3.02491700
H	-3.50086400	-2.21274600	4.29324200
H	-6.67006100	-3.11179800	1.52532600

H	-5.29234700	-1.20200000	-5.24554000
H	-5.63137600	5.13904200	1.16254400
H	-5.62445400	-3.39800000	3.76338900
Pd	-0.73460000	-0.00150000	-0.01536100
P	1.68732900	-0.00727300	0.03587400
C	2.33441800	-0.40480500	1.70642400
C	2.57805000	1.54673000	-0.39578000
C	2.42164700	-1.22585000	-1.12123200
C	1.55521200	-1.13828900	2.61520300
C	3.62181700	-0.02313900	2.12186500
C	2.57364800	2.64252300	0.48357800
C	3.24084900	1.71211800	-1.61975300
C	1.82420900	-1.43762200	-2.37206700
C	3.58982100	-1.94235100	-0.83244400
C	2.03126800	-1.47621200	3.87606100
H	0.56623400	-1.47421500	2.32084500
C	4.11141500	-0.35565000	3.37973900
H	4.25743200	0.55116800	1.45485900
C	3.20458400	3.83715600	0.16630500
H	2.05917600	2.57120200	1.43601200
C	3.87211400	2.90702900	-1.95507500
H	3.27456800	0.89526200	-2.33326600
C	2.37660000	-2.30328000	-3.30740100
H	0.89485800	-0.92969600	-2.61509000
C	4.14676700	-2.82490200	-1.75204700
H	4.07214900	-1.82814500	0.13344600
C	3.32316900	-1.08635800	4.30025700
H	1.38897600	-2.05434600	4.52953600
H	5.11353400	-0.03931100	3.64416800
C	3.88046800	4.00353000	-1.06558500
H	3.15687200	4.64913100	0.88173400
H	4.36347800	2.97594100	-2.91845600
C	3.56171500	-3.02185800	-3.02383900
H	1.86366400	-2.43804600	-4.25203900
H	5.03970700	-3.36866900	-1.46738100
C	-0.67880000	2.03664400	0.01837100
C	-0.50077000	2.77559700	-1.15992800

C	-0.83618600	2.73401800	1.22459000
C	-0.48890300	4.17451100	-1.13472600
H	-0.35789900	2.26442400	-2.10921200
C	-0.81659100	4.13305400	1.25273400
H	-0.98185500	2.19018000	2.15534100
C	-0.64616500	4.85888000	0.07226400
H	-0.34985600	4.72754700	-2.06159100
H	-0.94200400	4.65355600	2.20009200
I	-0.83153600	-2.83590100	-0.02240500
H	-0.63605400	5.94611000	0.09291400
C	5.02668400	5.39229800	-2.72965300
H	4.22665800	5.37343200	-3.48779700
H	5.52858200	6.36063900	-2.78557700
H	5.76213800	4.62412300	-2.99635300
C	5.18466700	-1.14400400	5.89788300
H	5.42436200	-0.07734400	5.80677400
H	5.36334500	-1.43420700	6.93507600
H	5.88476900	-1.70463900	5.25814600
C	3.36636900	-4.23980000	-5.14321500
H	3.13644800	-3.35219400	-5.74442400
H	3.96708700	-4.90876100	-5.76305100
H	2.41690000	-4.74603300	-4.90642400
N	3.79328600	-1.39802900	5.56604800
N	4.12714600	-3.88143500	-3.95729600
N	4.53248300	5.19027500	-1.37850400
C	3.02962500	-2.30102400	6.41112800
H	2.03057900	-1.89795300	6.61696300
H	2.90713800	-3.30022600	5.96464900
H	3.54291500	-2.41454000	7.36799000
C	5.19965400	-4.77084100	-3.54363100
H	4.89523700	-5.46907000	-2.74732900
H	5.52992900	-5.35557300	-4.40479000
H	6.06364700	-4.20084500	-3.18207500
C	4.30621500	6.36393400	-0.55133300
H	4.62906300	6.18552100	0.48119400
H	4.89882100	7.19430900	-0.94110900
H	3.24908100	6.67365200	-0.52759800

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P	-1.67942100	0.10154300	0.04558400
C	-2.96263100	-1.14182700	-0.34596200
C	-2.64503800	1.65801300	0.29864900
C	-2.60371500	-2.43862400	-0.75404000
C	-4.33345900	-0.85346900	-0.22711400
C	-1.03999200	-0.25416800	1.74372400
Pd	0.56543400	-0.47562700	-0.53841200
C	-2.94736800	2.14792800	1.57970200
C	-3.23280000	2.32857000	-0.79101100
C	-3.56434400	-3.40226400	-1.02952700
H	-1.55451500	-2.70949400	-0.84350400
C	-5.30239800	-1.81021600	-0.50203500
H	-4.65908800	0.13288400	0.08351800
C	-0.19797800	0.66370200	2.40100200
C	-1.28357400	-1.48172200	2.38041200
C	-0.75635100	0.69303700	-1.74681000
C	-3.75849000	3.26155300	1.77002700
H	-2.54564600	1.65468500	2.45691900
C	-4.05332600	3.43425500	-0.61754900
H	-3.06053100	1.97697300	-1.80190500
C	-4.94573900	-3.11919900	-0.90714700
H	-3.22571700	-4.38327900	-1.34013300
H	-6.34454300	-1.53157800	-0.39974400
C	0.36582400	0.37721900	3.63703400
H	0.01387200	1.62672000	1.94551000
C	-0.72670500	-1.77671300	3.61699000
H	-1.90149200	-2.22984900	1.89696500
C	-0.36446900	2.03829000	-1.91223500
C	-1.12571000	-0.05150800	-2.88573400
C	-4.33945000	3.93987700	0.67408400
H	-3.94043900	3.59806600	2.78373700
H	-4.47293200	3.90732100	-1.49735400
C	0.12144200	-0.85914900	4.28145100
H	1.01313100	1.11662700	4.09243500

H	-0.93857500	-2.74439600	4.05473500
C	-0.28627500	2.59963700	-3.18508100
H	-0.11083300	2.63982700	-1.04635800
C	-1.05851900	0.52420800	-4.15783100
H	-1.46096400	-1.07659200	-2.77650300
C	-0.63397100	1.84522900	-4.31124600
H	0.05288100	3.62611500	-3.29606000
H	-1.33776500	-0.06561600	-5.02724400
P	2.87319600	0.54813700	-0.52456100
C	3.98092700	-0.02666500	-1.88992800
C	3.89068600	0.25137900	0.99815100
C	2.93279400	2.39338500	-0.68432500
C	3.40150100	-0.72649100	-2.95797600
C	5.36676800	0.20217800	-1.89723300
C	4.81876200	1.17597700	1.50659000
C	3.72783000	-0.97719300	1.65942800
C	2.41720300	3.17966000	0.36359000
C	3.35505800	3.04307800	-1.85352200
C	4.18962800	-1.17426300	-4.02114600
H	2.33702900	-0.93991300	-2.94081900
C	6.15232900	-0.24813500	-2.95781400
H	5.83590500	0.72471800	-1.06849600
C	5.56812800	0.87840200	2.64662400
H	4.95385500	2.13607000	1.01796300
C	4.48664000	-1.27514300	2.79335700
H	3.01168400	-1.70309800	1.28251800
C	2.34119800	4.56717700	0.25164200
H	2.08435600	2.69997800	1.28080900
C	3.27088200	4.43407900	-1.96936600
H	3.75626000	2.46337300	-2.67839000
C	5.56390100	-0.93551700	-4.02338900
H	3.72797900	-1.72301400	-4.83760200
C	5.40625200	-0.34953500	3.29188200
H	6.28166700	1.60566700	3.02652200
H	4.35552100	-2.23590800	3.28459500
C	2.76651700	5.20162500	-0.91968500
H	1.94891100	5.15404200	1.07858200

H	3.60833800	4.91593000	-2.88372800
H	6.17846200	-1.29151600	-4.84644600
I	1.16810500	-3.29452600	-0.50631600
H	5.99577900	-0.58365400	4.17505100
H	2.70592800	6.28304200	-1.00973800
H	7.22451400	-0.06846000	-2.94986200
H	-0.58182300	2.28966100	-5.30184500
N	0.68195700	-1.15137100	5.51451200
N	-5.90401100	-4.08005400	-1.16624900
N	-5.15927700	5.03718400	0.85352500
C	-7.31103200	-3.71945200	-1.15638600
H	-7.55745300	-2.95931200	-1.91400800
H	-7.91027300	-4.60878000	-1.35989000
H	-7.61528500	-3.33051500	-0.17618800
C	-5.50689300	-5.36894700	-1.71064000
H	-4.81751600	-5.89028700	-1.03526500
H	-6.39324500	-5.99498700	-1.82878000
H	-5.01677300	-5.27812000	-2.69171600
C	1.74995100	-0.30380200	6.02449100
H	1.39525800	0.72155700	6.18409900
H	2.07873000	-0.68991300	6.99142100
H	2.61895400	-0.26563600	5.34960300
C	0.57756200	-2.50465000	6.03852900
H	1.05601700	-2.54415300	7.01920700
H	-0.47181500	-2.79205700	6.17187400
H	1.05638200	-3.25238200	5.38707700
C	-5.34144200	5.59393800	2.18344900
H	-4.39890600	5.95815700	2.62023900
H	-6.03733300	6.43288500	2.12815300
H	-5.76803800	4.85200800	2.87048100
C	-5.63281400	5.78463600	-0.29971900
H	-6.23138700	5.15191800	-0.96753400
H	-6.27045600	6.60204300	0.04136200
H	-4.80867000	6.21516800	-0.88856500

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P	-2.42001100	-0.10398000	-0.02648600
C	-3.13997000	-0.53828900	-1.67043900
C	-3.26731900	1.49432200	0.36901900
C	-3.17323600	-1.26745700	1.18952600
C	-2.38152200	-1.28319400	-2.58611500
C	-4.44316500	-0.14723800	-2.02618300
C	-3.23314000	2.54328100	-0.56576300
C	-3.91040100	1.70723800	1.59658000
C	-2.55282800	-1.41298700	2.43984300
C	-4.35727400	-1.96991400	0.93063100
C	-2.91655100	-1.63249300	-3.82762600
H	-1.38249500	-1.60829100	-2.31590000
C	-4.97410000	-0.49983100	-3.26732700
H	-5.04145000	0.44222800	-1.33884200
C	-3.82963800	3.76930600	-0.27966800
H	-2.73387300	2.40572400	-1.51890100
C	-4.50452700	2.93947900	1.88260400
H	-3.95779400	0.91228900	2.33280700
C	-3.11817900	-2.22732200	3.42024400
H	-1.61541700	-0.90075300	2.63760000
C	-4.91312800	-2.79745600	1.90846500
H	-4.84284800	-1.88492400	-0.03583400
C	-4.21137000	-1.24243100	-4.17142900
H	-2.31735700	-2.21319700	-4.52362200
H	-5.98286400	-0.19039400	-3.52759900
C	-4.46699000	3.97246700	0.94728300
H	-3.79092100	4.56891200	-1.01426600
H	-5.00125900	3.08464000	2.83836100
C	-4.29934400	-2.92390400	3.15506100
H	-2.62617800	-2.33206300	4.38338800
H	-5.82577700	-3.34597300	1.69127900
H	-4.62513600	-1.51371300	-5.13910900
H	-4.92951500	4.93021000	1.17031100
H	-4.73337900	-3.56956800	3.91377800
Pd	-0.00001300	-0.13935800	0.00001400
P	2.41998500	-0.10389100	0.02648900
C	3.13997300	-0.53812400	1.67045600

C	3.26721600	1.49444900	-0.36902900
C	3.17330500	-1.26730400	-1.18952600
C	2.38158100	-1.28299100	2.58620600
C	4.44317000	-0.14700900	2.02614100
C	3.23293300	2.54342100	0.56573300
C	3.91036500	1.70736500	-1.59655300
C	2.55308600	-1.41263000	-2.43997000
C	4.35722700	-1.96991400	-0.93051400
C	2.91665800	-1.63218500	3.82772900
H	1.38256000	-1.60815000	2.31604700
C	4.97415400	-0.49949900	3.26728900
H	5.04141200	0.44243100	1.33874000
C	3.82939200	3.76946800	0.27965000
H	2.73361800	2.40586000	1.51884500
C	4.50445500	2.93962700	-1.88256300
H	3.95783900	0.91240000	-2.33275900
C	3.11850900	-2.22693000	-3.42034700
H	1.61576900	-0.90027300	-2.63783900
C	4.91313800	-2.79741700	-1.90834600
H	4.84265000	-1.88508000	0.03603500
C	4.21147100	-1.24205900	4.17146900
H	2.31749800	-2.21285900	4.52378000
H	5.98291500	-0.19001400	3.52751500
C	4.46681100	3.97263200	-0.94726500
H	3.79059000	4.56908700	1.01423000
H	5.00124200	3.08478900	-2.83829200
C	4.29954900	-2.92367400	-3.15504800
H	2.62664400	-2.33151000	-4.38358400
H	5.82570200	-3.34604700	-1.69105500
C	-0.00009600	1.90287300	-0.00004400
C	0.17662200	2.62267700	-1.19030300
C	-0.17688200	2.62265000	1.19022400
C	0.17379400	4.02193000	-1.20080200
H	0.32912900	2.09938900	-2.13108900
C	-0.17417700	4.02190500	1.20073900
H	-0.32934600	2.09934800	2.13100900
C	-0.00022100	4.69829400	-0.00002800

H	0.31292000	4.58430800	-2.11929900
H	-0.31335200	4.58425700	2.11924400
I	0.00014500	-2.96343000	-0.00001100
H	4.92930400	4.93039300	-1.17028700
H	4.62527800	-1.51325700	5.13915500
H	4.73362600	-3.56930400	-3.91374900
F	-0.00028500	6.05362300	-0.00002700

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P	-2.27900600	0.06152700	0.29121700
C	-3.63820300	-0.70476200	-0.69262700
C	-3.15878000	1.41019400	1.23911700
C	-3.33343800	-1.70408600	-1.63228200
C	-4.98012900	-0.33635500	-0.49656900
C	-1.85939300	-1.13988800	1.65659200
Pd	-0.05059100	-0.41545400	-0.35814400
C	-3.49799600	1.26103200	2.59328700
C	-3.60436300	2.56358700	0.56548100
C	-4.35362400	-2.31457500	-2.36386400
H	-2.30370000	-2.02240400	-1.77672600
C	-5.99341100	-0.95146200	-1.23304900
H	-5.24223300	0.42491500	0.22841600
C	-0.98453300	-0.74678300	2.68831200
C	-2.35233500	-2.45364600	1.64316900
C	-1.23136800	1.29471300	-0.94613100
C	-4.22774300	2.24767300	3.26166200
H	-3.19874500	0.37337000	3.13645700
C	-4.34165400	3.54160300	1.23134900
H	-3.38929500	2.69735200	-0.48851600
C	-5.68371200	-1.93909600	-2.16956900
H	-4.09891400	-3.08813100	-3.08280200
H	-7.02649300	-0.65627500	-1.07041300
C	-0.61761400	-1.65058400	3.68524000
H	-0.60486800	0.26990500	2.72193800
C	-1.98593200	-3.34882900	2.64745800
H	-3.00650900	-2.78490300	0.84542100

C	-0.69864200	2.50997200	-0.46050700
C	-1.49016200	1.17247500	-2.32900400
C	-4.64791400	3.39206600	2.58586400
H	-4.46888000	2.11289000	4.31256000
H	-4.67597600	4.42167000	0.68883300
C	-1.11732600	-2.95411500	3.66678200
H	0.06373500	-1.33596300	4.47072300
H	-2.37553300	-4.36265400	2.62454300
C	-0.39486200	3.55356900	-1.32927900
H	-0.50951300	2.63808000	0.59931400
C	-1.20391700	2.22141200	-3.20368400
H	-1.91411700	0.25631100	-2.72265600
C	-0.65601100	3.39106200	-2.68839400
H	0.04656600	4.47694800	-0.97019600
H	-1.39525400	2.13890200	-4.26856700
P	2.32882000	0.26796400	0.22725600
C	3.50432200	0.22530700	-1.19788700
C	3.17139500	-0.75586800	1.51946000
C	2.52428300	1.98926400	0.88334500
C	2.97110600	0.16921700	-2.49385100
C	4.89922800	0.24828200	-1.03546700
C	4.11770700	-0.24050300	2.42156100
C	2.85373800	-2.12324000	1.57686600
C	1.98107900	2.30096300	2.14406300
C	3.08113000	3.02987200	0.12550100
C	3.81499400	0.15467900	-3.60688300
H	1.89476700	0.11260300	-2.62687900
C	5.74018700	0.22984500	-2.14776700
H	5.33009600	0.26999900	-0.03876400
C	4.73271900	-1.07363300	3.35813800
H	4.37199600	0.81487200	2.40144800
C	3.47765800	-2.95364700	2.50972300
H	2.12256600	-2.53855400	0.88792000
C	2.00565000	3.60576000	2.63478000
H	1.55215900	1.50999900	2.75459300
C	3.09968700	4.33990900	0.61435300
H	3.50718800	2.81852600	-0.84985300

C	5.19902500	0.18597200	-3.43579800
H	3.38798900	0.10293700	-4.60472900
C	4.41542100	-2.43271300	3.40328700
H	5.46173100	-0.65900200	4.05001600
H	3.22361400	-4.00996100	2.53681300
C	2.56401200	4.63369600	1.86841500
H	1.59096900	3.82072900	3.61647800
H	3.54167700	5.12941800	0.01172600
H	5.85627700	0.16584800	-4.30132400
I	0.31844900	-2.99207500	-1.51282100
H	4.89621400	-3.08085400	4.13167000
H	2.58303100	5.65146800	2.24882700
H	6.81825400	0.24339500	-2.00928800
H	-6.47571200	-2.41549500	-2.74133800
H	-5.21605800	4.15843100	3.10611500
H	-0.82852100	-3.65936200	4.44105800
F	-0.37977300	4.40705000	-3.52810400

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P	-2.42097800	-0.22987900	-0.02956000
C	-3.11782000	-0.61965500	-1.69366200
C	-3.26915100	1.35700100	0.40685800
C	-3.18711000	-1.42941300	1.14225900
C	-2.34716500	-1.34790200	-2.61266200
C	-4.41416800	-0.21714800	-2.06127600
C	-3.24657600	2.42877300	-0.50204700
C	-3.89767200	1.53950200	1.64716000
C	-2.58363500	-1.61094500	2.39610600
C	-4.36439000	-2.12803200	0.84534900
C	-2.86312400	-1.66905600	-3.86956700
H	-1.35359700	-1.68180800	-2.33305200
C	-4.92597000	-0.54129900	-3.31816700
H	-5.02193600	0.35890900	-1.37088700
C	-3.83931500	3.64742800	-0.17836600
H	-2.75961200	2.31573200	-1.46468600
C	-4.48755300	2.76422600	1.97080700

H	-3.93795700	0.72636900	2.36381700
C	-3.15942500	-2.45647400	3.34333100
H	-1.65096300	-1.10209800	2.62244500
C	-4.93058600	-2.98680000	1.78982300
H	-4.83721800	-2.01595000	-0.12472500
C	-4.15106800	-1.26706700	-4.22552000
H	-2.25491600	-2.23702900	-4.56823700
H	-5.92946300	-0.22306900	-3.58793700
C	-4.46087800	3.82026100	1.06106500
H	-3.80834200	4.46531300	-0.89277800
H	-4.97252800	2.88567400	2.93585700
C	-4.33413000	-3.14871100	3.04062100
H	-2.68018600	-2.58893600	4.30946900
H	-5.83786800	-3.53170000	1.54306800
H	-4.55009200	-1.51627200	-5.20523400
H	-4.91928800	4.77255200	1.31369800
H	-4.77621100	-3.81863400	3.77318800
Pd	0.00000700	-0.26641500	0.00001300
P	2.42103000	-0.22988100	0.02958000
C	3.11779100	-0.61973100	1.69370800
C	3.26910500	1.35709700	-0.40666700
C	3.18731300	-1.42925500	-1.14234200
C	2.34725700	-1.34840400	2.61247300
C	4.41392600	-0.21679000	2.06160500
C	3.24642000	2.42881400	0.50229900
C	3.89763400	1.53971400	-1.64694500
C	2.58380500	-1.61080300	-2.39617500
C	4.36469700	-2.12775200	-0.84550900
C	2.86315600	-1.66960900	3.86939100
H	1.35385000	-1.68262800	2.33267100
C	4.92565800	-0.54097400	3.31851600
H	5.02157500	0.35964900	1.37142800
C	3.83908000	3.64752800	0.17870200
H	2.75940800	2.31569000	1.46490700
C	4.48744500	2.76449400	-1.97050300
H	3.93799200	0.72662400	-2.36364900
C	3.15970000	-2.45616200	-3.34346800

H	1.65102700	-1.10213700	-2.62242300
C	4.93098200	-2.98633600	-1.79007800
H	4.83752900	-2.01573200	0.12455700
C	4.15089800	-1.26721200	4.22561400
H	2.25504700	-2.23793500	4.56786100
H	5.92898400	-0.22239800	3.58849800
C	4.46067800	3.82047300	-1.06069700
H	3.80801000	4.46537600	0.89315200
H	4.97243800	2.88602700	-2.93553400
C	4.33452100	-3.14822100	-3.04086200
H	2.68041500	-2.58863000	-4.30959400
H	5.83836700	-3.53110700	-1.54337700
C	-0.00001200	1.77383800	-0.00007300
C	0.15431800	2.49505500	-1.19207500
C	-0.15440100	2.49503500	1.19194000
C	0.15219300	3.89393100	-1.20277400
H	0.28779600	1.97309700	-2.13658300
C	-0.15234900	3.89390800	1.20265600
H	-0.28790300	1.97306500	2.13643700
C	-0.00009200	4.58018500	-0.00005700
H	0.27448700	4.44146800	-2.13223200
H	-0.27470200	4.44142700	2.13211700
I	0.00004200	-3.08701600	-0.00010500
H	4.91903400	4.77280800	-1.31325900
H	4.54986200	-1.51643900	5.20534700
H	4.77665400	-3.81799800	-3.77347100
Cl	-0.00017200	6.34664600	-0.00005500

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P	-2.28968600	-0.14033200	0.34532600
C	-3.63309500	-0.64623000	-0.81196100
C	-3.18838000	0.92322700	1.58970000
C	-3.31223600	-1.35851000	-1.97965700
C	-4.98093400	-0.36312900	-0.53073000
C	-1.84964400	-1.63092400	1.37165700
Pd	-0.04089800	-0.43265900	-0.39407900

C	-3.51460300	0.45079200	2.87037500
C	-3.65428200	2.19633300	1.20992900
C	-4.32272200	-1.76944800	-2.85068500
H	-2.27806500	-1.61491100	-2.19611300
C	-5.98416200	-0.77744000	-1.40748500
H	-5.25500300	0.17590900	0.36821500
C	-0.96168100	-1.49411800	2.45675000
C	-2.34469400	-2.90351500	1.04829600
C	-1.22961500	1.36576300	-0.51330100
C	-4.25574400	1.23874300	3.75539500
H	-3.19545300	-0.53458400	3.18663700
C	-4.40269100	2.97600500	2.09011300
H	-3.44597300	2.57972900	0.21746800
C	-5.65842700	-1.47788600	-2.57026100
H	-4.05592800	-2.32282000	-3.74659900
H	-7.02179600	-0.55154000	-1.17717800
C	-0.58474300	-2.61040800	3.20308800
H	-0.57823800	-0.51462700	2.72605400
C	-1.96876300	-4.01253600	1.80509000
H	-3.00940300	-3.03381700	0.20242400
C	-0.71659500	2.41436700	0.28128600
C	-1.47227400	1.61372600	-1.88163300
C	-4.69846700	2.50336900	3.37092500
H	-4.48761200	0.85516800	4.74522500
H	-4.75333600	3.95431200	1.77316700
C	-1.08718600	-3.87200800	2.87869400
H	0.10630500	-2.49293000	4.03306300
H	-2.36039700	-4.99179200	1.54483000
C	-0.40443000	3.64945200	-0.27860900
H	-0.54600100	2.26278700	1.34118800
C	-1.17892700	2.85657800	-2.44542000
H	-1.88911300	0.83553200	-2.51018900
C	-0.64171300	3.86023200	-1.63981900
H	0.02716400	4.43537300	0.33122900
H	-1.36240500	3.04004300	-3.49877700
P	2.33564600	0.11031500	0.32944400
C	3.48256000	0.44643500	-1.07962000

C	3.21862000	-1.19576300	1.30109200
C	2.51851400	1.60885300	1.40207900
C	2.92616700	0.66441100	-2.34826100
C	4.87870800	0.48673200	-0.93132600
C	4.16257400	-0.91277000	2.30275400
C	2.94058100	-2.53740500	0.99011600
C	1.99312000	1.57739900	2.70808500
C	3.04554200	2.81936200	0.92854200
C	3.74822400	0.93605600	-3.44458300
H	1.85010400	0.59572700	-2.47852600
C	5.69778800	0.75462400	-2.02757100
H	5.32827300	0.29814800	0.03921200
C	4.81322700	-1.94786800	2.97733500
H	4.38805400	0.11628300	2.56555800
C	3.59989700	-3.56841900	1.66186500
H	2.21308200	-2.77447200	0.21797400
C	2.00570300	2.71413100	3.51549200
H	1.58673600	0.64926100	3.10345000
C	3.05213700	3.96118700	1.73588800
H	3.45666100	2.87396400	-0.07411300
C	5.13320000	0.98286600	-3.28584800
H	3.30381800	1.09542700	-4.42322400
C	4.53472000	-3.27817600	2.65744400
H	5.53992000	-1.71218100	3.75092700
H	3.37625300	-4.60042500	1.40491500
C	2.53398400	3.91453300	3.03014800
H	1.60503800	2.66297600	4.52482100
H	3.47038900	4.88700200	1.34902700
H	5.77363100	1.18619600	-4.14024200
I	0.31572500	-2.65401500	-2.13641700
H	5.04332300	-4.08309800	3.18203700
H	2.54359600	4.80168000	3.65767000
H	6.77716300	0.77915000	-1.90137400
H	-6.44261300	-1.79815700	-3.25113400
H	-5.27532800	3.11465400	4.05961100
H	-0.79033000	-4.74174000	3.45807600
Cl	-0.27173900	5.42537900	-2.34360800

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P	-2.41200100	-0.52244600	-0.03378900
C	-3.08602100	-1.00086900	-1.68460100
C	-3.29038300	1.06862300	0.32201300
C	-3.17041900	-1.68076800	1.18334400
C	-2.30342500	-1.77789700	-2.55243700
C	-4.37720000	-0.61943100	-2.09040300
C	-3.27354800	2.09945500	-0.63334300
C	-3.93641200	1.29544800	1.54582100
C	-2.58005800	-1.79536400	2.45123200
C	-4.33186600	-2.41211300	0.90336400
C	-2.80256200	-2.16578900	-3.79722200
H	-1.31417300	-2.09739900	-2.24211900
C	-4.87164800	-1.00966200	-3.33546300
H	-4.99415000	-0.00849400	-1.43943200
C	-3.88947800	3.32139300	-0.37080900
H	-2.77303800	1.95261500	-1.58433200
C	-4.54971500	2.52326500	1.80796000
H	-3.97167500	0.51418300	2.29719400
C	-3.15349000	-2.60854700	3.42778800
H	-1.66011100	-1.25917900	2.66652000
C	-4.89561300	-3.23802200	1.87805500
H	-4.79343300	-2.35032600	-0.07654600
C	-4.08482300	-1.78245700	-4.19220300
H	-2.18539800	-2.77060500	-4.45596700
H	-5.87108100	-0.70620200	-3.63562300
C	-4.52902100	3.53822400	0.85240100
H	-3.86303500	4.10657900	-1.12128000
H	-5.04826200	2.67929300	2.76104700
C	-4.31218100	-3.33415300	3.14176100
H	-2.68480100	-2.68974200	4.40470600
H	-5.79047600	-3.80889100	1.64506100
H	-4.47032100	-2.08279500	-5.16295500
H	-5.00679300	4.49257200	1.05716600
H	-4.75200900	-3.97882200	3.89797200

Pd	0.01193200	-0.50968200	0.01610100
P	2.43036100	-0.42957900	0.02324600
C	3.16710400	-0.76806700	1.68087400
C	3.24525400	1.15967000	-0.46256800
C	3.18559200	-1.64457600	-1.13936600
C	2.41686000	-1.45238100	2.64873200
C	4.47594900	-0.36162500	1.99679100
C	3.21928500	2.24938500	0.42456300
C	3.84950300	1.32666700	-1.71690000
C	2.56405400	-1.84656200	-2.38136800
C	4.36692000	-2.33845300	-0.84822300
C	2.96557200	-1.72856900	3.90259700
H	1.41306700	-1.78732400	2.41046900
C	5.02093600	-0.64178900	3.25013200
H	5.06746200	0.18388800	1.26836900
C	3.78441400	3.47105600	0.06498500
H	2.75146700	2.14781800	1.39803400
C	4.41185800	2.55431100	-2.07609600
H	3.89124800	0.49977000	-2.41756800
C	3.12585400	-2.70760200	-3.32287600
H	1.62844500	-1.34080400	-2.60288000
C	4.91918200	-3.21281200	-1.78672100
H	4.85355500	-2.21134300	0.11307500
C	4.26631700	-1.32526400	4.20628200
H	2.37261100	-2.26293600	4.63981500
H	6.03397800	-0.32193500	3.47921500
C	4.38154300	3.62873700	-1.18833800
H	3.75183400	4.30277200	0.76332200
H	4.87713600	2.66431200	-3.05208400
C	4.30477800	-3.39520700	-3.02587600
H	2.63289900	-2.85520200	-4.27988900
H	5.82973100	-3.75408700	-1.54407600
C	-0.02765100	1.52385900	-0.06978000
C	0.10805000	2.19888200	-1.29368900
C	-0.18784400	2.28634400	1.09799400
C	0.08232500	3.59116700	-1.34924500
H	0.24192900	1.63827900	-2.21568700

C	-0.20640000	3.68037200	1.05023300
H	-0.30890800	1.79383900	2.05979700
C	-0.07247100	4.34555400	-0.17731200
H	0.18685900	4.11469400	-2.29479600
H	-0.33110600	4.25599500	1.96150800
I	0.07383700	-3.32757900	0.15386800
H	4.81734000	4.58359100	-1.46946500
H	4.69088300	-1.54023400	5.18336900
H	4.73617200	-4.07721100	-3.75364400
C	-0.08946700	5.82496500	-0.29403500
O	-0.01600200	6.44361100	-1.34017300
O	-0.19643300	6.44264100	0.91101000
C	-0.22340700	7.87381200	0.86096300
H	-1.07795100	8.22549700	0.27573100
H	-0.30915700	8.20232600	1.89776600
H	0.69361800	8.26366400	0.40993000

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P	-3.33062000	0.16756800	0.30435600
C	-4.23283100	-0.56398400	-1.09817300
C	-4.50832400	1.16187800	1.28543800
C	-3.61481900	-1.59336900	-1.82741600
C	-5.50906200	-0.10875900	-1.46991900
C	-2.72776000	-1.20126800	1.33982200
Pd	0.65720700	-0.14953900	-0.70807800
C	-4.98949100	0.69971800	2.51859200
C	-4.96238100	2.39631100	0.78542000
C	-4.26741400	-2.14747800	-2.92890000
H	-2.62273700	-1.96043300	-1.56699500
C	-6.15480800	-0.67741100	-2.56730100
H	-6.00339600	0.67538900	-0.90695000
C	-1.46451300	-1.11752800	1.94203800
C	-3.53694500	-2.33073800	1.55392700
C	-1.98916400	1.23514000	-0.22984300
C	-5.91512300	1.45772600	3.23847500
H	-4.63959500	-0.24473700	2.92099300

C	-5.88870100	3.14637300	1.50815700
H	-4.58039200	2.77668300	-0.15706200
C	-5.53462400	-1.69379700	-3.29846500
H	-3.76977500	-2.93106300	-3.49233600
H	-7.14348100	-0.32583800	-2.84861500
C	-1.01923300	-2.15625800	2.76120000
H	-0.81703500	-0.26734100	1.74810400
C	-3.08485700	-3.36026800	2.37698000
H	-4.50461200	-2.41476600	1.06760800
C	-1.70293400	2.39221700	0.51331900
C	-1.20316100	0.88622300	-1.38443600
C	-6.36680800	2.67774500	2.73500200
H	-6.27764100	1.09329300	4.19526100
H	-6.23156200	4.09927100	1.11550500
C	-1.82650600	-3.27249900	2.98005200
H	-0.03119000	-2.09611500	3.20686900
H	-3.70706300	-4.23652100	2.53439700
C	-0.67584500	3.25313800	0.12504600
H	-2.28870800	2.63891300	1.39226800
C	-0.11931400	1.75581700	-1.72656300
H	-1.59453000	0.20251700	-2.12845000
C	0.11472900	2.93152100	-0.98209100
H	-0.48851800	4.16086700	0.68963100
H	0.37350800	1.63010800	-2.68633900
P	2.74281600	-0.19546400	0.45404300
C	4.17476600	0.44740100	-0.52621900
C	3.40546800	-1.81809000	1.06687600
C	2.74622500	0.83521400	1.99564500
C	4.20365300	0.11733800	-1.89131500
C	5.22841200	1.20126600	0.01096500
C	4.68164300	-1.93893700	1.64435900
C	2.60854800	-2.96378100	0.94010200
C	2.71353000	0.26381400	3.27817400
C	2.64700200	2.23495300	1.88319200
C	5.27003100	0.52075400	-2.69538800
H	3.38447300	-0.45590700	-2.31940100
C	6.28936100	1.61319900	-0.79840900

H	5.21653700	1.48167600	1.05997500
C	5.14108600	-3.17430700	2.09805200
H	5.32165200	-1.06593700	1.73603300
C	3.07174700	-4.20290400	1.39448500
H	1.64086400	-2.89120700	0.45219100
C	2.59072700	1.06565700	4.41622100
H	2.79754500	-0.81233300	3.39292200
C	2.53984600	3.03230900	3.02278000
H	2.66120500	2.70165300	0.90237500
C	6.31471600	1.27170000	-2.15156000
H	5.28012900	0.25313500	-3.74893200
C	4.33425300	-4.31031200	1.97623400
H	6.13093500	-3.25293300	2.54101500
H	2.44575700	-5.08356500	1.27616200
C	2.50716600	2.45271200	4.29444400
H	2.57150100	0.60169500	5.39960400
H	2.48145500	4.11298700	2.91555700
H	7.14188700	1.59258200	-2.77980800
I	0.06669800	-2.60436100	-2.14377900
H	4.69641500	-5.27455100	2.32454500
H	2.42016100	3.07696000	5.18021300
H	7.09614300	2.20238300	-0.36918700
H	-6.04083200	-2.13100200	-4.15488300
H	-7.08571800	3.26624200	3.29805800
H	-1.47179600	-4.08298900	3.61064300
C	1.19101100	3.87926100	-1.42611600
O	2.36891200	3.79308000	-1.14893400
O	0.67997300	4.87068000	-2.18691000
C	1.63839400	5.83006500	-2.66929700
H	2.39401400	5.33826000	-3.28733900
H	1.06299200	6.54401600	-3.25911100
H	2.13468100	6.33037900	-1.83339800

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P	-2.48867600	-0.07593600	-0.04732000
C	-3.31987700	-0.44490000	-1.65298700

C	-3.04274800	1.65770600	0.29273700
C	-3.37827100	-1.04348800	1.24524900
C	-2.70538200	-1.30064300	-2.57916400
C	-4.56825900	0.11945500	-1.97129200
C	-2.86453700	2.64301400	-0.69357000
C	-3.58841700	2.03275600	1.52857800
C	-2.73853700	-1.24340100	2.47826600
C	-4.67576700	-1.53928800	1.06292500
C	-3.33041400	-1.59217000	-3.79338100
H	-1.74980900	-1.75410300	-2.33853300
C	-5.19004200	-0.17682600	-3.18439200
H	-5.05027600	0.80061400	-1.27712700
C	-3.22405500	3.96645200	-0.44865300
H	-2.44007700	2.37778900	-1.65627100
C	-3.94541900	3.36174200	1.77262400
H	-3.74286600	1.29128300	2.30493400
C	-3.39270300	-1.90503700	3.51663500
H	-1.71842700	-0.89605800	2.61698600
C	-5.32281900	-2.21576500	2.09908700
H	-5.18150300	-1.41310400	0.11139600
C	-4.57193300	-1.03332600	-4.09837700
H	-2.84325100	-2.25994600	-4.49858300
H	-6.15517400	0.26579700	-3.41594200
C	-3.76440500	4.33125900	0.78741100
H	-3.07639800	4.71477700	-1.22241800
H	-4.36921200	3.63346700	2.73582400
C	-4.68678800	-2.39510400	3.32793300
H	-2.88481200	-2.05340900	4.46569100
H	-6.32495700	-2.60528600	1.94125400
H	-5.05580200	-1.26077600	-5.04456000
H	-4.04077200	5.36459900	0.97860100
H	-5.19263900	-2.92254500	4.13214900
Pd	-0.10906400	-0.50621100	-0.04651400
P	2.29410500	-0.85782000	0.01609600
C	2.89650000	-1.29737200	1.70483800
C	3.37770700	0.56651000	-0.45811000
C	2.89206500	-2.19866800	-1.09955600

C	2.02328800	-1.92505500	2.60692800
C	4.21812200	-1.03654700	2.10727900
C	3.50056300	1.66763800	0.40659300
C	4.03246000	0.60779300	-1.69772500
C	2.26153000	-2.36792000	-2.34127100
C	3.98510800	-3.01205300	-0.77256400
C	2.46375100	-2.28438100	3.88201600
H	1.00715800	-2.15216700	2.30110200
C	4.65330500	-1.39698000	3.38324500
H	4.90617200	-0.54189300	1.42947600
C	4.25079200	2.78237900	0.03740100
H	2.99661900	1.66247400	1.36698100
C	4.78838500	1.72451800	-2.06385500
H	3.96027100	-0.23142600	-2.38096100
C	2.72882700	-3.31882200	-3.24795600
H	1.39107800	-1.76729400	-2.58846300
C	4.44154600	-3.97396100	-1.67577700
H	4.47616500	-2.90630100	0.18921900
C	3.77690400	-2.02025100	4.27389900
H	1.77650700	-2.77345300	4.56697500
H	5.67739500	-1.18724900	3.68043100
C	4.89735200	2.81433300	-1.20091300
H	4.30926500	3.63604100	0.70622400
H	5.29208500	1.73672500	-3.02688600
C	3.81874000	-4.12607400	-2.91526800
H	2.22919800	-3.44172400	-4.20493800
H	5.28326700	-4.60636500	-1.40647600
C	0.22444400	1.50339900	-0.04956400
C	0.53000000	2.18539000	-1.23644700
C	0.17255000	2.23875800	1.14436600
C	0.79788900	3.55556100	-1.23112600
H	0.58186900	1.64838500	-2.18027300
C	0.44297300	3.60760700	1.15888900
H	-0.08373000	1.74749600	2.07956400
C	0.76351200	4.26887200	-0.03041300
H	1.04140400	4.06759300	-2.15705800
H	0.40107700	4.16248300	2.09177700

I	-0.58512400	-3.28533800	-0.01304900
H	5.47872300	3.68564800	-1.49010600
H	4.11687700	-2.29770400	5.26817600
H	4.17484900	-4.87660500	-3.61585400
C	1.15500100	5.71530200	0.00444400
F	0.46760900	6.41003000	0.94108600
F	2.47278700	5.87441900	0.30421200
F	0.95506700	6.33251800	-1.18269900

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P	-2.28035400	-0.49448100	0.36672200
C	-3.59901400	-0.83371700	-0.87663400
C	-3.22224700	0.31138300	1.76192900
C	-3.25064600	-1.32468300	-2.14608400
C	-4.95616000	-0.63599700	-0.56745600
C	-1.78152100	-2.11533900	1.12617800
Pd	-0.00605900	-0.59863000	-0.41753600
C	-3.56910500	-0.39735300	2.92254900
C	-3.70314100	1.62582900	1.61273900
C	-4.24335500	-1.60527200	-3.08647800
H	-2.20871000	-1.51099800	-2.39383000
C	-5.94126700	-0.91867400	-1.51420600
H	-5.25182100	-0.26576700	0.40673100
C	-0.92789500	-2.13102800	2.24650500
C	-2.20484500	-3.33175800	0.56846200
C	-1.23499900	1.15357400	-0.19228100
C	-4.34617500	0.20003800	3.91863500
H	-3.23865700	-1.41987600	3.05758900
C	-4.48674200	2.21598900	2.60305700
H	-3.47885700	2.19130900	0.71532500
C	-5.58840600	-1.40041400	-2.77599500
H	-3.95475000	-1.98781700	-4.06133300
H	-6.98614000	-0.76123000	-1.26094400
C	-0.51121900	-3.34362000	2.79545100
H	-0.60465300	-1.19854700	2.69883600
C	-1.78858400	-4.53848600	1.12864400

H	-2.84153500	-3.33967300	-0.30842900
C	-0.75218000	2.05272800	0.78565700
C	-1.49805700	1.64194500	-1.49085700
C	-4.80370100	1.50778300	3.76468700
H	-4.59410800	-0.36511200	4.81291600
H	-4.84789500	3.23138700	2.46544500
C	-0.93965800	-4.54953100	2.23723600
H	0.15197800	-3.34357700	3.65592700
H	-2.12260300	-5.47306300	0.68721500
C	-0.48209100	3.37549500	0.45678500
H	-0.56548400	1.71009000	1.79716600
C	-1.24159700	2.97580500	-1.81091700
H	-1.89561900	0.97858200	-2.24980300
C	-0.72890500	3.84065600	-0.84187400
H	-0.06257100	4.04201000	1.20290700
H	-1.43150300	3.33710600	-2.81611600
P	2.34775000	-0.08867900	0.37575200
C	3.44404400	0.58820500	-0.94937000
C	3.31632800	-1.51308900	1.05637100
C	2.48627200	1.16842900	1.72935800
C	2.84586100	1.07260200	-2.12173800
C	4.84284800	0.63297400	-0.83040000
C	4.28441700	-1.37567800	2.06572200
C	3.08118000	-2.78574800	0.51033400
C	1.97776600	0.84962800	3.00288100
C	2.97050600	2.46679600	1.51382200
C	3.62827300	1.60907200	-3.14696800
H	1.76799400	1.00952000	-2.23815200
C	5.62267300	1.16549600	-1.85660800
H	5.32569500	0.24138400	0.06004600
C	5.00324100	-2.48503700	2.51517600
H	4.47449000	-0.40323300	2.50942300
C	3.80807900	-3.89055000	0.95778500
H	2.33417000	-2.91089900	-0.26912400
C	1.96542300	1.79397800	4.02848200
H	1.60460200	-0.15312300	3.19684300
C	2.95196500	3.41633300	2.54050600

H	3.36804800	2.74076900	0.54213400
C	5.01617100	1.65738200	-3.01577900
H	3.15122700	1.97477000	-4.05216500
C	4.76841100	-3.74488200	1.96057900
H	5.74826200	-2.36228200	3.29742300
H	3.61680800	-4.86682600	0.52032700
C	2.45136900	3.08528400	3.79964500
H	1.57870200	1.52226500	5.00752200
H	3.33604000	4.41551800	2.35164700
H	5.62587900	2.06726100	-3.81680700
I	0.40832300	-2.46748200	-2.52011100
H	5.33007500	-4.60759900	2.30990100
H	2.44122100	3.82303600	4.59744600
H	6.70451300	1.19074300	-1.75412600
H	-6.35866000	-1.61780900	-3.51117600
H	-5.40817400	1.97132900	4.53953100
H	-0.61126100	-5.49344300	2.66306800
C	-0.49675800	5.29154800	-1.16204900
F	-1.53949700	6.06162800	-0.76483900
F	0.59997800	5.77287900	-0.53500900
F	-0.33485700	5.50173000	-2.48557800

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P	-2.41014700	-0.37934300	-0.03236600
C	-3.08619100	-0.81493000	-1.69364000
C	-3.28951000	1.20194300	0.36401200
C	-3.16509900	-1.56764700	1.15763700
C	-2.29812800	-1.55396300	-2.58905000
C	-4.38401700	-0.43703200	-2.08149200
C	-3.28051600	2.25348700	-0.56845900
C	-3.92935900	1.40023700	1.59608800
C	-2.56923200	-1.71437000	2.41964300
C	-4.32849000	-2.29092500	0.86488300
C	-2.79848900	-1.90910400	-3.84310100
H	-1.30320300	-1.86954400	-2.29343300
C	-4.87989200	-0.79481900	-3.33560300

H	-5.00517200	0.14617000	-1.40934000
C	-3.89836600	3.46781900	-0.27612400
H	-2.78582800	2.12861700	-1.52558600
C	-4.54471800	2.62024700	1.88828400
H	-3.95926600	0.60238700	2.33020300
C	-3.13918100	-2.55077400	3.37848100
H	-1.64729500	-1.18524400	2.64371400
C	-4.88864200	-3.14019200	1.82141600
H	-4.79453800	-2.20512600	-0.11109800
C	-4.08767900	-1.53058000	-4.21962800
H	-2.17693000	-2.48467600	-4.52352500
H	-5.88448400	-0.49480500	-3.62161100
C	-4.53225500	3.65596100	0.95485000
H	-3.87917700	4.26865200	-1.01011300
H	-5.03975700	2.75343100	2.84669100
C	-4.29989700	-3.26795900	3.07983500
H	-2.66608200	-2.65666100	4.35090000
H	-5.78497400	-3.70446200	1.57825200
H	-4.47430400	-1.80558300	-5.19739100
H	-5.01410000	4.60331800	1.18182600
H	-4.73708300	-3.93070700	3.82180000
Pd	0.01414200	-0.36697000	0.01533300
P	2.43177500	-0.28566800	0.02701500
C	3.16198400	-0.66054900	1.67972700
C	3.24497600	1.31551400	-0.42117900
C	3.19358600	-1.47357500	-1.15887400
C	2.41082000	-1.37507300	2.62495100
C	4.46678700	-0.25524000	2.01329600
C	3.21968300	2.38412300	0.49132300
C	3.84748100	1.51207600	-1.67200900
C	2.57718000	-1.65070800	-2.40718800
C	4.37551500	-2.17056600	-0.87770700
C	2.95452200	-1.68119700	3.87401100
H	1.41061200	-1.71040000	2.37226600
C	5.00665400	-0.56518900	3.26188400
H	5.05920500	0.31214100	1.30255700
C	3.78487000	3.61365600	0.15988300

H	2.75283800	2.25914100	1.46260500
C	4.40886300	2.74800800	-2.00320700
H	3.88865500	0.70160100	-2.39160200
C	3.14478700	-2.49036000	-3.36439100
H	1.64132600	-1.14238400	-2.62168500
C	4.93362500	-3.02349000	-1.83231100
H	4.85805200	-2.06249000	0.08797100
C	4.25109400	-1.27813300	4.19547000
H	2.36112500	-2.23888300	4.59339300
H	6.01661200	-0.24581900	3.50481700
C	4.38000100	3.80112200	-1.09028700
H	3.75504200	4.42875500	0.87774500
H	4.87239200	2.88120300	-2.97709300
C	4.32435700	-3.18110800	-3.07738900
H	2.65591500	-2.61899900	-4.32620700
H	5.84465100	-3.56746600	-1.59768900
C	-0.02725500	1.66784300	-0.01240800
C	0.10727900	2.38052600	-1.21613100
C	-0.19440400	2.39569000	1.17520200
C	0.06783700	3.77214000	-1.23136900
H	0.24971300	1.84703100	-2.15300600
C	-0.22883300	3.79098900	1.16289800
H	-0.31075200	1.87639700	2.12342800
C	-0.10171200	4.50020800	-0.04182900
H	0.16965600	4.32474500	-2.16062300
H	-0.36428500	4.32195600	2.10123300
I	0.07321800	-3.18672400	0.07393500
H	4.81517400	4.76242200	-1.34935300
H	4.67182100	-1.51646700	5.16878600
H	4.76023600	-3.84647500	-3.81775200
C	-0.14506400	5.99005400	-0.11666900
O	-0.04416300	6.57402800	-1.18793100
C	-0.32349900	6.78520600	1.17047900
H	-0.32305200	7.84902300	0.92610300
H	-1.26768900	6.52696000	1.66499400
H	0.48390400	6.57598000	1.88244500

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P	-2.36655100	-0.14079400	0.30249300
C	-3.60818400	-0.59014300	-0.98213300
C	-3.36879000	0.92392900	1.46587300
C	-3.19110500	-1.16248700	-2.19455000
C	-4.98215100	-0.39801300	-0.75085800
C	-2.02242800	-1.62741900	1.35199200
Pd	-0.04524000	-0.51967300	-0.34957300
C	-3.83938100	0.43911900	2.69490400
C	-3.75793900	2.21355900	1.05914500
C	-4.13215500	-1.52673000	-3.15899700
H	-2.13691100	-1.35563600	-2.37066700
C	-5.91562900	-0.76856100	-1.71860700
H	-5.32936300	0.03623900	0.17909000
C	-1.23137400	-1.50164200	2.51023100
C	-2.50390700	-2.89208600	0.98083300
C	-1.13612400	1.33001200	-0.32840600
C	-4.65504500	1.23141600	3.50827100
H	-3.57579800	-0.55830700	3.02566200
C	-4.58094800	2.99664100	1.86620600
H	-3.42735500	2.60803600	0.10409300
C	-5.49352600	-1.32890200	-2.92591600
H	-3.79142500	-1.97214800	-4.08917500
H	-6.97414600	-0.61659500	-1.52605800
C	-0.93436300	-2.62440700	3.28238400
H	-0.85980900	-0.52831300	2.81685000
C	-2.20983000	-4.00657200	1.76478300
H	-3.08833800	-3.01065100	0.07564700
C	-0.67010200	2.28556900	0.60361800
C	-1.28662200	1.72683800	-1.68007300
C	-5.02590600	2.51106300	3.09867600
H	-5.00062500	0.83983000	4.46112200
H	-4.87288200	3.98824200	1.53147100
C	-1.42383100	-3.87854900	2.91192900
H	-0.31740300	-2.51715100	4.17006100
H	-2.58793600	-4.98057900	1.46786800

C	-0.28451700	3.55260000	0.18685100
H	-0.58959900	2.02848100	1.65413400
C	-0.91851600	3.00706800	-2.08320900
H	-1.68986800	1.03132300	-2.40727700
C	-0.40449600	3.93294400	-1.16216400
H	0.12058700	4.24141000	0.92086000
H	-1.01794900	3.31252300	-3.11992300
P	2.34994700	-0.05667200	0.30199000
C	3.49743600	0.04688400	-1.14270700
C	3.12839800	-1.33338000	1.39538000
C	2.69763300	1.51194800	1.22592200
C	2.94141900	0.24002600	-2.41545700
C	4.89247800	-0.05665000	-1.01730600
C	4.13237700	-1.03822000	2.33343200
C	2.69973600	-2.66393200	1.25721000
C	2.17585400	1.66260500	2.52426500
C	3.37715400	2.59734900	0.65394700
C	3.76424900	0.35030700	-3.53873500
H	1.86181900	0.27477300	-2.52658400
C	5.71221500	0.04894200	-2.14063300
H	5.34048700	-0.23011200	-0.04330200
C	4.69676400	-2.05085600	3.11149800
H	4.47117400	-0.01530500	2.46617300
C	3.27248500	-3.67411900	2.03230000
H	1.92427600	-2.90893600	0.53623900
C	2.34284400	2.85176100	3.23297400
H	1.64846600	0.83389300	2.99149600
C	3.53966000	3.79271800	1.36160500
H	3.79147000	2.50908100	-0.34498900
C	5.14938900	0.25655900	-3.40306300
H	3.31857000	0.49272500	-4.51937400
C	4.26969000	-3.37177100	2.96132300
H	5.47197800	-1.80567800	3.83327000
H	2.93270700	-4.69886800	1.90764600
C	3.02622500	3.92495700	2.65242500
H	1.94407900	2.94008900	4.24054600
H	4.08223300	4.61613100	0.90347300

H	5.78969500	0.33367800	-4.27799500
I	0.23347000	-2.84477800	-1.95543800
H	4.71136400	-4.15968500	3.56621400
H	3.16111400	4.85113400	3.20482400
H	6.79030300	-0.03696900	-2.03136400
H	-6.22377700	-1.61322000	-3.67885700
H	-5.66132700	3.12543200	3.73075800
H	-1.19061500	-4.75294600	3.51299800
C	-0.00966600	5.28903900	-1.66021800
O	-0.18551400	5.59894000	-2.82982400
C	0.61954400	6.27053500	-0.68422400
H	-0.08093800	6.52712000	0.12018600
H	1.51195300	5.84169800	-0.21307500
H	0.89004000	7.17825700	-1.22646800

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P	-2.42259400	-0.18456100	-0.02825800
C	-3.12374700	-0.58306900	-1.68756000
C	-3.26273900	1.40842200	0.40026300
C	-3.18204300	-1.37488600	1.15630900
C	-2.35320600	-1.30674500	-2.61017700
C	-4.42523000	-0.19004600	-2.04774700
C	-3.25231900	2.46906700	-0.52205300
C	-3.86878200	1.60807200	1.64905800
C	-2.57431400	-1.54464200	2.40980100
C	-4.35834500	-2.07879400	0.86814500
C	-2.87447500	-1.63310600	-3.86356900
H	-1.35561400	-1.63327900	-2.33645500
C	-4.94226800	-0.51973600	-3.30094200
H	-5.03279800	0.38308000	-1.35471900
C	-3.83428700	3.69415500	-0.20250000
H	-2.78571200	2.34135400	-1.49312200
C	-4.44808700	2.83899300	1.96820300
H	-3.89992700	0.80340500	2.37570300
C	-3.14522400	-2.38398300	3.36539700
H	-1.64234400	-1.03157100	2.62963200

C	-4.91961500	-2.93117000	1.82128500
H	-4.83397500	-1.97609500	-0.10154000
C	-4.16750900	-1.24109600	-4.21199000
H	-2.26646500	-2.19742500	-4.56531100
H	-5.94956600	-0.20907600	-3.56507900
C	-4.43292900	3.88428100	1.04573000
H	-3.81463500	4.50316200	-0.92739100
H	-4.91587700	2.97394500	2.93985600
C	-4.31911400	-3.08144400	3.07158500
H	-2.66304200	-2.50739900	4.33123900
H	-5.82619000	-3.48029800	1.58162100
H	-4.57064400	-1.49448700	-5.18889000
H	-4.88291200	4.84140000	1.29483000
H	-4.75742200	-3.74643500	3.81081600
Pd	-0.00000400	-0.21655400	0.00017000
P	2.42257100	-0.18449500	0.02822300
C	3.12423000	-0.58306500	1.68728800
C	3.26264300	1.40850800	-0.40036300
C	3.18160900	-1.37479500	-1.15663500
C	2.35387500	-1.30647600	2.61026400
C	4.42591600	-0.19024900	2.04695900
C	3.25222000	2.46911200	0.52200700
C	3.86871500	1.60820000	-1.64913000
C	2.57372900	-1.54410700	-2.41011500
C	4.35763800	-2.07923000	-0.86866600
C	2.87554100	-1.63280900	3.86349900
H	1.35611500	-1.63283000	2.33694900
C	4.94335500	-0.51992000	3.29999300
H	5.03333300	0.38270000	1.35364900
C	3.83420500	3.69420400	0.20252000
H	2.78559000	2.34135600	1.49305900
C	4.44804100	2.83913500	-1.96821200
H	3.89986900	0.80356400	-2.37580700
C	3.14422500	-2.38353600	-3.36588300
H	1.64196600	-1.03060000	-2.62982100
C	4.91849100	-2.93169300	-1.82198300
H	4.83337600	-1.97687700	0.10100100

C	4.16878500	-1.24103200	4.21140000
H	2.26767200	-2.19692300	4.56552900
H	5.95080900	-0.20942400	3.56372900
C	4.43287300	3.88437800	-1.04569600
H	3.81455100	4.50318200	0.92744200
H	4.91585200	2.97412200	-2.93985000
C	4.31784700	-3.08153600	-3.07226300
H	2.66192200	-2.50658500	-4.33171100
H	5.82485700	-3.48122300	-1.58245300
C	-0.00006700	1.81961500	0.00010700
C	0.15684900	2.54064600	-1.19472900
C	-0.15699300	2.54063000	1.19496200
C	0.15552100	3.93416300	-1.20322500
H	0.29126700	2.01492300	-2.13657400
C	-0.15569700	3.93414100	1.20347500
H	-0.29139100	2.01489000	2.13679900
C	-0.00009400	4.64343300	0.00012700
H	0.27967800	4.47934700	-2.13447100
H	-0.27986100	4.47931700	2.13472600
I	0.00014000	-3.03135700	0.00049100
H	4.88286700	4.84150600	-1.29474300
H	4.57222800	-1.49440200	5.18817800
H	4.75582400	-3.74660000	-3.81162900
C	-0.00011100	6.07596800	0.00013700
N	-0.00013600	7.24025300	0.00014800

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P	-2.31662400	-0.05172100	0.32033400
C	-3.63253500	-0.65350200	-0.81883700
C	-3.23722400	1.12915200	1.43142200
C	-3.28780800	-1.43768300	-1.93223500
C	-4.98729800	-0.36675100	-0.57415000
C	-1.87977500	-1.42659400	1.48474900
Pd	-0.02245500	-0.45141800	-0.38987400
C	-3.60054900	0.78069400	2.74104500
C	-3.67995000	2.36272600	0.91830100

C	-4.28175300	-1.91806700	-2.78635900
H	-2.24838100	-1.69653500	-2.11761400
C	-5.97344800	-0.85141700	-1.43359500
H	-5.27921000	0.22938800	0.28214100
C	-1.02200300	-1.18043000	2.57455500
C	-2.36516200	-2.72590600	1.27019100
C	-1.16908800	1.34444100	-0.60517400
C	-4.35931000	1.65322400	3.52617900
H	-3.29791500	-0.17221600	3.15775900
C	-4.44479500	3.22655900	1.69995900
H	-3.43995500	2.64873900	-0.09982600
C	-5.62405100	-1.62432500	-2.54257500
H	-3.99664200	-2.52656700	-3.63976300
H	-7.01648900	-0.62283600	-1.23264100
C	-0.66257400	-2.21976200	3.43229400
H	-0.64890600	-0.17794600	2.76034400
C	-2.00523100	-3.75630300	2.13730500
H	-3.00663700	-2.93737100	0.42253700
C	-0.68881800	2.45078100	0.13521600
C	-1.40596600	1.51132600	-1.99086400
C	-4.77996700	2.87817900	3.01088000
H	-4.62165300	1.36688600	4.54090700
H	-4.77745800	4.17313500	1.28326700
C	-1.15287800	-3.50905200	3.21540300
H	0.00446700	-2.02094900	4.26629300
H	-2.38627800	-4.75798900	1.96071400
C	-0.38183300	3.64818800	-0.49417500
H	-0.53239400	2.36458700	1.20442600
C	-1.11261500	2.71760900	-2.62140200
H	-1.81537100	0.69445300	-2.57345700
C	-0.59343500	3.79244200	-1.87992300
H	0.03158800	4.47232500	0.07730900
H	-1.28402100	2.83119300	-3.68716200
P	2.33379000	0.16085500	0.28787500
C	3.49015200	0.35227800	-1.14079400
C	3.19477700	-1.05203400	1.39082700
C	2.52937000	1.75292100	1.21268800

C	2.94652200	0.40629200	-2.43203900
C	4.88331500	0.44074500	-0.98327200
C	4.18452600	-0.68438100	2.31844900
C	2.85278700	-2.40832300	1.26497600
C	2.03771000	1.84119300	2.52882700
C	3.03883400	2.91505500	0.61486900
C	3.77732700	0.56447100	-3.54407500
H	1.87394300	0.30067000	-2.56460700
C	5.71096500	0.59633600	-2.09438800
H	5.32429300	0.37886800	0.00723300
C	4.81947600	-1.65211800	3.09880800
H	4.45583100	0.35973500	2.44126400
C	3.49623200	-3.37350700	2.04214200
H	2.08870100	-2.70870100	0.55295200
C	2.06546000	3.04804100	3.22673200
H	1.64880000	0.95154100	3.01821800
C	3.06143600	4.12679600	1.31254300
H	3.42568700	2.87679100	-0.39825000
C	5.15850200	0.66151000	-3.37695500
H	3.34275800	0.59799800	-4.53933400
C	4.47844600	-2.99936900	2.96076500
H	5.58240200	-1.35189100	3.81277400
H	3.22360600	-4.41919400	1.92725300
C	2.57631400	4.19908300	2.61859100
H	1.69186300	3.08996600	4.24680700
H	3.46572000	5.01358000	0.83119600
H	5.80580100	0.77832200	-4.24222400
I	0.29745500	-2.82704500	-1.90584000
H	4.97553100	-3.75210100	3.56739300
H	2.59880200	5.14052300	3.16079900
H	6.78766500	0.66101700	-1.96026800
H	-6.39546100	-1.99833600	-3.21040900
H	-5.37014000	3.55557700	3.62192700
H	-0.86925900	-4.31808400	3.88259400
C	-0.29597600	5.03644700	-2.52390300
N	-0.05708800	6.05074600	-3.04256600

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P	-2.42255000	-0.32761200	-0.02803100
C	-3.12755100	-0.73500500	-1.68317000
C	-3.25809200	1.26987600	0.39193400
C	-3.17818500	-1.50968300	1.16687100
C	-2.35702600	-1.45615800	-2.60768300
C	-4.43282100	-0.34981100	-2.03836600
C	-3.25594600	2.32094600	-0.54138900
C	-3.85015200	1.48324800	1.64512800
C	-2.56739100	-1.66940400	2.42022800
C	-4.35372900	-2.21779600	0.88608700
C	-2.88208700	-1.78802400	-3.85807100
H	-1.35635500	-1.77643600	-2.33798000
C	-4.95366900	-0.68522900	-3.28839200
H	-5.04025800	0.22195600	-1.34407300
C	-3.83221200	3.55039200	-0.22787400
H	-2.80169600	2.18204500	-1.51684100
C	-4.42339200	2.71849800	1.95815300
H	-3.87472700	0.68598600	2.38015600
C	-3.13467300	-2.50305200	3.38291900
H	-1.63607600	-1.15277400	2.63456700
C	-4.91136800	-3.06438000	1.84648200
H	-4.83140200	-2.12302600	-0.08337000
C	-4.17890500	-1.40420500	-4.20136300
H	-2.27401800	-2.35020300	-4.56145300
H	-5.96380200	-0.38067700	-3.54871800
C	-4.41629400	3.75444300	1.02505200
H	-3.82042600	4.35133500	-0.96194000
H	-4.87974000	2.86450700	2.93359000
C	-4.30791300	-3.20469400	3.09651000
H	-2.65032600	-2.61863900	4.34863600
H	-5.81740000	-3.61688400	1.61265700
H	-4.58497400	-1.66191400	-5.17589900
H	-4.86125400	4.71499100	1.26975000
H	-4.74342000	-3.86521400	3.84136500
Pd	0.00002700	-0.35870500	0.00015300

P	2.42259700	-0.32739400	0.02804000
C	3.12800900	-0.73473900	1.68301600
C	3.25798000	1.27013400	-0.39204500
C	3.17796400	-1.50942600	-1.16706600
C	2.35765400	-1.45566500	2.60784600
C	4.43343100	-0.34967800	2.03778200
C	3.25578100	2.32125400	0.54122300
C	3.85003300	1.48346200	-1.64525000
C	2.56706100	-1.66884700	-2.42041000
C	4.35333600	-2.21787600	-0.88643000
C	2.88304100	-1.78744900	3.85812000
H	1.35685800	-1.77584100	2.33849100
C	4.95461200	-0.68502900	3.28768900
H	5.04074100	0.22193000	1.34324400
C	3.83199200	3.55070200	0.22763900
H	2.80151900	2.18238100	1.51667500
C	4.42322600	2.71871800	-1.95834400
H	3.87464000	0.68615700	-2.38022900
C	3.13405100	-2.50255200	-3.38321900
H	1.63588300	-1.15192600	-2.63465100
C	4.91068200	-3.06452500	-1.84693800
H	4.83110400	-2.12332400	0.08300200
C	4.18002000	-1.40378400	4.20097900
H	2.27509300	-2.34944600	4.56175300
H	5.96486800	-0.38058800	3.54766900
C	4.41607700	3.75471000	-1.02529600
H	3.82017100	4.35169100	0.96165600
H	4.87956900	2.86469500	-2.93378700
C	4.30710400	-3.20455100	-3.09693500
H	2.64962600	-2.61790800	-4.34892400
H	5.81657900	-3.61730100	-1.61323400
C	-0.00007700	1.67557100	0.00007600
C	0.15047600	2.39645800	-1.19734400
C	-0.15068100	2.39642400	1.19752300
C	0.14816900	3.78991100	-1.20817300
H	0.27983800	1.86985700	-2.13916200
C	-0.14856100	3.78987000	1.20837800

H	-0.27995300	1.86978400	2.13933200
C	-0.00025700	4.47147700	0.00010000
H	0.26424300	4.35235100	-2.12702800
H	-0.26468200	4.35228700	2.12723900
I	0.00018400	-3.17139900	0.00034900
H	4.86101000	4.71526000	-1.27003300
H	4.58634400	-1.66143600	5.17542300
H	4.74237400	-3.86512600	-3.84186900
N	-0.00039300	5.93466700	0.00010600
O	0.09651800	6.51258800	-1.08527500
O	-0.09741400	6.51256200	1.08548800

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P	-2.34501800	-0.21892800	0.32857500
C	-3.59064100	-0.70888300	-0.93529100
C	-3.34287900	0.83170200	1.49882800
C	-3.17809100	-1.29733700	-2.14183500
C	-4.96458000	-0.53034900	-0.69246800
C	-1.92427000	-1.68656500	1.36790900
Pd	0.00978100	-0.54086900	-0.36981500
C	-3.76439500	0.35068400	2.74702200
C	-3.77593500	2.10524600	1.08571600
C	-4.12436700	-1.69192600	-3.08891000
H	-2.12330100	-1.47922200	-2.32789900
C	-5.90279400	-0.93033800	-1.64373200
H	-5.30780500	-0.08450500	0.23339100
C	-1.10853100	-1.52981500	2.50539300
C	-2.37961200	-2.96648200	1.01575700
C	-1.12628800	1.26244000	-0.33519700
C	-4.57731600	1.13309500	3.57229600
H	-3.46431000	-0.63465500	3.08318700
C	-4.59460300	2.87838400	1.90636900
H	-3.48403100	2.49498500	0.11622300
C	-5.48578000	-1.50731400	-2.84494500
H	-3.78740100	-2.14970900	-4.01441000
H	-6.96109400	-0.78858000	-1.44285000

C	-0.75996700	-2.63939700	3.27490200
H	-0.75846100	-0.54453800	2.79825700
C	-2.03227300	-4.06741400	1.79692000
H	-2.98676600	-3.10675800	0.12885800
C	-0.71082100	2.25974500	0.58335500
C	-1.32418500	1.63639400	-1.68992000
C	-4.99172200	2.39755100	3.15690100
H	-4.88583200	0.74616200	4.53953800
H	-4.91953600	3.85844800	1.56863200
C	-1.22089600	-3.90945000	2.92240700
H	-0.12523200	-2.50946900	4.14677600
H	-2.38934300	-5.05363600	1.51499800
C	-0.40953700	3.54324500	0.15592000
H	-0.59559300	2.01805400	1.63370800
C	-1.03648600	2.92844600	-2.12138000
H	-1.69882800	0.91167100	-2.40310300
C	-0.57764300	3.86520000	-1.19531300
H	-0.03784600	4.29183500	0.84369900
H	-1.16319800	3.21816900	-3.15740100
P	2.35519700	0.03419000	0.30713600
C	3.49184800	0.27506600	-1.13007000
C	3.21404400	-1.23659300	1.34512500
C	2.58090800	1.58168700	1.29556500
C	2.93065600	0.39710300	-2.40899700
C	4.88799000	0.33882200	-0.98943300
C	4.23282200	-0.92100200	2.26079500
C	2.84156100	-2.58065500	1.18195600
C	2.13713300	1.61228800	2.63085300
C	3.06696200	2.76917400	0.72893400
C	3.74724500	0.59733700	-3.52470500
H	1.85514600	0.31065800	-2.53041800
C	5.70163400	0.53524700	-2.10444300
H	5.34265200	0.22551000	-0.00985400
C	4.86572500	-1.92734100	2.99228600
H	4.52857100	0.11243300	2.41354300
C	3.48252500	-3.58456500	1.91081100
H	2.05670600	-2.84132800	0.47716800

C	2.19374200	2.78817800	3.37853900
H	1.76203100	0.70322700	3.09505900
C	3.11604400	3.94993000	1.47574400
H	3.41321400	2.77554900	-0.29952700
C	5.13191200	0.66803100	-3.37410200
H	3.29865600	0.68348500	-4.51053600
C	4.49343500	-3.26200000	2.81754600
H	5.65123100	-1.66681900	3.69725100
H	3.18562500	-4.62002500	1.76699500
C	2.68259400	3.96450100	2.80177300
H	1.85891300	2.78595800	4.41288600
H	3.49491700	4.85870600	1.01598500
H	5.76824300	0.81684200	-4.24258100
I	0.32461500	-2.83670200	-2.00078000
H	4.98877100	-4.04484000	3.38630600
H	2.72568300	4.88207100	3.38218700
H	6.78089600	0.57947800	-1.98341400
H	-6.21994100	-1.81468500	-3.58481800
H	-5.62370700	3.00448900	3.79932300
H	-0.94631600	-4.77312600	3.52138200
N	-0.27461000	5.22359200	-1.64614500
O	-0.45527200	5.48794100	-2.83684500
O	0.14419000	6.02616100	-0.80836500

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P	-2.42126700	-0.09601500	-0.02396500
C	-3.12463800	-0.47750300	-1.68808500
C	-3.27532300	1.48607400	0.42098900
C	-3.18668200	-1.30224700	1.14225300
C	-2.35699100	-1.20212000	-2.61242200
C	-4.42116000	-0.07172100	-2.05116500
C	-3.24225400	2.56687200	-0.47653700
C	-3.92657600	1.65301600	1.65166500
C	-2.58032800	-1.49038000	2.39371500
C	-4.36434000	-1.99984900	0.84456800
C	-2.87608800	-1.51661800	-3.86973800

H	-1.36308000	-1.53816400	-2.33653000
C	-4.93626000	-0.38914100	-3.30847600
H	-5.02672500	0.50164900	-1.35660800
C	-3.84958400	3.77802200	-0.15214700
H	-2.73406500	2.46740300	-1.42941200
C	-4.53029500	2.87068600	1.97649800
H	-3.97415000	0.83298000	2.35990500
C	-3.15344100	-2.34133500	3.33772200
H	-1.64739000	-0.98216100	2.62028600
C	-4.92791100	-2.86415900	1.78558700
H	-4.83951300	-1.88267400	-0.12378400
C	-4.16431600	-1.11145600	-4.22106100
H	-2.26995500	-2.08190100	-4.57242900
H	-5.94004400	-0.06843700	-3.57443200
C	-4.49557000	3.93500500	1.07681600
H	-3.81217700	4.60200600	-0.85942500
H	-5.03323600	2.97959700	2.93386600
C	-4.32845400	-3.03264100	3.03408800
H	-2.67171100	-2.47887500	4.30194400
H	-5.83543500	-3.40832400	1.53791100
H	-4.56577300	-1.35552300	-5.20112700
H	-4.96744300	4.88092100	1.32939300
H	-4.76837500	-3.70695800	3.76398000
Pd	-0.00254900	-0.14313300	0.00018800
P	2.41766700	-0.10953100	0.03114500
C	3.11629100	-0.52328600	1.68969200
C	3.27973500	1.47691000	-0.38330300
C	3.18036700	-1.29816200	-1.15471600
C	2.34460900	-1.26204500	2.59939300
C	4.41357300	-0.12865300	2.06226000
C	3.24999900	2.54100400	0.53405800
C	3.93361500	1.66380400	-1.60967000
C	2.57664900	-1.46024900	-2.41111300
C	4.35312600	-2.00769800	-0.86612100
C	2.86044700	-1.60112500	3.85165300
H	1.35022900	-1.59009100	2.31570200
C	4.92535200	-0.47058000	3.31449100

H	5.02227100	0.45498800	1.37911400
C	3.86343200	3.75521300	0.23318400
H	2.74049100	2.42579400	1.48445400
C	4.54312100	2.88456900	-1.91106700
H	3.97856700	0.85665400	-2.33270300
C	3.14767300	-2.29758300	-3.36846300
H	1.64769100	-0.94201400	-2.63150300
C	4.91460000	-2.85823900	-1.82083000
H	4.82579500	-1.91044900	0.10563600
C	4.14936700	-1.20672600	4.21248700
H	2.25121300	-2.17713300	4.54285400
H	5.92977000	-0.15825900	3.58792900
C	4.51174800	3.93219600	-0.99185200
H	3.83013200	4.56555700	0.95638800
H	5.04795100	3.00906100	-2.86552500
C	4.31782500	-3.00096200	-3.07382400
H	2.66816200	-2.41505000	-4.33644200
H	5.81830000	-3.41193200	-1.58039700
C	0.00468100	1.89746400	-0.00005300
C	0.15363800	2.61348700	-1.19519900
C	-0.14065300	2.62325100	1.18872300
C	0.15639600	4.01160100	-1.19844200
H	0.27295700	2.08675200	-2.13951000
C	-0.12927200	4.02211100	1.18135200
H	-0.27638300	2.10523800	2.13556900
C	0.02119900	4.74147500	-0.01038200
H	0.27195200	4.54210900	-2.14256000
H	-0.24820500	4.56096900	2.12017800
I	-0.00897800	-2.97273600	-0.02010700
H	4.98851600	4.88038900	-1.22605000
H	4.54831700	-1.46991100	5.18862300
H	4.75602300	-3.66465500	-3.81441000
C	0.06444700	6.25305700	-0.01397900
H	1.09734200	6.62585200	0.02541200
H	-0.39065500	6.66678200	-0.92124600
H	-0.46481000	6.67204300	0.84897800

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P	-2.27254700	0.05065500	0.29809600
C	-3.64059900	-0.68572700	-0.69711800
C	-3.14495200	1.36722200	1.29717500
C	-3.34312300	-1.66011700	-1.66490400
C	-4.98072500	-0.32132000	-0.48339700
C	-1.85063200	-1.19927400	1.61968500
Pd	-0.04941400	-0.40537600	-0.38583500
C	-3.46765700	1.17843500	2.65025700
C	-3.59812600	2.53966600	0.66287300
C	-4.36849400	-2.25002200	-2.40601300
H	-2.31475600	-1.97572200	-1.82423700
C	-5.99942100	-0.91521300	-1.22994900
H	-5.23742900	0.42044600	0.26343700
C	-0.96311000	-0.84979100	2.65626900
C	-2.36036800	-2.50583900	1.57044400
C	-1.23745400	1.32133100	-0.91176000
C	-4.18982100	2.14459900	3.35583400
H	-3.16115500	0.27583300	3.16392800
C	-4.32832500	3.49694300	1.36562500
H	-3.39276400	2.70412600	-0.38863700
C	-5.69692700	-1.87818400	-2.19401800
H	-4.11905800	-3.00464500	-3.14663900
H	-7.03112300	-0.62317900	-1.05315500
C	-0.59998500	-1.78843700	3.62178800
H	-0.56972100	0.16022500	2.71859800
C	-1.99716500	-3.43654400	2.54324900
H	-3.02581300	-2.80421500	0.76906800
C	-0.70508400	2.52484000	-0.40006400
C	-1.51224400	1.24336000	-2.29243800
C	-4.61883600	3.30767200	2.71865000
H	-4.41818200	1.97912700	4.40523900
H	-4.66920300	4.39244000	0.85315500
C	-1.11591200	-3.08466000	3.56723300
H	0.09181400	-1.50661400	4.41055900
H	-2.39985500	-4.44425100	2.49205100

C	-0.42107400	3.58853100	-1.24973200
H	-0.49928300	2.62321300	0.66022300
C	-1.23779500	2.32638700	-3.12940000
H	-1.93546700	0.33818400	-2.71216500
C	-0.68676800	3.51189600	-2.62741800
H	0.02459600	4.49029200	-0.83685500
H	-1.45178100	2.24163600	-4.19237900
P	2.32533300	0.26016600	0.23744600
C	3.52561700	0.22951600	-1.16810600
C	3.14439200	-0.79168100	1.52396100
C	2.52596700	1.96857000	0.92518200
C	3.01775500	0.11522700	-2.47003800
C	4.91577300	0.31174800	-0.98340700
C	4.08537500	-0.30061200	2.44489700
C	2.81501500	-2.15713000	1.55412800
C	1.98739000	2.25920700	2.19277400
C	3.08054600	3.02227700	0.18371000
C	3.88170000	0.10046300	-3.56802500
H	1.94705600	0.01150800	-2.61828400
C	5.77647800	0.29511500	-2.08026400
H	5.32798400	0.37889900	0.01925700
C	4.68320800	-1.15504600	3.37329700
H	4.34827900	0.75281100	2.44634900
C	3.42197000	-3.00919800	2.47867100
H	2.08776500	-2.55422600	0.85049200
C	2.01549100	3.55498200	2.70658600
H	1.55910700	1.45835300	2.79050300
C	3.10364600	4.32305800	0.69607500
H	3.50238600	2.82797500	-0.79699800
C	5.26002900	0.19197400	-3.37533900
H	3.47438900	0.00170100	-4.57057700
C	4.35434300	-2.51202500	3.39119000
H	5.40801600	-0.75873100	4.08022200
H	3.15879900	-4.06360600	2.48437900
C	2.57344900	4.59544100	1.95726900
H	1.60392200	3.75291600	3.69316200
H	3.54544700	5.12253600	0.10641300

H	5.93291800	0.17261100	-4.22886700
I	0.31694100	-2.94938900	-1.61761500
H	4.82193900	-3.17682400	4.11315800
H	2.59610700	5.60609900	2.35610400
H	6.85061900	0.35556100	-1.92448700
H	-6.49303800	-2.33843600	-2.77333100
H	-5.18144700	4.05793500	3.26769100
H	-0.82997700	-3.81708800	4.31700400
C	-0.41068800	4.68846800	-3.53227100
H	-0.34742000	4.38138200	-4.58101700
H	-1.20619600	5.44246400	-3.45813500
H	0.52880700	5.18519200	-3.26533500

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P	-2.42685400	-0.19391300	-0.02139800
C	-3.15252300	-0.52095700	-1.68738600
C	-3.25716200	1.38557700	0.47244000
C	-3.19212000	-1.42196100	1.12198500
C	-2.39718000	-1.20810500	-2.64937700
C	-4.45529800	-0.10551900	-2.01594300
C	-3.21602300	2.48877200	-0.39711300
C	-3.89455300	1.53007000	1.71299100
C	-2.57596600	-1.64227000	2.36346100
C	-4.37602500	-2.10642700	0.81889800
C	-2.93468400	-1.47774900	-3.90949300
H	-1.39807800	-1.55007000	-2.40127800
C	-4.98915700	-0.37870400	-3.27572100
H	-5.05108400	0.44143000	-1.29212500
C	-3.80046900	3.70036000	-0.03500100
H	-2.71986400	2.40537900	-1.35794100
C	-4.47581700	2.74813000	2.07544700
H	-3.94806500	0.69282200	2.40040000
C	-3.14525500	-2.51170900	3.29278200
H	-1.63819500	-1.14446400	2.59332200
C	-4.93586100	-2.98935800	1.74478600
H	-4.85903500	-1.96505200	-0.14231000

C	-4.22942900	-1.06481800	-4.22583800
H	-2.33769400	-2.01455600	-4.64173000
H	-5.99777800	-0.05170900	-3.51431500
C	-4.43181400	3.83531000	1.20420600
H	-3.75666900	4.54241800	-0.72029600
H	-4.96754800	2.83979900	3.04039300
C	-4.32655600	-3.18977200	2.98374700
H	-2.65591900	-2.67366000	4.24936400
H	-5.84830800	-3.52312300	1.49259700
H	-4.64534800	-1.27462000	-5.20781000
H	-4.88402700	4.78221600	1.48681000
H	-4.76376500	-3.87844700	3.70176400
Pd	-0.01154100	-0.27045900	-0.00877700
P	2.41094300	-0.26391800	0.03767500
C	3.08612200	-0.72664600	1.69351800
C	3.28915100	1.32552300	-0.33014400
C	3.18319100	-1.42954800	-1.16495500
C	2.30956500	-1.51345300	2.55813900
C	4.36923500	-0.32683400	2.10663500
C	3.25539400	2.37028100	0.60919800
C	3.95792800	1.53434900	-1.54491500
C	2.59412100	-1.56598400	-2.43123100
C	4.35276700	-2.14480500	-0.87711400
C	2.80651800	-1.89255800	3.80646400
H	1.32680200	-1.84725900	2.24200100
C	4.86156600	-0.70788200	3.35552200
H	4.98198200	0.29081600	1.45805100
C	3.87903700	3.58707000	0.34124500
H	2.73331500	2.23904500	1.55057000
C	4.57836400	2.75743400	-1.81327400
H	4.00588500	0.74247000	-2.28438400
C	3.17640900	-2.38412700	-3.39844600
H	1.66779200	-1.04328100	-2.65195500
C	4.92562000	-2.97588700	-1.84208100
H	4.81418400	-2.06616700	0.10172800
C	4.08073400	-1.49038100	4.20884300
H	2.19397200	-2.50534500	4.46221600

H	5.85496700	-0.39008500	3.66104900
C	4.54282700	3.78548000	-0.87230300
H	3.83979700	4.38265100	1.08020500
H	5.09546600	2.89861100	-2.75885400
C	4.34317400	-3.09336600	-3.10445900
H	2.70808200	-2.48237200	-4.37400600
H	5.82682900	-3.53402600	-1.60256500
C	0.01929400	1.76914500	0.08734500
C	0.18890600	2.54352000	-1.06310300
C	-0.12696900	2.43928900	1.31271000
C	0.21214100	3.94508700	-1.01066400
H	0.31921500	2.06613600	-2.03173900
C	-0.09662800	3.83077900	1.38394300
H	-0.27100300	1.87658000	2.23224500
C	0.07329600	4.59331900	0.22028000
H	0.35099900	4.50685600	-1.92827200
H	-0.20975300	4.34848100	2.33243100
I	-0.05929700	-3.09505200	-0.14689800
H	5.02886100	4.73512800	-1.08049800
H	4.46462200	-1.78388600	5.18237300
H	4.78995800	-3.74208300	-3.85315000
O	0.09124600	5.95376000	0.39486600
C	0.28110200	6.76639400	-0.74749700
H	0.27389700	7.79832100	-0.38964000
H	1.24254600	6.56041500	-1.23820100
H	-0.52655100	6.63449100	-1.48134600

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P	-2.33511200	0.00849300	0.26883400
C	-3.63720200	-0.44988900	-0.95531200
C	-3.24539500	1.16165400	1.43174500
C	-3.28776200	-1.20472300	-2.08753400
C	-4.98213900	-0.09197600	-0.76086300
C	-2.09555000	-1.47681600	1.37548200
Pd	-0.08242100	-0.42829800	-0.36348000
C	-3.66084300	0.75688200	2.70949800

C	-3.62205600	2.44282900	0.98578800
C	-4.26561800	-1.58159900	-3.00968800
H	-2.25839700	-1.52207200	-2.23272500
C	-5.95349900	-0.47312900	-1.68752900
H	-5.27912000	0.48037200	0.10991500
C	-1.22100400	-1.39272600	2.47561600
C	-2.73049600	-2.69673200	1.09949200
C	-1.17865400	1.42796400	-0.56610700
C	-4.40302400	1.61417300	3.52710200
H	-3.41092500	-0.23036900	3.07766900
C	-4.37391800	3.29149400	1.79661600
H	-3.33899600	2.77798800	-0.00584800
C	-5.59816500	-1.21487300	-2.81537600
H	-3.97711900	-2.16929100	-3.87662600
H	-6.98945400	-0.18877700	-1.52356300
C	-0.99013200	-2.50785300	3.28079900
H	-0.72817500	-0.45360100	2.70987300
C	-2.49972300	-3.80553100	1.91357800
H	-3.38926700	-2.79016600	0.24397800
C	-0.61985700	2.44966000	0.22739900
C	-1.32437600	1.66710900	-1.95352200
C	-4.75998600	2.88350200	3.07586700
H	-4.70324000	1.28034700	4.51670000
H	-4.65684000	4.27354400	1.42722800
C	-1.62868700	-3.71770200	3.00085200
H	-0.30567900	-2.43055200	4.12097700
H	-2.99716300	-4.74458400	1.68745000
C	-0.18012300	3.64617100	-0.33153700
H	-0.52150700	2.31244600	1.29847300
C	-0.90753300	2.86683100	-2.51530500
H	-1.77098800	0.91173200	-2.58981800
C	-0.32180100	3.85920300	-1.71187500
H	0.28000900	4.38938700	0.30848800
H	-1.01712600	3.05635200	-3.57850900
P	2.35629900	0.01053100	0.28302900
C	3.53421500	-0.01464600	-1.14179800
C	3.09716200	-1.19149100	1.48340500

C	2.71793100	1.63764600	1.09583700
C	3.00267700	0.07271000	-2.43658800
C	4.92599700	-0.11605100	-0.98270000
C	4.09431700	-0.84527100	2.41107800
C	2.64329300	-2.52015000	1.44002500
C	2.16684400	1.89176500	2.36567100
C	3.42797000	2.66897200	0.46390000
C	3.84649800	0.08147900	-3.54978000
H	1.92546400	0.10315000	-2.57009700
C	5.76681700	-0.11164900	-2.09538700
H	5.35462100	-0.20903800	0.01086500
C	4.62695200	-1.80621100	3.27256600
H	4.45218600	0.17812800	2.46975600
C	3.18417300	-3.47926700	2.29855000
H	1.87241700	-2.80381500	0.72835200
C	2.33065600	3.12887100	2.98749200
H	1.61722100	1.10638000	2.87958800
C	3.58824300	3.91225600	1.08425300
H	3.86735300	2.50116800	-0.51393200
C	5.22822200	-0.00865500	-3.38115300
H	3.41956000	0.14122300	-4.54722400
C	4.17446000	-3.12616000	3.21709100
H	5.39702400	-1.52197100	3.98554000
H	2.82501600	-4.50369700	2.24712800
C	3.04220800	4.14805400	2.34648500
H	1.90677000	3.29695300	3.97444800
H	4.15462000	4.69232000	0.58089500
H	5.88478400	-0.01081000	-4.24750100
I	0.18123600	-2.87813100	-1.77955400
H	4.59111800	-3.87385600	3.88732000
H	3.17420100	5.11186600	2.83120100
H	6.84213000	-0.19481100	-1.95932200
H	-6.35708600	-1.50941200	-3.53547900
H	-5.33913700	3.54853700	3.71090000
H	-1.44582500	-4.58793000	3.62513900
O	0.06253500	4.99075700	-2.35733100
C	0.70259300	6.01446900	-1.60731200

H	0.95189400	6.79742900	-2.32546500
H	0.03523500	6.42567700	-0.83866300
H	1.62011000	5.64740800	-1.13090700

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0 1

P	-2.44498800	-0.22815600	-0.03916500
C	-3.17224600	-0.62161600	-1.69083600
C	-3.22312100	1.40389700	0.36077100
C	-3.26388100	-1.36312600	1.16218200
C	-2.44604000	-1.41139200	-2.59524400
C	-4.44645500	-0.15850500	-2.06425000
C	-3.11504400	2.46254800	-0.55688300
C	-3.89185500	1.62830000	1.57258400
C	-2.66186700	-1.54483100	2.41669600
C	-4.47387000	-2.01320800	0.88749900
C	-2.98422000	-1.73342400	-3.84261100
H	-1.47070300	-1.79225200	-2.31104100
C	-4.98068100	-0.48368500	-3.31164600
H	-5.01961100	0.46523200	-1.38569500
C	-3.66685800	3.70916300	-0.27058000
H	-2.59010300	2.31704800	-1.49459900
C	-4.44039500	2.88127600	1.85924600
H	-3.99483600	0.82642100	2.29542000
C	-3.26993500	-2.34180100	3.38560500
H	-1.70488800	-1.07527100	2.62601000
C	-5.07349600	-2.82356200	1.85393900
H	-4.94691400	-1.90091700	-0.08254200
C	-4.25012300	-1.27106800	-4.20421800
H	-2.41032200	-2.34958800	-4.52946600
H	-5.96693700	-0.11824400	-3.58546700
C	-4.33150300	3.92339200	0.93980500
H	-3.56949900	4.51643800	-0.99110800
H	-4.95842000	3.03529900	2.80233200
C	-4.47737300	-2.98529100	3.10495700
H	-2.79094500	-2.47514200	4.35182200
H	-6.00643800	-3.33139700	1.62410900

H	-4.66626300	-1.52130000	-5.17661100
H	-4.75987300	4.89710100	1.16279100
H	-4.94519800	-3.61785000	3.85463900
Pd	-0.03281900	-0.39683600	-0.01114000
P	2.38621100	-0.47734900	0.02861200
C	3.05582000	-0.88208900	1.70179300
C	3.32589300	1.05623300	-0.41699100
C	3.10637600	-1.72767800	-1.12069500
C	2.24858800	-1.57151200	2.61931500
C	4.36381000	-0.52937000	2.07846600
C	3.33171500	2.14622500	0.46980000
C	4.00604600	1.17835200	-1.63718900
C	2.49750200	-1.90559700	-2.37235900
C	4.25663500	-2.46525200	-0.81195100
C	2.74005200	-1.90352000	3.88323400
H	1.24453300	-1.86622700	2.33301400
C	4.85114400	-0.86372300	3.34246900
H	5.00014800	0.01610200	1.38904800
C	4.00530300	3.32188400	0.14570300
H	2.80100900	2.08278100	1.41328800
C	4.67622900	2.36089900	-1.96222000
H	4.02418800	0.35022100	-2.33734800
C	3.04151000	-2.78724900	-3.30554200
H	1.58524500	-1.36473500	-2.60748300
C	4.79050700	-3.35981900	-1.74186500
H	4.73294400	-2.35484300	0.15665700
C	4.03990400	-1.55071600	4.24816700
H	2.10312900	-2.44106500	4.58044800
H	5.86430300	-0.58391600	3.61901700
C	4.68009900	3.43432300	-1.07280000
H	3.99765800	4.15295400	0.84573900
H	5.20088800	2.43461400	-2.91129300
C	4.18872200	-3.51892700	-2.99058200
H	2.55810300	-2.91670900	-4.27004900
H	5.67658000	-3.93460800	-1.48570200
C	0.07435600	1.64237100	-0.01500200
C	0.28471400	2.36053000	-1.19751600

C	-0.05883800	2.38051600	1.16585200
C	0.35206100	3.75540900	-1.20861200
H	0.41591700	1.83736200	-2.14230600
C	0.01600200	3.77572400	1.17341700
H	-0.22689900	1.87389700	2.11399200
C	0.20934900	4.50297000	-0.02023800
H	0.52622700	4.25457500	-2.15523000
H	-0.08843900	4.29102300	2.12156800
I	-0.18118300	-3.22455200	0.01167200
H	5.20519500	4.35206600	-1.32473600
H	4.41997200	-1.80798700	5.23339900
H	4.60540900	-4.21678500	-3.71196800
N	0.24257800	5.90521300	-0.03027400
C	0.36213600	6.60096600	1.23848100
H	0.34896200	7.67853500	1.05711500
H	-0.48779000	6.36814100	1.88949400
H	1.28726800	6.35444100	1.78909600
C	0.80243200	6.57156500	-1.19424700
H	0.20991800	6.35692400	-2.09082600
H	0.77148300	7.65232300	-1.03576500
H	1.84632600	6.27966400	-1.40117700

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0 1

P	-2.31793100	-0.14999100	0.32794600
C	-3.64062100	-0.35519900	-0.94252600
C	-3.19047200	0.78072900	1.70080000
C	-3.31002400	-0.88928000	-2.19930800
C	-4.97998200	-0.03051900	-0.66972100
C	-2.11999300	-1.82954400	1.13380000
Pd	-0.09009500	-0.46346000	-0.38124600
C	-3.55323500	0.16756900	2.90982400
C	-3.58122400	2.11720000	1.49072300
C	-4.30008000	-1.07938300	-3.16483100
H	-2.28538000	-1.18387500	-2.41169400
C	-5.96417600	-0.22404200	-1.64035600
H	-5.26294300	0.36966800	0.29675100

C	-1.20863600	-1.98682500	2.19499900
C	-2.81963000	-2.95082200	0.66526600
C	-1.16238500	1.40698400	-0.26585400
C	-4.25803800	0.87416200	3.88887300
H	-3.28946900	-0.86563200	3.09814200
C	-4.29679200	2.81579600	2.46150500
H	-3.33516100	2.61367000	0.55870800
C	-5.62708800	-0.74445900	-2.89089900
H	-4.02596800	-1.49791500	-4.12921500
H	-6.99590600	0.03189600	-1.41415300
C	-1.00807100	-3.23880300	2.77561000
H	-0.66095700	-1.12824200	2.57270600
C	-2.61834600	-4.19943400	1.25431300
H	-3.51089000	-2.85754300	-0.16429100
C	-0.61214400	2.29895400	0.68046200
C	-1.31282800	1.87772500	-1.58847700
C	-4.63050300	2.19904900	3.66994400
H	-4.51723000	0.37957700	4.82118000
H	-4.59147700	3.84476400	2.27326400
C	-1.71266000	-4.34915900	2.30572700
H	-0.29514900	-3.34547600	3.58855800
H	-3.16755100	-5.05943600	0.88086800
C	-0.20144300	3.57321800	0.32626900
H	-0.49322400	1.98790400	1.71268600
C	-0.91942100	3.16024500	-1.95135900
H	-1.74741300	1.23365800	-2.34480100
C	-0.34333900	4.04360000	-1.00517200
H	0.24748500	4.20006200	1.08671300
H	-1.05533700	3.46922100	-2.98081300
P	2.34606600	-0.16612000	0.33894800
C	3.51994400	0.08922800	-1.06580200
C	3.10143500	-1.57647900	1.27490900
C	2.70799900	1.27438300	1.44959100
C	2.99027600	0.49067600	-2.30091800
C	4.90663400	-0.09871900	-0.94822100
C	4.04977900	-1.40872000	2.29788800
C	2.70989200	-2.87844600	0.91980600

C	2.10936300	1.30585600	2.72296500
C	3.47415400	2.37922600	1.05076900
C	3.83206500	0.72027200	-3.39151600
H	1.91473200	0.59516200	-2.41083300
C	5.74553700	0.12726100	-2.03960600
H	5.33143500	-0.43142000	-0.00548300
C	4.59436700	-2.51704900	2.95006800
H	4.36167900	-0.41172000	2.59318600
C	3.26340000	-3.98324800	1.56914000
H	1.97627600	-3.02677900	0.13155700
C	2.28188100	2.39718300	3.57325600
H	1.51210800	0.46041300	3.05756100
C	3.63975600	3.47881800	1.89895200
H	3.95234300	2.38111000	0.07671700
C	5.20967200	0.54064900	-3.26239500
H	3.40690700	1.02113100	-4.34532700
C	4.20385100	-3.80716900	2.58619900
H	5.32585700	-2.36977500	3.74092100
H	2.95226000	-4.98308800	1.27815600
C	3.04722900	3.49295700	3.16187000
H	1.81955500	2.39290700	4.55720900
H	4.24635400	4.32015800	1.57218800
H	5.86418600	0.70956700	-4.11373900
I	0.16129900	-2.62021200	-2.22408200
H	4.62950800	-4.66937100	3.09345700
H	3.18332700	4.34474500	3.82310800
H	6.81687400	-0.02624500	-1.93752600
H	-6.39585100	-0.89357600	-3.64467000
H	-5.18098200	2.74677800	4.43027000
H	-1.55335700	-5.32595600	2.75414400
N	0.05186600	5.31728900	-1.35704200
C	0.77706800	6.13902600	-0.39995300
H	1.02715200	7.09359900	-0.86605500
H	0.16670400	6.35014800	0.48759600
H	1.70985100	5.66260400	-0.06467300
C	0.00208500	5.73211600	-2.74982100
H	-1.01946400	5.67103700	-3.14513400

H	0.32443900	6.77206500	-2.82523700
H	0.65360500	5.12171200	-3.39322100

P(*para*−H−phenyl)$_2$(*para*−F−phenyl)

0 1

P	-0.38500000	-0.00178200	-1.25285300
C	-1.16667200	-1.44633600	-0.39338300
C	-1.16276400	1.44790900	-0.39859800
C	1.33138500	-0.01302500	-0.55542000
C	-1.03063700	-2.70175600	-1.01119200
C	-1.90381000	-1.36223100	0.79792000
C	-2.34760500	1.95440700	-0.96024400
C	-0.63388700	2.08390000	0.73510000
C	2.32167700	0.66985200	-1.28302000
C	1.70801600	-0.67225100	0.62610200
C	-1.59491000	-3.84398800	-0.44349600
H	-0.48193100	-2.78241000	-1.94690000
C	-2.47916500	-2.50450900	1.36039400
H	-2.03328700	-0.40129700	1.28665000
C	-2.99735400	3.05079200	-0.39290300
H	-2.76019900	1.48774800	-1.85191300
C	-1.27819000	3.18857800	1.29715000
H	0.28707300	1.71873600	1.17942300
C	3.64331000	0.71703200	-0.84121700
H	2.05631900	1.16911300	-2.21161500
C	3.02841100	-0.64436800	1.07747700
H	0.96539100	-1.21765300	1.20022600
C	-2.32353500	-3.74744300	0.74446400
H	-1.47533500	-4.80666500	-0.93380900
H	-3.04940700	-2.42113800	2.28220400
C	-2.46214000	3.67243100	0.73770300
H	-3.91460500	3.42586000	-0.83944100
H	-0.85319100	3.67090700	2.17382800
C	3.97404300	0.05484700	0.33602200
H	4.41295800	1.24399900	-1.39579700
H	3.33007500	-1.15304100	1.98759500
F	5.25201000	0.08569000	0.76739300

H	-2.96135600	4.53284300	1.17542100
H	-2.77264000	-4.63452100	1.18322200

P(*para*−H−phenyl)(*para*−F−phenyl)$_2$

0 1

P	-0.00054200	0.38174500	1.30213300
C	1.44899000	-0.50061700	0.55944400
C	-0.00023200	1.98963700	0.38064600
C	-1.44149900	-0.51617700	0.56168300
C	1.97729100	-1.58369800	1.28392100
C	2.06762500	-0.14243400	-0.64941500
C	0.76858300	3.03242800	0.92620500
C	-0.73428800	2.23940300	-0.78915800
C	-2.68355300	-0.36457800	1.20315400
C	-1.37072500	-1.35482200	-0.56239600
C	3.07314900	-2.30549200	0.81319500
H	1.52805300	-1.86459600	2.23331100
C	3.17256900	-0.84716200	-1.12990800
H	1.68920600	0.69866700	-1.22202200
C	0.82085000	4.28192300	0.30851600
H	1.32627200	2.86371000	1.84469500
C	-0.69112900	3.49434000	-1.40168800
H	-1.34568500	1.45340100	-1.22204900
C	-3.82703200	-1.00739900	0.73121400
H	-2.75739300	0.26243300	2.08831100
C	-2.50308700	-2.01532700	-1.04166700
H	-0.42212400	-1.50112800	-1.06954400
C	3.65456900	-1.92104300	-0.39031100
H	3.48505000	-3.14389900	1.36545000
H	3.65973300	-0.57589300	-2.06107600
C	0.08833000	4.51659400	-0.85761000
H	1.42409100	5.07478200	0.74303400
H	-1.26790700	3.67167100	-2.30592300
C	-3.71489400	-1.82648900	-0.38712400
H	-4.78940400	-0.89316000	1.21942300
H	-2.45747800	-2.66831600	-1.90740200
F	4.72195500	-2.60591900	-0.84949300

F	-4.81274200	-2.46194400	-0.84555400
H	0.11970500	5.49239600	-1.33500300

P(*para*−F−phenyl)$_3$

0 1

P	0.00055200	-0.00083900	1.37575900
C	-0.37035700	1.62654200	0.57300100
C	-1.22398800	-1.13489000	0.57263500
C	1.59515000	-0.49324400	0.57250000
C	0.11351600	2.77932400	1.21670800
C	-1.12228100	1.78574600	-0.60226100
C	-2.46395600	-1.29190900	1.21696300
C	-0.98712800	-1.86484400	-0.60330800
C	2.35051300	-1.49043600	1.21472600
C	2.11047700	0.08038900	-0.60112200
C	-0.12143900	4.05180800	0.69833500
H	0.67925000	2.68130700	2.13998200
C	-1.37672700	3.05311400	-1.12901700
H	-1.52036500	0.91409900	-1.11241100
C	-3.44943900	-2.13047000	0.69858900
H	-2.66094800	-0.75364700	2.14086400
C	-1.95844000	-2.71777000	-1.13015200
H	-0.03364500	-1.77384400	-1.11429300
C	3.57007100	-1.92309700	0.69641400
H	1.98204000	-1.93281400	2.13703100
C	3.33539400	-0.33274200	-1.12774800
H	1.55627600	0.86283300	-1.11023800
C	-0.86733400	4.16612000	-0.47004500
H	0.25083400	4.94585600	1.18785400
H	-1.95991300	3.18658800	-2.03456500
C	-3.17673300	-2.83280700	-0.47055300
H	-4.40954100	-2.25483700	1.18875800
H	-1.78342500	-3.28884300	-2.03633700
C	4.04339400	-1.33227900	-0.47038100
H	4.15730800	-2.69380700	1.18498900
H	3.74353100	0.10726300	-2.03205100
F	-1.10953800	5.39314300	-0.97404600

F	5.22719500	-1.73588300	-0.97434100
F	-4.11919800	-3.65491600	-0.97468800

P(*para*−H−phenyl)$_2$(*para*−Cl−phenyl)

0 1

P	-0.76470300	-0.00261800	1.26806700
C	-1.47233500	-1.46539200	0.37800900
C	0.98316900	0.03241000	0.65148600
C	-1.53131300	1.42946700	0.37703900
C	-2.66150400	-2.00670500	0.89582100
C	-0.89097800	-2.07530900	-0.74476000
C	1.92579700	-0.73339300	1.35865000
C	1.43151000	0.79579800	-0.43688600
C	-1.49725200	2.67427400	1.02889800
C	-2.16167900	1.34427300	-0.87423400
C	-3.26482500	-3.11269100	0.29661300
H	-3.11401500	-1.56002300	1.77823600
C	-1.48887700	-3.18951300	-1.33815000
H	0.03431900	-1.68257000	-1.15554700
C	3.26832500	-0.75951500	0.98454800
H	1.60837200	-1.31707800	2.21947500
C	2.77486400	0.79064000	-0.81770600
H	0.72967400	1.40625900	-0.99656400
C	-2.05737900	3.80708300	0.43789700
H	-1.03258500	2.75360400	2.00909300
C	-2.73237100	2.47617600	-1.46102200
H	-2.21150900	0.39018200	-1.39026600
C	-2.67778400	-3.70849900	-0.82195900
H	-4.18626200	-3.51529000	0.70915100
H	-1.02412400	-3.65154500	-2.20547400
C	3.68139900	0.00820600	-0.10451900
H	3.98755800	-1.35707900	1.53469900
H	3.11394800	1.38551100	-1.65948600
C	-2.67870900	3.70973000	-0.80927200
H	-2.01826100	4.76208200	0.95534400
H	-3.21926600	2.39263300	-2.42937200
Cl	5.37455400	-0.00484100	-0.57890800

H	-3.12435300	4.58886000	-1.26715300
H	-3.14070700	-4.57622600	-1.28441300

P(*para*−H−phenyl)(*para*−Cl−phenyl)$_2$

0 1

P	-0.00146000	0.75965700	1.36406500
C	-1.42664300	-0.21120600	0.68562400
C	1.45938100	-0.15255900	0.68015700
C	-0.03475300	2.30012500	0.33656300
C	-2.68148300	-0.00183500	1.28245900
C	-1.33232000	-1.15647800	-0.34702200
C	1.96344200	-1.21791700	1.44563300
C	2.11345100	0.17184800	-0.51802100
C	0.65874800	3.41305400	0.84235400
C	-0.72089900	2.43247400	-0.88094800
C	-3.81365200	-0.69271200	0.85345300
H	-2.77728700	0.70932100	2.09942400
C	-2.45391700	-1.86561400	-0.78082900
H	-0.37478000	-1.34958500	-0.82073600
C	3.06906400	-1.95493500	1.02429200
H	1.48862300	-1.47518400	2.38944600
C	3.22925400	-0.54850300	-0.94851200
H	1.75541200	0.99749300	-1.12517100
C	0.68460100	4.61863800	0.14075200
H	1.17715200	3.33434900	1.79521100
C	-0.70415000	3.64283000	-1.57783000
H	-1.27458300	1.59011100	-1.28470500
C	-3.68732900	-1.62342900	-0.17798500
H	-4.77886300	-0.52154900	1.31826300
H	-2.37232900	-2.59665700	-1.57849800
C	3.69478100	-1.60991200	-0.17391000
H	3.44850200	-2.77820300	1.62029600
H	3.73111600	-0.29022200	-1.87522500
C	0.00065800	4.73651800	-1.07130600
H	1.22897200	5.46784400	0.54529500
H	-1.24303600	3.73003800	-2.51780500
Cl	5.09781900	-2.52240900	-0.71018600

Cl	-5.10415100	-2.51127400	-0.71933000
H	0.01125900	5.67767200	-1.61453900

P(*para*−Cl−phenyl)$_3$

0 1

P	0.00002300	-0.00008500	1.54868900
C	-0.20042300	1.65597900	0.74329400
C	-1.33394200	-1.00179300	0.74364600
C	1.53454200	-0.65449800	0.74376800
C	0.42018300	2.74915300	1.37148900
C	-0.95157400	1.89517400	-0.41756200
C	-2.59072600	-1.01107200	1.37228300
C	-1.16582200	-1.77161200	-0.41745200
C	2.17265500	-1.73645300	1.37380600
C	2.11540200	-0.12569800	-0.41898300
C	0.31814200	4.03833900	0.85116900
H	0.98922800	2.59400700	2.28496000
C	-1.07343600	3.18190700	-0.94502600
H	-1.45382000	1.07359700	-0.91891900
C	-3.65630800	-1.74397100	0.85214900
H	-2.74055200	-0.44087700	2.28592300
C	-2.21937300	-2.52043000	-0.94473700
H	-0.20332000	-1.79549700	-0.91909700
C	3.34026000	-2.29256800	0.85358600
H	1.75503100	-2.15008800	2.28857000
C	3.29075100	-0.66338600	-0.94636200
H	1.65323200	0.71820000	-0.92179400
C	-0.43256300	4.24297600	-0.30678800
H	0.80380600	4.87556200	1.34117300
H	-1.65815600	3.35947700	-1.84161000
C	-3.45849200	-2.49616300	-0.30603500
H	-4.62403200	-1.74220600	1.34247400
H	-2.08109100	-3.11534000	-1.84154700
C	3.89110600	-1.74673300	-0.30612700
H	3.82389200	-3.13016200	1.34495600
H	3.73542700	-0.24753700	-1.84448800
Cl	-4.78931600	-3.43475200	-0.96444100

Cl	5.36950000	-2.42947500	-0.96470200
Cl	-0.58031800	5.86465200	-0.96542500

P(*para*−H−phenyl)$_2$(*para*−COOMe−phenyl)

0 1

P	1.42987000	-0.02985200	-1.27194800
C	2.11643700	-1.43559300	-0.28027300
C	-0.36114400	-0.05788000	-0.79509200
C	2.07134800	1.46130500	-0.38015100
C	3.34065900	-1.97616100	-0.70853900
C	1.48982200	-1.99876200	0.84307100
C	-1.17348900	-1.02537100	-1.41655400
C	-0.96253000	0.85360000	0.08643200
C	2.08769900	2.66994200	-1.09705900
C	2.56244500	1.45388700	0.93489000
C	3.93303400	-3.03706800	-0.02267700
H	3.82891200	-1.56529300	-1.58917600
C	2.07745000	-3.06761500	1.52321700
H	0.53715300	-1.60523200	1.18486300
C	-2.53546400	-1.09356500	-1.14847700
H	-0.73175200	-1.72905700	-2.11813900
C	-2.33126200	0.79636700	0.34894800
H	-0.35966300	1.61323000	0.57344400
C	2.56096400	3.84403000	-0.50978800
H	1.73151800	2.68831100	-2.12453100
C	3.04691800	2.62621300	1.51875200
H	2.57153400	0.52865600	1.50311000
C	3.30080300	-3.58683200	1.09461900
H	4.88158100	-3.44081500	-0.36695300
H	1.57806300	-3.49428500	2.38937800
C	-3.12676800	-0.17989100	-0.26374300
H	-3.16317800	-1.84179600	-1.62141500
H	-2.78447500	1.50561700	1.03281800
C	3.04410000	3.82374600	0.80027100
H	2.56256800	4.77035000	-1.07829900
H	3.42680500	2.60319500	2.53702400
H	3.42262700	4.73462300	1.25655200

H	3.75566300	-4.41959500	1.62444700
C	-4.59158900	-0.29212900	-0.02007100
O	-5.31374500	-1.12627600	-0.53175700
O	-5.04672600	0.64444200	0.84534700
C	-6.45330600	0.58857900	1.12147400
H	-6.72106400	-0.37521800	1.56313400
H	-6.64582400	1.39970700	1.82458600
H	-7.03151700	0.72923400	0.20414600

P(*para*–H–phenyl)(*para*–COOMe–phenyl)$_2$

0 1

P	0.01151200	1.41917700	-1.41731600
C	1.46065000	0.40703300	-0.85910700
C	-1.42784100	0.38086100	-0.88530600
C	0.00535600	2.80805000	-0.19363700
C	2.72600300	0.79173000	-1.33942200
C	1.37288800	-0.72343900	-0.03138300
C	-1.81246400	-0.66420600	-1.74621500
C	-2.18390800	0.60512900	0.27566000
C	-0.63482500	3.99586500	-0.58512600
C	0.61039100	2.75504200	1.07246200
C	3.86880400	0.08230700	-0.98730700
H	2.81249700	1.65225600	-1.99841400
C	2.51524700	-1.44460000	0.31466000
H	0.40734800	-1.04545800	0.34542400
C	-2.90172500	-1.47370500	-1.44412600
H	-1.25387100	-0.84028300	-2.66244800
C	-3.28497300	-0.19644900	0.57577900
H	-1.91273400	1.41026800	0.95086600
C	-0.68673800	5.09567300	0.27246500
H	-1.08988600	4.05969700	-1.57073700
C	0.56742700	3.85894500	1.92615500
H	1.12080200	1.85089200	1.39077800
C	3.77139000	-1.04422300	-0.15852100
H	4.84702600	0.37791700	-1.35220600
H	2.43611700	-2.31653400	0.95455100
C	-3.64875900	-1.24387600	-0.28008000

H	-3.19795400	-2.28397000	-2.10228400
H	-3.86213200	-0.01433700	1.47563700
C	-0.08329700	5.02958700	1.52988800
H	-1.18834800	6.00584300	-0.04545400
H	1.04324400	3.80393900	2.90190300
H	-0.11405200	5.88810800	2.19549700
C	5.02649800	-1.77339900	0.17845300
O	6.13324600	-1.45493300	-0.21172500
C	-4.81228900	-2.13476900	-0.01032600
O	-5.15675600	-3.05346700	-0.72860700
O	4.80535100	-2.84327300	0.97693200
O	-5.45668100	-1.81271600	1.13529300
C	-6.58903200	-2.63539800	1.45161200
H	-6.28539500	-3.67927200	1.56856500
H	-6.98285500	-2.24260000	2.38959700
H	-7.34230000	-2.57292900	0.66157900
C	5.97672200	-3.58971200	1.33734100
H	6.68371300	-2.95714200	1.88098100
H	5.62169300	-4.40236600	1.97194300
H	6.46996300	-3.98524000	0.44529900

P(*para*−COOMe−phenyl)$_3$

0 1

P	-0.00070100	0.00028500	1.71921000
C	0.69301500	-1.51822200	0.91597300
C	0.96815800	1.36015100	0.91655400
C	-1.66260700	0.15917000	0.91609100
C	0.39756800	-2.74926500	1.52805500
C	1.51266100	-1.51395000	-0.22456800
C	2.18522700	1.71478700	1.52525000
C	0.55213100	2.07275400	-0.21997800
C	-2.58138700	1.02938600	1.52927100
C	-2.06842900	-0.55152900	-0.22534600
C	0.88612900	-3.94454800	1.00743200
H	-0.21739000	-2.76988800	2.42453700
C	2.01263100	-2.70672900	-0.74182600
H	1.76196600	-0.57598500	-0.71047600

C	2.97673000	2.73519200	1.00500400
H	2.51275600	1.18873900	2.41872300
C	1.33577300	3.10190500	-0.73673700
H	-0.38721200	1.82367600	-0.70330100
C	-3.86088800	1.20405100	1.00886400
H	-2.29201100	1.57129800	2.42641900
C	-3.35142800	-0.38794200	-0.74244500
H	-1.38051900	-1.23551700	-0.71215700
C	1.70132400	-3.92909000	-0.13294400
H	0.64796600	-4.88818800	1.48529000
H	2.64594000	-2.71104200	-1.62310000
C	2.55321900	3.43835100	-0.13145400
H	3.91555300	2.99669500	1.48014500
H	1.02087000	3.65620800	-1.61499000
C	-4.25475900	0.49167200	-0.13245600
H	-4.55930300	1.88123200	1.48758200
H	-3.67157700	-0.93322600	-1.62443600
C	2.26447200	-5.17185000	-0.73402700
O	2.97653900	-5.19737700	-1.71907900
O	1.89438400	-6.28506900	-0.06076000
C	2.40309000	-7.51819300	-0.59071000
H	3.49639100	-7.51823600	-0.58135100
H	2.01315900	-8.29968800	0.06217700
H	2.05800100	-7.66629300	-1.61752300
C	3.34841500	4.54727200	-0.73208500
O	3.01230800	5.18061600	-1.71389300
O	4.50069600	4.77843800	-0.06249300
C	-5.61260600	0.62557200	-0.73346900
O	-5.99031500	0.02299400	-1.71950100
O	-6.39228300	1.50095700	-0.05870900
C	5.31490500	5.83506500	-0.59241900
H	4.77069000	6.78323400	-0.57830700
H	6.18922400	5.88407500	0.05735400
H	5.61131900	5.61248100	-1.62099300
C	-7.71463400	1.67701200	-0.58845000
H	-8.26057200	0.72975900	-0.58111600
H	-8.19711300	2.40372600	0.06587300

H	-7.67051000	2.05207300	-1.61448600

P(*para*−H−phenyl)$_2$(*para*−CF$_3$−phenyl)

0 1

P	1.34588400	-0.00321300	-1.27756500
C	2.02323800	-1.46660100	-0.36663100
C	-0.42049200	0.02223900	-0.71088700
C	2.08450000	1.43248300	-0.37043100
C	3.20100600	-2.03965600	-0.87556100
C	1.43222700	-2.04318700	0.76909900
C	-1.31199100	-0.85106400	-1.35917500
C	-0.92788100	0.88347700	0.27318800
C	2.09445600	2.66769900	-1.04088500
C	2.65345500	1.35892400	0.91071900
C	3.78382200	-3.14574100	-0.25613700
H	3.66026200	-1.61824800	-1.76675500
C	2.00972500	-3.15681100	1.38289100
H	0.51526800	-1.62499300	1.17358900
C	-2.66230100	-0.87898200	-1.02286800
H	-0.94438100	-1.51670800	-2.13632400
C	-2.28293000	0.86830200	0.60583500
H	-0.26311400	1.57006700	0.78721700
C	2.63755400	3.80365900	-0.43957000
H	1.67812200	2.73704800	-2.04327200
C	3.20742100	2.49332600	1.50789300
H	2.66896200	0.41197500	1.44179000
C	3.18746300	-3.70835600	0.87439900
H	4.69644500	-3.57401300	-0.66223700
H	1.53820400	-3.59300000	2.25983000
C	-3.15175000	-0.01463800	-0.03828800
H	-3.33618900	-1.56721600	-1.52287200
H	-2.66179800	1.53488400	1.37401300
C	3.19763900	3.71792100	0.83688200
H	2.63311100	4.75138600	-0.97154200
H	3.64703600	2.41922700	2.49930400
H	3.63021500	4.59906000	1.30330800
H	3.63445800	-4.57579500	1.35272100

C	-4.62163600	0.00516400	0.27996200
F	-5.29667500	0.86114800	-0.52324300
F	-5.18849500	-1.21145800	0.11640900
F	-4.85772100	0.39537300	1.55262100

P(*para*–H–phenyl)(*para*–CF_3–phenyl)$_2$

0 1

P	0.00054500	1.25791000	-1.41259800
C	1.42943300	0.25687200	-0.78370200
C	-1.45704500	0.30592900	-0.77496100
C	0.04228300	2.74492000	-0.31184900
C	2.69352400	0.54657600	-1.32627900
C	1.32742600	-0.77778100	0.15847100
C	-1.90530000	-0.77232400	-1.55817300
C	-2.16192600	0.62011700	0.39654100
C	-0.58833900	3.90511700	-0.79215600
C	0.67335200	2.79109100	0.94171100
C	3.82444900	-0.16085200	-0.92773600
H	2.79290700	1.33344200	-2.06984100
C	2.45560500	-1.49778600	0.55245200
H	0.36348100	-1.02599900	0.59091900
C	-3.00979200	-1.52792400	-1.17383400
H	-1.38523200	-1.02199500	-2.47976200
C	-3.27682600	-0.12594200	0.77952900
H	-1.84075000	1.45089700	1.01646000
C	-0.60582700	5.07522100	-0.03195300
H	-1.06319400	3.89172600	-1.77038700
C	0.66469900	3.96510500	1.69746500
H	1.17755700	1.90996300	1.32736400
C	3.70581800	-1.18853400	0.01285800
H	4.79615700	0.08107500	-1.34602800
H	2.36536800	-2.29178400	1.28672900
C	-3.70020700	-1.20277800	-0.00230200
H	-3.33758400	-2.36539800	-1.78111400
H	-3.81065100	0.12253600	1.69119300
C	0.02300500	5.10767300	1.21437100
H	-1.10061600	5.96271600	-0.41729900

H	1.16020400	3.98648600	2.66461900
H	0.01887700	6.02065200	1.80372600
C	4.91521700	-1.99855200	0.39476700
C	-4.93442600	-1.97393600	0.38075500
F	6.04612800	-1.25900000	0.35922500
F	5.10321300	-3.04157200	-0.44710800
F	4.80466600	-2.51373800	1.63916800
F	-4.86951400	-3.26087300	-0.02713600
F	-6.04768400	-1.44216300	-0.17592200
F	-5.12963400	-1.98001600	1.71805500

P(*para*–CF_3–phenyl)$_3$

0 1

P	0.00093000	-0.00000600	1.75317500
C	1.66816700	0.07725600	0.94733700
C	-0.89969000	1.40528200	0.94738200
C	-0.76631600	-1.48212600	0.94727700
C	2.70379900	-0.64485100	1.56492900
C	1.96535100	0.82605500	-0.20163200
C	-0.79206400	2.66344000	1.56461400
C	-1.69716800	1.28793800	-0.20126000
C	-1.91411600	-2.01307600	1.56075500
C	-0.26254500	-2.11880300	-0.19719800
C	3.99419500	-0.63678500	1.04105900
H	2.49894200	-1.21681200	2.46644800
C	3.25872100	0.84670200	-0.72341100
H	1.18574500	1.39774600	-0.69492600
C	-1.44488700	3.77659700	1.04087000
H	-0.19359900	2.77253600	2.46560300
C	-2.36235300	2.39742600	-0.72291300
H	-1.80187600	0.32703000	-0.69479100
C	-2.55274800	-3.13442000	1.03713800
H	-2.31058900	-1.54583900	2.45873700
C	-0.89179900	-3.24923600	-0.71855800
H	0.62544100	-1.73330500	-0.68788400
C	4.27367400	0.11300100	-0.10497100
H	4.78257300	-1.20760000	1.52073400

H	3.47640300	1.42449200	-1.61585900
C	-2.23459600	3.64332400	-0.10472600
H	-1.34457200	4.74494300	1.52014900
H	-2.97171900	2.29682200	-1.61525500
C	-2.03907900	-3.75639000	-0.10441300
H	-3.44504900	-3.52755000	1.51328300
H	-0.49727500	-3.73038200	-1.60768400
C	-2.99586400	4.82941000	-0.63468300
C	-2.68705300	-5.00802500	-0.63393400
C	5.68153600	0.17844500	-0.63466800
F	6.36050200	-0.96518000	-0.39628500
F	6.38372900	1.18023800	-0.05685600
F	5.70721600	0.39803100	-1.96748900
F	-2.17335700	-6.11717300	-0.05388400
F	-2.50714500	-5.14181200	-1.96627400
F	-4.01745700	-5.02198000	-0.39826200
F	-4.21579600	4.93423600	-0.05908400
F	-3.19617300	4.74281800	-1.96798500
F	-2.34700500	5.98982300	-0.39389800

P(*para*−H−phenyl)$_2$(*para*−Ac−phenyl)

0 1

P	1.04777700	-0.03096600	-1.26558700
C	1.73367900	-1.47016700	-0.32330500
C	-0.71813500	-0.00676100	-0.70506700
C	1.77941200	1.42876100	-0.39141700
C	2.91256900	-2.05058200	-0.82088100
C	1.14854200	-2.02000600	0.82876500
C	-1.58059800	-0.97831600	-1.25100400
C	-1.26049300	0.95339200	0.16123200
C	1.82053200	2.63919800	-1.10418300
C	2.31324500	1.39509800	0.90649000
C	3.50200600	-3.13804100	-0.17520300
H	3.36716700	-1.64999700	-1.72395200
C	1.73266900	-3.11507800	1.46892900
H	0.23022700	-1.59587800	1.22384900
C	-2.92949300	-1.00062200	-0.92357600

H	-1.18559400	-1.72170500	-1.93965500
C	-2.61933100	0.93854400	0.48018900
H	-0.62097200	1.71685600	0.59224300
C	2.36017100	3.79051000	-0.52885400
H	1.43159300	2.67668100	-2.11916700
C	2.86378900	2.54400900	1.47797400
H	2.30453800	0.46729000	1.47052600
C	2.91141400	-3.67422500	0.97105000
H	4.41518000	-3.57278000	-0.57313000
H	1.26554000	-3.53110800	2.35794400
C	-3.47035300	-0.03874200	-0.05347200
H	-3.59502900	-1.75143600	-1.33720200
H	-3.00790600	1.69563600	1.15491800
C	2.88539000	3.74427100	0.76417700
H	2.38056600	4.71872700	-1.09388500
H	3.27655500	2.50066800	2.48269000
H	3.31566600	4.63682900	1.21067600
H	3.36352900	-4.52739100	1.46981500
C	-4.93461300	-0.10432300	0.25756900
O	-5.63603700	-0.98004600	-0.22731100
C	-5.53556300	0.93790300	1.18813700
H	-5.05731300	0.90965500	2.17468900
H	-5.39913500	1.94994400	0.78835700
H	-6.60200800	0.73392100	1.29827300

P(*para*–H–phenyl)(*para*–Ac–phenyl)$_2$

0 1

P	0.01483700	1.02267200	-1.39207200
C	1.43787700	0.02215600	-0.75327300
C	-1.45151200	0.08001900	-0.76667800
C	0.05966000	2.51420300	-0.29747700
C	2.71722500	0.35411000	-1.23941100
C	1.32063100	-1.05548100	0.13696900
C	-1.84887000	-1.05169300	-1.50576600
C	-2.22224300	0.45665600	0.34273100
C	-0.52411900	3.68914500	-0.79987000
C	0.65076600	2.54674500	0.97600100

C	3.84061900	-0.35423800	-0.83292500
H	2.82744100	1.17350700	-1.94588400
C	2.44814000	-1.77523600	0.53513000
H	0.34606500	-1.33843100	0.52172900
C	-2.96184400	-1.79358000	-1.13174900
H	-1.27900900	-1.34783500	-2.38355000
C	-3.34919200	-0.28046100	0.70945700
H	-1.94369800	1.32896500	0.92509200
C	-0.53407100	4.86182700	-0.04299400
H	-0.96745600	3.68517400	-1.79281700
C	0.64973400	3.72245700	1.72867500
H	1.11815200	1.65275500	1.37822000
C	3.72122500	-1.43262700	0.05914700
H	4.82887400	-0.09902500	-1.20153400
H	2.32467300	-2.60493600	1.22475600
C	-3.73079600	-1.41587000	-0.01845300
H	-3.26737600	-2.66982800	-1.69436100
H	-3.92583200	0.03713400	1.57310700
C	0.05523100	4.88080700	1.22261000
H	-0.99157600	5.76144500	-0.44599700
H	1.11466900	3.73365200	2.71111400
H	0.05757800	5.79546600	1.80945600
C	4.96645500	-2.16881500	0.45513700
O	6.05524400	-1.82695500	0.01853600
C	-4.92838800	-2.24716600	0.33315800
O	-5.21372400	-3.23550500	-0.32627300
C	-5.78163300	-1.83998300	1.52398000
H	-5.19124300	-1.82932100	2.44819600
H	-6.19365500	-0.83273300	1.38842300
H	-6.60035800	-2.55410200	1.62732100
C	4.85145300	-3.34741100	1.40876100
H	4.41366700	-3.04003100	2.36621100
H	4.20732800	-4.13108200	0.99204200
H	5.84895100	-3.75456300	1.58248500

P(*para*−Ac−phenyl)$_3$

0 1

P	0.00023800	0.00006200	1.63648100
C	-0.67478400	-1.52697000	0.83421100
C	1.66010700	0.17892800	0.83396400
C	-0.98471400	1.34800500	0.83396500
C	-1.78947300	-2.12404500	1.44684900
C	-0.12907000	-2.13857400	-0.30758900
C	2.73511900	-0.48555200	1.44808600
C	1.91623500	0.95513000	-0.30949600
C	-0.94770900	2.61099600	1.44860600
C	-1.78414800	1.18181200	-0.31010300
C	-2.35701300	-3.28415500	0.92402000
H	-2.21342900	-1.67911500	2.34386800
C	-0.68922000	-3.30366600	-0.82263800
H	0.73689700	-1.70153400	-0.79494000
C	4.02355300	-0.39678500	0.92522400
H	2.56226400	-1.07347300	2.34631200
C	3.20525400	1.05274100	-0.82464000
H	1.10425400	1.48463700	-0.79809400
C	-1.66889100	3.68232900	0.92565400
H	-0.35286100	2.75513600	2.34733800
C	-2.51327500	2.24922000	-0.82534400
H	-1.83592200	0.21401700	-0.79909900
C	-1.81081900	-3.89041400	-0.21712000
H	-3.22103100	-3.71814700	1.41781200
H	-0.27402700	-3.78095100	-1.70455800
C	4.27482100	0.37719000	-0.21752900
H	4.83189900	-0.92617500	1.42023600
H	3.41049000	1.64923900	-1.70783700
C	-2.46394300	3.51305400	-0.21770400
H	-1.61537200	4.64690100	1.42108200
H	-3.13182900	2.12880100	-1.70900500
C	-2.36950300	-5.14572300	-0.82153700
O	-1.85274300	-5.63948500	-1.81209100
C	5.64123000	0.52115500	-0.82206100
O	5.80989400	1.21372100	-1.81399700
C	-3.27187500	4.62433500	-0.82232400
O	-3.95538500	4.42421000	-1.81469300

C	6.80905200	-0.20935500	-0.17953400
H	6.95169900	0.11151100	0.85949300
H	6.63838600	-1.29261800	-0.16623600
H	7.71331100	0.00664000	-0.75096700
C	-3.58834400	-5.78960200	-0.18111700
H	-3.38437700	-6.07308500	0.85855500
H	-4.44019100	-5.09895200	-0.17012600
H	-3.85346600	-6.68076400	-0.75243900
C	-3.22382800	6.00079700	-0.17940500
H	-3.57382600	5.96356800	0.85934500
H	-2.20043500	6.39478300	-0.16520400
H	-3.86269800	6.67596000	-0.75113100

P(*para*–H–phenyl)$_2$(*para*–CN–phenyl)

0 1

P	0.65324300	-0.00246500	-1.24818600
C	1.33816100	-1.47758900	-0.36399500
C	-1.09478100	0.03704800	-0.62998500
C	1.43292900	1.42507200	-0.36461300
C	2.47091700	-2.08546800	-0.93090700
C	0.79686800	-2.02685700	0.80986900
C	-1.98468000	-0.91959800	-1.15420600
C	-1.59722900	1.00034700	0.25842900
C	1.47219800	2.64984000	-1.05273000
C	2.00301900	1.35438300	0.91632000
C	3.05886800	-3.20026900	-0.33196500
H	2.89040200	-1.68475900	-1.85069000
C	1.37916900	-3.14865300	1.40340100
H	-0.08549100	-1.58139200	1.25980400
C	-3.32533100	-0.93185700	-0.78939900
H	-1.62177300	-1.66455600	-1.85793900
C	-2.94211900	1.00601600	0.62301600
H	-0.93412200	1.75246700	0.67283700
C	2.04553200	3.78011700	-0.46831600
H	1.05538900	2.71541900	-2.05512400
C	2.58696800	2.48232600	1.49611200
H	1.99714900	0.41457000	1.46008200

C	2.51235600	-3.73556200	0.83621500
H	3.93613600	-3.65629500	-0.78307900
H	0.94678400	-3.56346400	2.31028900
C	-3.81553400	0.03717200	0.10454200
H	-4.00047700	-1.67845400	-1.19543800
H	-3.32007600	1.75457400	1.31241000
C	2.60628200	3.69748200	0.80781200
H	2.06396500	4.72012500	-1.01338500
H	3.02747000	2.41104400	2.48725900
H	3.06224500	4.57364000	1.26106100
H	2.96321700	-4.60934900	1.29897900
C	-5.19879600	0.03694800	0.48080400
N	-6.32117700	0.03543000	0.78761700

P(*para*–H–phenyl)(*para*–CN–phenyl)$_2$

0 1

P	-0.00174000	0.65233200	1.33752500
C	-1.41480700	-0.33706600	0.65671300
C	1.46996900	-0.24026100	0.65036400
C	-0.07478600	2.19623800	0.32260600
C	-2.68603700	-0.07959300	1.20117500
C	-1.29441700	-1.33581800	-0.32263200
C	1.89833800	-1.39017100	1.33926400
C	2.21314300	0.19291200	-0.45873400
C	0.49037000	3.35170300	0.88788600
C	-0.66685500	2.28605700	-0.94786700
C	-3.80770000	-0.77898400	0.77024000
H	-2.79740200	0.67538800	1.97526900
C	-2.40883500	-2.05163600	-0.75459800
H	-0.32430300	-1.56042300	-0.75389500
C	3.01722100	-2.10268800	0.92289500
H	1.35121000	-1.72918400	2.21543600
C	3.34367800	-0.50506500	-0.87791900
H	1.90915900	1.08219100	-1.00097400
C	0.48160100	4.56255700	0.19383600
H	0.93407500	3.30247200	1.87939600
C	-0.68412500	3.49981700	-1.63713300

H	-1.12056200	1.40829300	-1.39859500
C	-3.67431900	-1.77485700	-0.21292500
H	-4.78462800	-0.56956900	1.19401300
H	-2.30643700	-2.82176200	-1.51265000
C	3.75077600	-1.66056500	-0.19203600
H	3.33574200	-2.99153800	1.45799100
H	3.91259000	-0.16287800	-1.73667900
C	-0.10775700	4.63870000	-1.06954700
H	0.92513900	5.44655900	0.64386000
H	-1.14870000	3.55560700	-2.61804000
H	-0.12390200	5.58266400	-1.60748300
C	4.91194200	-2.38299900	-0.62315600
N	5.85293800	-2.97000700	-0.97426700
C	-4.82430400	-2.50724700	-0.65703700
N	-5.75786100	-3.09985000	-1.01843200

P(*para*−CN−phenyl)$_3$

0 1

P	-0.00035500	0.00067800	1.50074200
C	1.24199600	1.11564000	0.69675400
C	-1.58721600	0.51866500	0.69658000
C	0.34434400	-1.63268700	0.69671300
C	2.50575500	1.19787800	1.30859900
C	0.99192000	1.90105900	-0.43986600
C	-2.29333700	1.56855400	1.31064500
C	-2.13961500	-0.08860200	-0.44253800
C	-0.21250400	-2.76891700	1.31059000
C	1.14661500	-1.80771800	-0.44216900
C	3.50093400	2.02076200	0.79202900
H	2.71088500	0.61527500	2.20305800
C	1.97675900	2.73804500	-0.95949900
H	0.02190800	1.86352000	-0.92498100
C	-3.50412500	2.01764000	0.79396400
H	-1.89355800	2.03573700	2.20701200
C	-3.35721600	0.34443500	-0.96231000
H	-1.61947700	-0.90733300	-0.92918600
C	0.00358700	-4.04207500	0.79397000

H	-0.81734200	-2.65602500	2.20668200
C	1.37997400	-3.07880200	-0.96194300
H	1.59586600	-0.94808600	-0.92891800
C	3.23950700	2.79984600	-0.34809900
H	4.47445500	2.07452300	1.26847200
H	1.77571300	3.34284300	-1.83803700
C	-4.04532100	1.40374900	-0.34850400
H	-4.03991000	2.83117900	1.27221600
H	-3.77851800	-0.13046400	-1.84265000
C	0.80610000	-4.20412500	-0.34828900
H	-0.43358800	-4.91265100	1.27210300
H	2.00194900	-3.20636100	-1.84222600
C	-5.29806300	1.85365400	-0.88236900
N	-6.31313600	2.21984400	-1.31642600
C	1.04247100	-5.51411500	-0.88204900
N	1.23260700	-6.57636900	-1.31603200
C	4.25657600	3.65858400	-0.88182700
N	5.08225600	4.35350300	-1.31568000

P(*para*–H–phenyl)$_2$(*para*–NO$_2$–phenyl)

0 1

P	1.00728500	-0.02053800	-1.25142600
C	1.68117000	-1.48371100	-0.34096700
C	-0.75084000	0.01934800	-0.66597600
C	1.76739100	1.42256800	-0.37685600
C	2.80546700	-2.11344900	-0.90050800
C	1.14292800	-2.00101500	0.84907600
C	-1.60389500	-1.01399100	-1.10199800
C	-1.29758700	1.06267000	0.09879800
C	1.84441700	2.62798000	-1.09504500
C	2.28631000	1.38101500	0.92694400
C	3.38799400	-3.21914800	-0.27950200
H	3.22235600	-1.73732400	-1.83169400
C	1.71988400	-3.11333700	1.46481100
H	0.26671500	-1.53852300	1.29383900
C	-2.95342900	-1.02218500	-0.77022200
H	-1.20529100	-1.82353900	-1.70783400

C	-2.65131000	1.07461500	0.43113500
H	-0.66294300	1.87207200	0.44329500
C	2.40442200	3.76903400	-0.51809500
H	1.46770800	2.67003800	-2.11438600
C	2.85698300	2.51909200	1.49939100
H	2.25164900	0.45590500	1.49426300
C	2.84464700	-3.72252100	0.90407000
H	4.25849700	-3.69283900	-0.72539100
H	1.29016800	-3.50340800	2.38381500
C	-3.46080900	0.02917800	-0.00547500
H	-3.61541300	-1.81546300	-1.09512700
H	-3.08254300	1.87210800	1.02398000
C	2.91377600	3.71557200	0.78071500
H	2.45243900	4.69412500	-1.08631500
H	3.25772600	2.47078400	2.50859000
H	3.35912600	4.59982400	1.22871700
H	3.29135400	-4.58899500	1.38422300
N	-4.88693300	0.03331600	0.34650200
O	-5.30800200	0.97482100	1.01916800
O	-5.57667400	-0.90609700	-0.05115100

P(*para*−H−phenyl)(*para*−NO_2−phenyl)$_2$

0 1

P	0.01169500	0.96086300	-1.37551300
C	1.42156100	-0.05099300	-0.72119600
C	-1.46559800	0.05312500	-0.72245000
C	0.09225200	2.47425900	-0.31794100
C	2.69796700	0.24379900	-1.23608000
C	1.29416700	-1.09603100	0.20871400
C	-1.85558700	-1.11278000	-1.40954400
C	-2.25450300	0.49958400	0.34993000
C	-0.41554000	3.66125000	-0.87166500
C	0.63540600	2.50978300	0.97709800
C	3.82104000	-0.46608600	-0.82431200
H	2.81306800	1.03578800	-1.97138200
C	2.40824600	-1.82422200	0.62324000
H	0.32059800	-1.34746900	0.61598000

C	-2.98344600	-1.83049600	-1.02571000
H	-1.27210400	-1.46092500	-2.25803700
C	-3.39519800	-0.20135300	0.73842800
H	-1.97878100	1.39975600	0.88866200
C	-0.39764800	4.85179300	-0.14304700
H	-0.82129700	3.65272000	-1.88036900
C	0.66114500	3.70252800	1.70120100
H	1.04370600	1.60595600	1.41980800
C	3.65685100	-1.49528800	0.10187200
H	4.80852100	-0.24586000	-1.21081100
H	2.32447500	-2.63092600	1.34131200
C	-3.74038400	-1.35934700	0.04664000
H	-3.28961700	-2.73160100	-1.54271100
H	-4.01169500	0.13109100	1.56472800
C	0.14258800	4.87416300	1.14394900
H	-0.79619500	5.76127600	-0.58415900
H	1.08698800	3.71682500	2.70091700
H	0.16532600	5.80180900	1.70926600
N	-4.94120700	-2.10542800	0.45550800
O	-5.21917400	-3.12595300	-0.17324300
O	-5.59234100	-1.66369600	1.40152900
N	4.83726200	-2.25800300	0.53890100
O	5.92683700	-1.94453300	0.06080200
O	4.66208800	-3.16075300	1.35639500

P(*para*–NO_2–phenyl)$_3$

0 1

P	0.00042600	-0.00007100	1.63132700
C	-0.85374700	1.43468800	0.82778000
C	-0.81525700	-1.45716500	0.82823900
C	1.67000700	0.02215600	0.82783700
C	-0.68371700	2.69058600	1.43917100
C	-1.67849900	1.33836100	-0.30515300
C	-1.99011700	-1.93513200	1.43756700
C	-0.31784600	-2.12572900	-0.30255200
C	2.67255300	-0.75311300	1.43928600
C	1.99900300	0.78441400	-0.30521000

C	-1.30020200	3.82789900	0.92575600
H	-0.06804600	2.77876900	2.33040500
C	-2.31189600	2.46631000	-0.82429300
H	-1.83130400	0.37923000	-0.78874100
C	-2.66742600	-3.03724300	0.92401300
H	-2.37570500	-1.44415500	2.32716500
C	-0.97842200	-3.23802100	-0.82157300
H	0.59086200	-1.78058900	-0.78448900
C	3.96573000	-0.78804000	0.92584800
H	2.44099300	-1.33037800	2.33050300
C	3.29254200	0.76887000	-0.82430800
H	1.24479300	1.39627700	-0.78889100
C	-2.10920600	3.69508600	-0.20113400
H	-1.17508400	4.80111400	1.38423600
H	-2.95032400	2.40844300	-1.69746400
C	-2.14617200	-3.67401300	-0.20064600
H	-3.57461200	-3.41332200	1.38071200
H	-0.60775500	-3.76391900	-1.69301100
C	4.25528200	-0.02105700	-0.20106000
H	4.74596300	-1.38304900	1.38432100
H	3.56173800	1.35057800	-1.69753000
N	5.62385200	-0.04324300	-0.74750500
O	6.45212500	-0.74962300	-0.17541800
O	5.84987800	0.64463500	-1.74149900
N	-2.77432600	4.89134700	-0.74760100
O	-3.48381600	4.74294400	-1.74102700
O	-2.57641200	5.96193800	-0.17580000
N	-2.85021400	-4.84780300	-0.74708000
O	-3.87890700	-5.20849000	-0.17787200
O	-2.36521300	-5.39055200	-1.73828800

P(*para*–H–phenyl)$_2$(*para*–OMe–phenyl)

0 1

P	0.80541200	-0.00540300	-1.28792400
C	1.59390700	-1.39977000	-0.35391100
C	-0.96018300	-0.08194400	-0.74771000
C	1.43399100	1.48494700	-0.38089400

C	2.88172700	-1.79037900	-0.76063400
C	0.97861600	-2.10791500	0.68954200
C	-1.85381700	-0.80787000	-1.55960200
C	-1.47971800	0.55096200	0.38850800
C	1.30567300	2.72558600	-1.02909200
C	2.04874400	1.44951400	0.88040800
C	3.54481800	-2.84197400	-0.12834700
H	3.36572800	-1.26753700	-1.58264300
C	1.63748000	-3.16931600	1.31527900
H	-0.02062200	-1.83180000	1.01233700
C	-3.20015600	-0.91395600	-1.23871600
H	-1.48528600	-1.29353500	-2.46016400
C	-2.83511400	0.46367400	0.72004500
H	-0.82351100	1.13115700	1.03060700
C	1.75868700	3.89918800	-0.42652400
H	0.85083800	2.76942600	-2.01615500
C	2.51259600	2.62337600	1.47961400
H	2.16970000	0.50116500	1.39526500
C	2.92217800	-3.53669700	0.91163800
H	4.54213900	-3.12608600	-0.45428600
H	1.14466300	-3.70880500	2.12035800
C	-3.70211900	-0.27546700	-0.09393300
H	-3.88807800	-1.47521800	-1.86354600
H	-3.19810500	0.97277000	1.60592700
C	2.36617200	3.85050500	0.83054500
H	1.64750000	4.84947500	-0.94248000
H	2.98864200	2.57715400	2.45598600
H	2.72895800	4.76241900	1.29758600
H	3.43274100	-4.36322500	1.39896700
C	-5.60571800	0.20150800	1.26853700
H	-5.16101000	-0.17016800	2.20127400
H	-5.49039700	1.29264100	1.22493900
H	-6.66787400	-0.04958500	1.25101900
O	-5.03797300	-0.42913000	0.13191800

P(*para*–H–phenyl)(*para*–OMe–phenyl)$_2$

0 1

P	-0.00433800	0.68929300	1.31656200
C	-0.09115900	2.28614000	0.37593800
C	-1.39299600	-0.29550500	0.59524200
C	1.49502600	-0.10545000	0.58225400
C	0.70940600	3.34447600	0.84102800
C	-0.92857100	2.51695200	-0.72579400
C	-2.61816500	-0.27145900	1.27551700
C	-1.30479900	-1.08802500	-0.56466700
C	2.14238000	-1.08841300	1.34293000
C	2.04409800	0.21722300	-0.67327800
C	0.69117700	4.58811100	0.21067700
H	1.35029800	3.19157600	1.70666200
C	-0.95581200	3.76668100	-1.35091600
H	-1.56412700	1.71877200	-1.09698500
C	-3.72983700	-0.98428100	0.81928000
H	-2.71195500	0.31413700	2.18730800
C	-2.39725500	-1.81114100	-1.02676500
H	-0.36685200	-1.14546400	-1.10897000
C	3.28046400	-1.75111800	0.87673200
H	1.75477400	-1.34506400	2.32620700
C	3.18071800	-0.42536100	-1.14801500
H	1.57978100	0.98638600	-1.28350100
C	-0.14481100	4.80368800	-0.88811300
H	1.32157400	5.39183000	0.58267900
H	-1.61195300	3.92725200	-2.20288800
C	-3.62043600	-1.76155700	-0.34002300
H	-4.65926100	-0.93488500	1.37531000
H	-2.32977400	-2.42570400	-1.91947700
C	3.80577000	-1.41820500	-0.37767400
H	3.74822500	-2.50714300	1.49726200
H	3.60719200	-0.17560800	-2.11491200
C	-5.88961500	-2.49856900	-0.22210100
H	-6.32155100	-1.48951300	-0.18776600
H	-6.53768100	-3.14781400	-0.81379300
C	5.58928500	-2.99736300	-0.19965900
H	5.97183500	-2.61498900	0.75604200
H	4.93924600	-3.86120200	-0.00687500

H	6.42831000	-3.31016100	-0.82400100
O	4.91336000	-1.98869000	-0.93260800
O	-4.63056600	-2.50560100	-0.87501500
H	-5.81705400	-2.89342600	0.80000600
H	-0.16751500	5.77500500	-1.37531500

P(*para*–OMe–phenyl)$_3$

0 1

P	-0.00159800	0.00022400	1.43384500
C	0.84670400	1.43724400	0.63413900
C	-1.66976400	0.01575300	0.63340200
C	0.81957600	-1.45185900	0.63323500
C	1.97374500	1.96112400	1.28225100
C	0.42940000	2.06102700	-0.55630900
C	-2.69057200	0.71985300	1.28671500
C	-1.99732100	-0.64872400	-0.56312900
C	0.72111700	-2.68800500	1.28653500
C	1.55825600	-1.40288400	-0.56361800
C	2.68398500	3.04741100	0.76564700
H	2.30889900	1.51564400	2.21629500
C	1.11822900	3.14909300	-1.07891800
H	-0.44983900	1.69462500	-1.07788700
C	-3.98637800	0.79044600	0.76965200
H	-2.47525600	1.22575000	2.22527700
C	-3.28372600	-0.59736800	-1.08642200
H	-1.23729700	-1.21918300	-1.08880500
C	1.30835900	-3.84514500	0.76923200
H	0.17569500	-2.75484500	2.22527800
C	2.15745400	-2.54227500	-1.08714900
H	1.67144100	-0.45933300	-1.08925900
C	2.25418700	3.64831200	-0.42383800
H	3.55245300	3.41785500	1.29860900
H	0.79543400	3.63266800	-1.99609200
C	-4.28784400	0.12667100	-0.42581600
H	-4.74442300	1.34935700	1.30677700
H	-3.53809600	-1.11192400	-2.00825400
C	2.03349600	-3.77392300	-0.42643300

H	1.20402300	-4.78113100	1.30639800
H	2.72988900	-2.50497600	-2.00919600
C	-6.57044000	0.83009000	-0.39730900
H	-6.34380200	1.90197400	-0.32136200
H	-7.44496500	0.69136300	-1.03581200
C	2.56763400	-6.10197800	-0.39766100
H	3.01725100	-6.09327600	0.60426100
H	1.52637700	-6.44252200	-0.32100500
H	3.12522900	-6.78964400	-1.03635900
C	4.01199800	5.26560000	-0.39941700
H	3.78910100	5.64662900	0.60617400
H	4.82420500	4.52944700	-0.33255500
H	4.32843700	6.09396800	-1.03613400
O	2.85967300	4.71729100	-1.01759000
O	2.65715600	-4.83168900	-1.02140200
O	-5.51575700	0.11617600	-1.02071300
H	-6.78791600	0.43718900	0.60489200

P(*para*−H−phenyl)$_2$(*para*−Me−phenyl)

0 1

P	0.41385500	0.00097200	-1.25193200
C	1.17827600	-1.45335400	-0.39344300
C	-1.30743200	0.02101100	-0.57089500
C	1.20352000	1.43802800	-0.38695100
C	2.37815500	-1.95011900	-0.93141500
C	0.62496100	-2.10251500	0.72107600
C	-2.28806400	-0.68686700	-1.28604200
C	-1.70449400	0.70926000	0.58528400
C	1.10348700	2.69114800	-1.01579100
C	1.91224200	1.35003000	0.82131700
C	3.01872800	-3.04950200	-0.35966700
H	2.81001900	-1.47305200	-1.80837400
C	1.26008400	-3.21071600	1.28697500
H	-0.30732900	-1.74369500	1.14662500
C	-3.61101800	-0.72127000	-0.84951800
H	-2.01168300	-1.21624300	-2.19522200
C	-3.03308200	0.68053000	1.01211600

H	-0.97349100	1.27285200	1.15746400
C	1.67578300	3.82746700	-0.44389900
H	0.57634600	2.77425400	-1.96359100
C	2.49537600	2.48577300	1.38862600
H	2.01264400	0.39054400	1.31963100
C	2.45899600	-3.68471000	0.75143900
H	3.94806700	-3.41653800	-0.78763800
H	0.81634900	-3.70320600	2.14868700
C	-4.00919300	-0.03316500	0.30510100
H	-4.34834600	-1.28353900	-1.41880000
H	-3.31547700	1.22185000	1.91287500
C	2.37609800	3.72678100	0.76058200
H	1.58441700	4.78852000	-0.94348600
H	3.04292200	2.39918700	2.32386800
H	2.83137800	4.60896600	1.20303200
H	2.95098300	-4.54763900	1.19257300
C	-5.45214000	-0.03604600	0.75315400
H	-6.02886500	0.74594300	0.24084900
H	-5.93905700	-0.99249500	0.53309500
H	-5.53839000	0.14912600	1.82910000

P(*para*−H−phenyl)(*para*−Me−phenyl)$_2$

0 1

P	0.00040200	0.41718000	1.31222300
C	-1.43668800	-0.49612200	0.58475800
C	1.45524100	-0.46327000	0.57932100
C	-0.01256200	2.01469300	0.37092500
C	-2.68483400	-0.32952700	1.20841500
C	-1.36271500	-1.35898500	-0.51863600
C	1.98857300	-1.53899000	1.30915700
C	2.07419600	-0.11868100	-0.63145500
C	0.75896800	3.06705700	0.89370400
C	-0.76098700	2.24797600	-0.79310200
C	-3.81888100	-0.98503300	0.73311800
H	-2.76837400	0.32079500	2.07641100
C	-2.49957800	-2.02195600	-0.98399900
H	-0.41190000	-1.51634800	-1.01914800

C	3.08630600	-2.25474600	0.83546800
H	1.53870300	-1.81803900	2.25942300
C	3.18034000	-0.83210900	-1.09622600
H	1.69223800	0.71243400	-1.21690500
C	0.79958000	4.30917800	0.26041900
H	1.32856800	2.91116900	1.80718800
C	-0.72975300	3.49552400	-1.42137200
H	-1.37337800	1.45358600	-1.20891300
C	-3.74593600	-1.84832200	-0.36912000
H	-4.77424500	-0.83166700	1.23082200
H	-2.41593200	-2.68529300	-1.84259300
C	3.70628500	-1.91069200	-0.37393900
H	3.47416100	-3.08802400	1.41784800
H	3.64176100	-0.54554900	-2.03917700
C	0.05223800	4.52737600	-0.89952800
H	1.40547400	5.10929700	0.67792500
H	-1.31757300	3.65951300	-2.32116700
H	0.07444700	5.49743900	-1.38923400
C	-4.96789100	-2.59142700	-0.85654500
H	-5.12476500	-3.51650900	-0.28540900
H	-5.87543300	-1.98735400	-0.74734700
H	-4.87229900	-2.87263500	-1.91065000
C	4.92271200	-2.66064400	-0.86469400
H	5.84279900	-2.26371400	-0.41471000
H	4.87017600	-3.72407800	-0.60627700
H	5.03186600	-2.58053400	-1.95144800

P(*para*–Me–phenyl)$_3$

0 1

P	0.00010100	0.00148700	1.40016800
C	0.02392300	-1.66752300	0.59754700
C	1.43387800	0.85603700	0.59757300
C	-1.45713200	0.81442200	0.59678800
C	-0.70440700	-2.69219100	1.22523900
C	0.73541800	-1.98604800	-0.56857800
C	2.68649200	0.73208700	1.22239100
C	1.35348800	1.63665200	-0.56490800

C	-1.98699200	1.95216100	1.22878700
C	-2.08304500	0.36102000	-0.57364300
C	-0.73604100	-3.98032100	0.69486500
H	-1.25250500	-2.47791500	2.14013800
C	0.70930700	-3.28081000	-1.08982800
H	1.31478500	-1.21952500	-1.07466100
C	3.81827300	1.34810300	0.69240500
H	2.77544000	0.14626800	2.13467100
C	2.48844900	2.26107900	-1.08566200
H	0.39938100	1.75988900	-1.06870500
C	-3.08786100	2.62177500	0.69854100
H	-1.53173000	2.31673000	2.14700400
C	-3.19256700	1.02913600	-1.09488400
H	-1.70374700	-0.51983300	-1.08310200
C	-0.02470500	-4.29997100	-0.47017300
H	-1.31455700	-4.75260600	1.19776300
H	1.26880300	-3.50180000	-1.99670500
C	3.73889100	2.12922300	-0.46926200
H	4.77703400	1.22879000	1.19295900
H	2.39960000	2.86043400	-1.98960600
C	-3.71488200	2.16881300	-0.47085600
H	-3.47274000	3.50458900	1.20499500
H	-3.65944600	0.65777200	-2.00498900
C	4.95911700	2.83106200	-1.01838800
H	5.13216200	3.78737600	-0.50642100
H	5.86353800	2.22673500	-0.88635500
H	4.84977400	3.04899700	-2.08603300
C	-4.93449000	2.87138200	-1.02033900
H	-5.84943500	2.53413800	-0.51464700
H	-4.87026900	3.95623200	-0.88029600
H	-5.06271100	2.67451500	-2.08996400
C	-0.02527700	-5.70740400	-1.01994500
H	0.73991100	-6.32570200	-0.53122000
H	-0.98999500	-6.20115700	-0.85887500
H	0.18616500	-5.71833500	-2.09448300

P(*para*–H–phenyl)$_2$(*para*–NMe$_2$–phenyl)

0 1

P	1.07673000	-0.03393700	-1.28181600
C	1.83886300	-1.44857400	-0.35468800
C	-0.67037500	-0.02198900	-0.69656000
C	1.79695500	1.43637300	-0.40865800
C	3.12989100	-1.84724100	-0.74420200
C	1.19450300	-2.17213800	0.65986200
C	-1.63939400	-0.61788900	-1.52006400
C	-1.12164800	0.56248000	0.49777000
C	1.69325200	2.67791100	-1.05949800
C	2.45358900	1.38487100	0.83078100
C	3.76739600	-2.92039800	-0.12241100
H	3.63750900	-1.31261200	-1.54424000
C	1.82779200	-3.25551000	1.27488200
H	0.19268800	-1.88989700	0.96889700
C	-2.98408400	-0.65677900	-1.16803900
H	-1.33675400	-1.05806900	-2.46773600
C	-2.46367400	0.54160800	0.86234900
H	-0.41349600	1.05777000	1.15634200
C	2.21152700	3.83649600	-0.48108700
H	1.20519100	2.73407500	-2.02996100
C	2.98239000	2.54331100	1.40593500
H	2.55632100	0.43541700	1.34755500
C	3.11571600	-3.63027900	0.88951900
H	4.76784100	-3.20940800	-0.43449000
H	1.31214400	-3.80589200	2.05810900
C	-3.43437500	-0.08397400	0.04424700
H	-3.68529800	-1.12582300	-1.84797100
H	-2.75515000	1.02020000	1.78993900
C	2.86045700	3.77171100	0.75443300
H	2.11838800	4.78761500	-0.99925500
H	3.48948100	2.48401900	2.36591200
H	3.27357800	4.67165400	1.20261400
H	3.60655700	-4.47341400	1.36872000
N	-4.77034800	-0.13406900	0.41657600
C	-5.76070500	-0.60374700	-0.53720100
H	-5.81104500	0.01996700	-1.44418600

H	-5.55051600	-1.63449700	-0.84719600
H	-6.74433400	-0.59733700	-0.06329600
C	-5.22400600	0.64093300	1.55885800
H	-4.70523400	0.33329300	2.47485800
H	-5.07016800	1.72424100	1.42914400
H	-6.29062200	0.46319200	1.71008600

P(*para*–H–phenyl)(*para*–NMe$_2$–phenyl)$_2$

0 1

P	0.01953000	1.07512600	-1.39674700
C	1.44582300	0.10326800	-0.74293500
C	-1.45114500	0.14608800	-0.78094300
C	-0.00056200	2.57844900	-0.30692000
C	2.68319300	0.24128900	-1.39266600
C	1.38966000	-0.79789700	0.33134400
C	-2.05509300	-0.77748400	-1.64919800
C	-2.02895600	0.29575500	0.48963900
C	-0.89796500	3.60687100	-0.64616100
C	0.85439500	2.77524300	0.78758800
C	3.81492800	-0.45543900	-0.98273100
H	2.76472600	0.90703100	-2.24936400
C	2.50853500	-1.51163800	0.74961100
H	0.44817100	-0.95921700	0.84886100
C	-3.16372100	-1.52839200	-1.27362900
H	-1.64735900	-0.91598000	-2.64829200
C	-3.14375100	-0.43992900	0.88028600
H	-1.60412400	1.00612800	1.19352300
C	-0.95463800	4.78464900	0.09766600
H	-1.55705600	3.48187600	-1.50263900
C	0.80624800	3.96058400	1.52707000
H	1.56219900	1.99942800	1.06313200
C	3.76086800	-1.34812900	0.11262800
H	4.73980900	-0.30987700	-1.52825800
H	2.40097200	-2.20302100	1.57729900
C	-3.74839200	-1.37142200	0.00442100
H	-3.57981700	-2.23167900	-1.98535800
H	-3.54415900	-0.28323300	1.87516900

C	-0.09911200	4.96654200	1.18790700
H	-1.65951700	5.56496200	-0.17867800
H	1.47799300	4.09477100	2.37163300
H	-0.13511700	5.88790700	1.76356600
N	-4.87772200	-2.08958100	0.37761100
N	4.88975000	-2.03353300	0.54602500
C	-5.34167900	-3.17704500	-0.46626900
H	-5.61017800	-2.81360800	-1.46568700
H	-4.59196500	-3.97586000	-0.58653300
H	-6.23908200	-3.61476500	-0.02419300
C	-5.32517900	-2.04814400	1.75880200
H	-4.57235600	-2.43387700	2.46540100
H	-5.57725600	-1.02430200	2.06063300
H	-6.22925800	-2.65214100	1.85989500
C	4.74360200	-3.10194100	1.51953700
H	4.31327100	-2.72505300	2.45507200
H	4.10568800	-3.92599800	1.16055400
H	5.72944300	-3.50955600	1.75298400
C	6.09377300	-2.00687000	-0.26658900
H	5.94535800	-2.43998600	-1.26922000
H	6.45938800	-0.98086100	-0.39291000
H	6.87808600	-2.57462700	0.23842300

P(*para*–NMe$_2$–phenyl)$_3$

0 1

P	0.00011400	0.00026900	-1.66400200
C	-0.26375500	-1.64574700	-0.86586000
C	-1.29348600	1.05181200	-0.86599700
C	1.55762600	0.59465100	-0.86601500
C	0.25811000	-2.77878900	-1.51084600
C	-0.98118700	-1.86544700	0.31940800
C	-2.53631900	1.16462600	-1.51006500
C	-1.12458500	1.78467800	0.31816500
C	2.27890000	1.61190700	-1.51181300
C	2.10565200	0.08432600	0.32021500
C	0.10266800	-4.06070600	-0.99444200
H	0.79595500	-2.65850100	-2.44904800

C	-1.15592400	-3.14239100	0.84651200
H	-1.42711700	-1.02321700	0.84105200
C	-3.56892200	1.94007900	-0.99378100
H	-2.70150400	0.63728200	-2.44739300
C	-2.14324000	2.57435300	0.84514900
H	-0.17180800	1.75112400	0.83911800
C	3.46683300	2.11816100	-0.99536000
H	1.90649200	2.01673500	-2.45063300
C	3.29882700	0.57145900	0.84743500
H	1.59840900	-0.72198400	0.84259700
C	-0.60316400	-4.27767600	0.21136700
H	0.52427200	-4.89517800	-1.54242800
H	-1.73088900	-3.25007300	1.75896300
C	-3.40341800	2.66154500	0.21095100
H	-4.50298700	1.99065400	-1.54091700
H	-1.94865900	3.12735600	1.75677700
C	4.00668700	1.61656100	0.21137700
H	3.97938800	2.89958600	-1.54400700
H	3.67871600	0.12829500	1.76069100
N	5.18214000	2.13215100	0.75109500
N	-0.74433000	-5.55345600	0.75096500
N	-4.43778900	3.42157700	0.75036800
C	-5.62133700	3.67714100	-0.05232800
H	-5.40171600	4.22747800	-0.98211600
H	-6.11946000	2.73940000	-0.32522300
H	-6.33021200	4.26563300	0.53428500
C	-4.14990700	4.33316400	1.84421000
H	-3.76495100	3.79049700	2.71561000
H	-3.41440000	5.10965200	1.57648100
H	-5.07458800	4.82810400	2.14903600
C	5.99810200	3.02513700	-0.05347200
H	6.36646600	2.55570600	-0.98061500
H	5.43669700	3.92492300	-0.33109600
H	6.86121200	3.34615000	0.53385200
C	5.82619200	1.42740100	1.84611400
H	5.16313400	1.36716100	2.71713400
H	6.12982200	0.40152200	1.57970100

H	6.71759600	1.98005900	2.15094500
C	-0.37675600	-6.70640800	-0.05280700
H	-0.96569200	-6.79109800	-0.98105000
H	0.68369300	-6.66951300	-0.32847500
H	-0.53089400	-7.61443000	0.53429600
C	-1.67731200	-5.75932400	1.84532700
H	-1.39885500	-5.15491200	2.71661700
H	-2.71747400	-5.50977500	1.57817800
H	-1.64421100	-6.80765300	2.15004400

P(*para*–F–phenyl)$_2$(*para*–Cl–phenyl)

0 1

P	0.38123500	0.00107600	1.41948800
C	1.10673700	1.47931700	0.57302800
C	-1.32917800	-0.05912000	0.70807700
C	1.22462600	-1.41174600	0.57064400
C	2.23987000	2.06158000	1.16798700
C	0.58909600	2.06740000	-0.59271200
C	-2.31832200	0.69819300	1.35888700
C	-1.70804400	-0.83397400	-0.39830300
C	1.20884600	-2.65231500	1.23248400
C	1.89973200	-1.31968300	-0.65739300
C	2.85600200	3.18130100	0.61127400
H	2.64434400	1.63617500	2.08308000
C	1.18688600	3.19518100	-1.15717800
H	-0.29356700	1.64782100	-1.06546600
C	-3.63841300	0.70536700	0.91183900
H	-2.05600200	1.29008900	2.23257700
C	-3.02855700	-0.84750300	-0.85198400
H	-0.96993700	-1.43944500	-0.91509000
C	1.82470100	-3.77536900	0.68211100
H	0.71162500	-2.74108400	2.19525600
C	2.53129600	-2.43115900	-1.21727100
H	1.94084800	-0.37075000	-1.18308300
C	2.31472700	3.73120800	-0.54587200
H	3.73199800	3.63512100	1.06309700
H	0.79233800	3.65911500	-2.05548600

C	-3.98230300	-0.07278700	-0.19402700
H	-4.39388700	1.29647300	1.41864000
H	-3.31382700	-1.45123500	-1.70726800
C	2.47922300	-3.64315800	-0.53789500
H	1.81483200	-4.73664100	1.18542500
H	3.05885600	-2.36946900	-2.16371700
F	2.89657800	4.82050800	-1.08646500
F	3.08742000	-4.72024200	-1.07389800
Cl	-5.64610000	-0.08300700	-0.75995200

P(*para*–F–phenyl)(*para*–Cl–phenyl)$_2$

0 1

P	-0.00066100	0.38007200	1.47535700
C	1.47379500	-0.45073500	0.72118800
C	-0.07120400	1.99372300	0.57169300
C	-1.41114400	-0.55868800	0.72501200
C	1.99462600	-1.56507900	1.40111600
C	2.12340800	-0.02213700	-0.44610400
C	0.56530800	3.09102800	1.17801800
C	-0.73537700	2.19805000	-0.64904000
C	-2.66943500	-0.41298400	1.33360100
C	-1.30160700	-1.42276000	-0.37504800
C	3.11219200	-2.24853000	0.92486400
H	1.52359500	-1.90387600	2.32078700
C	3.25099300	-0.68805900	-0.93014900
H	1.75303800	0.84318300	-0.98694700
C	0.56272900	4.35069300	0.58068800
H	1.06648500	2.96034200	2.13386600
C	-0.75711800	3.45474200	-1.25521900
H	-1.24775300	1.37185900	-1.13226400
C	-3.79062900	-1.08651500	0.85181500
H	-2.77664400	0.23350000	2.20130700
C	-2.41230300	-2.11381200	-0.86295800
H	-0.34070000	-1.56638600	-0.85943400
C	3.73318500	-1.79988800	-0.24116300
H	3.50445600	-3.11016900	1.45462600
H	3.74929800	-0.34898300	-1.83239900

C	-0.10293100	4.51054700	-0.62991000
H	1.05332400	5.20215600	1.04083400
H	-1.27071500	3.62417300	-2.19613900
C	-3.64974200	-1.93556000	-0.24626800
H	-4.75868800	-0.96493900	1.32618600
H	-2.31904400	-2.78205000	-1.71271800
Cl	-5.05250500	-2.80074000	-0.85517600
Cl	5.15075800	-2.64416400	-0.84507600
F	-0.12061500	5.72658600	-1.21073300

P(*para*–F–phenyl)$_2$(*para*–COOMe–phenyl)

0 1

P	-1.03965200	-0.01994000	1.45632800
C	-1.76923900	-1.43869600	0.51799000
C	0.72638600	-0.05851400	0.89549700
C	-1.72657900	1.45677900	0.57727600
C	-2.96132500	-1.99013700	1.01904500
C	-1.20438500	-2.00657600	-0.63631900
C	1.56315700	-1.02577600	1.48414400
C	1.28927500	0.84653100	-0.01729900
C	-1.75283600	2.66675800	1.29266000
C	-2.24595200	1.44173100	-0.72763400
C	-3.58774600	-3.06082000	0.38264200
H	-3.40411100	-1.57995500	1.92318100
C	-1.81259400	-3.08521000	-1.27957600
H	-0.27614800	-1.61040500	-1.03652900
C	2.91101500	-1.10000200	1.15364800
H	1.15234700	-1.72435000	2.20925700
C	2.64430200	0.78297700	-0.34270600
H	0.66775900	1.60671100	-0.47939400
C	-2.25921100	3.83468400	0.72336700
H	-1.37626100	2.69573800	2.31211100
C	-2.76686000	2.59820800	-1.30857300
H	-2.25187900	0.51784600	-1.29762000
C	-2.99843200	-3.59207800	-0.75946800
H	-4.50869200	-3.49133800	0.76204300
H	-1.38245400	-3.53368100	-2.16934200

C	3.46364400	-0.19305000	0.23761700
H	3.55757600	-1.84789600	1.60098300
H	3.06795600	1.48737200	-1.05009300
C	-2.76079600	3.77809500	-0.57225100
H	-2.28103100	4.77296000	1.26797400
H	-3.17436600	2.59643100	-2.31445800
F	-3.59046700	-4.63403900	-1.37661400
F	-3.26288800	4.89845300	-1.12891200
C	4.91584700	-0.31196200	-0.07289600
O	5.65664800	-1.14691600	0.40956400
O	5.33333200	0.61870600	-0.96231900
C	6.72585200	0.55714400	-1.30325300
H	6.96944200	-0.40934600	-1.75280600
H	6.88784500	1.36482200	-2.01782500
H	7.34600700	0.69962400	-0.41411400

P(*para*−F−phenyl)(*para*−COOMe−phenyl)$_2$

0 1

P	-0.00999800	0.59532100	1.50136800
C	1.48551500	-0.22522300	0.77880400
C	-0.13686100	2.18076800	0.56383000
C	-1.39811600	-0.39733600	0.77455700
C	1.89471900	-1.43879000	1.36490500
C	2.27075900	0.32713100	-0.24571200
C	0.31031000	3.34324800	1.21517200
C	-0.66374900	2.29818600	-0.73417400
C	-2.67766800	-0.18099400	1.31950400
C	-1.25025900	-1.35679000	-0.24068000
C	3.03763500	-2.09939400	0.92708800
H	1.31428000	-1.87031900	2.17638400
C	3.42625400	-0.31621400	-0.68680200
H	1.98132600	1.26569200	-0.70602000
C	0.25358200	4.58840300	0.58978400
H	0.70326800	3.27567800	2.22627000
C	-0.73562600	3.53674900	-1.36975300
H	-1.02803200	1.41776800	-1.25493500
C	-3.78489400	-0.88359300	0.85536000

H	-2.80778700	0.54263000	2.11986700
C	-2.34816300	-2.07684000	-0.70928500
H	-0.27329700	-1.54807500	-0.67188800
C	3.79007200	-1.52324800	-0.09602400
H	3.35856700	-3.03615800	1.36585500
H	4.04003800	0.09811500	-1.47736300
C	-0.27176800	4.66265400	-0.69547000
H	0.59711500	5.49148300	1.08323400
H	-1.14367900	3.64130000	-2.36978100
C	-3.60081800	-1.82617900	-0.15530700
H	-4.77480200	-0.72346500	1.26457600
H	-2.24884100	-2.81802100	-1.49300300
F	-0.33993300	5.86020500	-1.30479700
N	-4.76443900	-2.58088600	-0.64877200
O	-5.85780700	-2.33803200	-0.13963200
O	-4.57163600	-3.40622700	-1.54055100
N	5.00645300	-2.20909500	-0.56116700
O	5.65277000	-1.67504700	-1.46164300
O	5.30061800	-3.27490000	-0.02139500

P(*para*−F−phenyl)$_2$(*para*−CF$_3$−phenyl)

0 1

P	-0.95632400	-0.00107600	1.44484700
C	-1.65922400	-1.47400700	0.57246000
C	0.78122000	0.03351300	0.79640700
C	-1.75278600	1.42184700	0.56994000
C	-2.79460900	-2.07268100	1.14596600
C	-1.12604000	-2.03887200	-0.59824300
C	1.70419100	-0.84203100	1.39619600
C	1.24012200	0.90509100	-0.20195300
C	-1.78101600	2.65112700	1.25191100
C	-2.35281300	1.34793500	-0.69780300
C	-3.39747500	-3.18716800	0.56448300
H	-3.21105300	-1.66477800	2.06354500
C	-1.71069300	-3.16054800	-1.18740500
H	-0.24124800	-1.60607800	-1.05497300
C	3.03755100	-0.86199400	0.99810100

H	1.37507600	-1.51566100	2.18367000
C	2.57873900	0.89764900	-0.59652300
H	0.55096700	1.59443700	-0.67883200
C	-2.36733000	3.78153900	0.68408900
H	-1.34258400	2.72510100	2.24401600
C	-2.95407600	2.46637700	-1.27589600
H	-2.35928900	0.40771700	-1.24038400
C	-2.84109600	-3.71399900	-0.59610000
H	-4.27485500	-3.65419200	0.99978800
H	-1.30451900	-3.60674400	-2.08947500
C	3.47862400	0.01245000	-0.00051600
H	3.73590900	-1.55197900	1.46071400
H	2.91998300	1.57239400	-1.37502800
C	-2.94736400	3.66733700	-0.57463700
H	-2.39120700	4.73436900	1.20268600
H	-3.42415800	2.41897900	-2.25293600
F	-3.40999400	-4.79751900	-1.16055100
F	-3.52674400	4.75080000	-1.12843300
C	4.93294500	0.03855600	-0.38493600
F	5.50279300	-1.18263500	-0.27652500
F	5.64464900	0.87345200	0.40809100
F	5.11136500	0.45921800	-1.65688700

P(*para*–F–phenyl)(*para*–CF_3–phenyl)$_2$

0 1

P	-0.00050200	0.90582700	-1.55805600
C	-1.46249900	0.01378000	-0.84839400
C	0.05959200	2.47069200	-0.57484500
C	1.42318600	-0.05392200	-0.85691100
C	-1.90592800	-1.12888800	-1.53762000
C	-2.17685400	0.43038900	0.28454300
C	-0.53044400	3.60808000	-1.15320400
C	0.67018100	2.60056200	0.68394900
C	2.68614200	0.17587000	-1.42962200
C	1.31718100	-1.00356300	0.17067100
C	-3.01463400	-1.84670900	-1.09758600
H	-1.37860900	-1.45955000	-2.42912000

C	-3.29624800	-0.27805800	0.72234100
H	-1.86024400	1.31226200	0.83194100
C	-0.53342500	4.83647100	-0.49349300
H	-0.98978100	3.53412200	-2.13564900
C	0.68529900	3.82449600	1.35283800
H	1.14536000	1.74164200	1.14783700
C	3.81287900	-0.50671200	-0.97880800
H	2.78802800	0.89515700	-2.23840800
C	2.44108600	-1.69830700	0.61835200
H	0.35342400	-1.20528200	0.62716100
C	-3.71456600	-1.41912100	0.03487600
H	-3.33840700	-2.73423400	-1.63153000
H	-3.83737500	0.05041700	1.60384300
C	0.07865800	4.92279200	0.75213100
H	-0.98788300	5.71901600	-0.93151300
H	1.15756700	3.93732700	2.32337400
C	3.69059000	-1.44882300	0.04685400
H	4.78396200	-0.31175400	-1.42216300
H	2.34819600	-2.42591600	1.41819200
F	0.09078600	6.10709700	1.39376700
C	4.89383900	-2.23692400	0.49014700
C	-4.95302200	-2.15353800	0.47310900
F	4.79420400	-2.62416100	1.78093500
F	6.03489000	-1.52353600	0.36554600
F	5.05180600	-3.36121000	-0.24640700
F	-5.16786100	-2.03049700	1.80154200
F	-6.05843900	-1.68207200	-0.14921000
F	-4.87903100	-3.47362000	0.19281600

P(*para*–F–phenyl)$_2$(*para*–Ac–phenyl)

0 1

P	-0.66042100	-0.02148100	1.43164700
C	-1.37697600	-1.47798300	0.54304700
C	1.07403100	0.00852900	0.78125000
C	-1.45299500	1.41806200	0.58039400
C	-2.51355600	-2.07749100	1.11302900
C	-0.85426700	-2.02765900	-0.63968400

C	1.96735300	-0.95831300	1.28440800
C	1.56749400	0.97067600	-0.11138300
C	-1.51233300	2.62625500	1.29669100
C	-2.01883600	1.37545700	-0.70451600
C	-3.12769600	-3.17811400	0.51698700
H	-2.92183800	-1.68148900	2.03942500
C	-1.45024000	-3.13539700	-1.24353000
H	0.03204600	-1.59443700	-1.09300800
C	3.29822800	-0.97405600	0.88983300
H	1.61137400	-1.70304600	1.99262700
C	2.90886500	0.96221700	-0.49807800
H	0.90409900	1.73135600	-0.51004000
C	-2.09642000	3.76708900	0.74683700
H	-1.10033900	2.67504500	2.30156700
C	-2.61716100	2.50385800	-1.26538700
H	-2.00101700	0.45133100	-1.27389800
C	-2.58154400	-3.69004400	-0.65499100
H	-4.00590300	-3.64597300	0.94972900
H	-1.05208100	-3.57024500	-2.15467600
C	3.78995000	-0.01038800	-0.00700700
H	3.98748300	-1.72102200	1.27019900
H	3.25961600	1.72080300	-1.19148700
C	-2.64203700	3.68384700	-0.52932700
H	-2.14464500	4.70387600	1.29230600
H	-3.06136600	2.48044700	-2.25533800
F	-3.16152200	-4.76010900	-1.23387800
F	-3.21870000	4.77713300	-1.06687500
C	5.23797000	-0.06942600	-0.39051800
O	5.96520300	-0.94203300	0.06011200
C	5.78740600	0.97488000	-1.34960600
H	5.26019200	0.94562200	-2.31084000
H	5.66801500	1.98622700	-0.94258000
H	6.84762700	0.77476100	-1.51350600

P(*para*−F−phenyl)(*para*−Ac−phenyl)$_2$

0 1

P	-0.01361100	0.63112900	1.50959100

C	1.49388000	-0.16615300	0.78719100
C	-0.15630600	2.21591100	0.56766500
C	-1.38517800	-0.38135700	0.78132800
C	1.95079000	-1.34239800	1.40753500
C	2.23791600	0.35719600	-0.28338000
C	0.33225200	3.37589500	1.19308700
C	-0.73550400	2.33601700	-0.70700900
C	-2.65670600	-0.23693100	1.36176100
C	-1.23210500	-1.29308900	-0.27759900
C	3.09855400	-1.98983900	0.95743700
H	1.40381700	-1.75375500	2.25272500
C	3.39205000	-0.28348300	-0.72506100
H	1.91288100	1.26904400	-0.77403100
C	0.26618000	4.61932800	0.56505600
H	0.76642800	3.30736700	2.18726200
C	-0.81836800	3.57334600	-1.34506500
H	-1.13146100	1.45779000	-1.20774300
C	-3.74662300	-0.96356500	0.88777900
H	-2.79266100	0.44730000	2.19583400
C	-2.31920300	-2.02595600	-0.74463600
H	-0.25825100	-1.43068500	-0.73717500
C	3.83653600	-1.46586700	-0.11530300
H	3.42034000	-2.90009000	1.45410400
H	3.97005900	0.11527000	-1.55266100
C	-0.31194100	4.69551700	-0.69710000
H	0.64252100	5.51974200	1.03932300
H	-1.26591800	3.67846300	-2.32811000
C	-3.59041600	-1.87029200	-0.17158800
H	-4.71658000	-0.82617800	1.35587700
H	-2.20840500	-2.73000900	-1.56323700
F	-0.39057200	5.89331200	-1.30889300
C	5.08535100	-2.11089200	-0.63975500
O	5.69464500	-1.61443400	-1.57514600
C	-4.72267600	-2.68769400	-0.72040900
O	-4.53588900	-3.46494100	-1.64428900
C	-6.10531600	-2.53120000	-0.10822900
H	-6.09553000	-2.78494500	0.95871700

H	-6.46106200	-1.49737500	-0.19450600
H	-6.79594700	-3.19530800	-0.63062500
C	5.57875400	-3.39278000	0.01177900
H	5.79501100	-3.23681100	1.07562500
H	4.82428700	-4.18594600	-0.05506600
H	6.48820200	-3.71591500	-0.49754600

P(*para*–F–phenyl)$_2$(*para*–CN–phenyl)

0 1

P	0.27098100	0.00124100	1.39701200
C	0.94417300	1.50695600	0.55985400
C	-1.43643400	-0.09856400	0.68067200
C	1.15789200	-1.38665700	0.55555500
C	2.00670800	2.16919100	1.19901400
C	0.45924600	2.03353100	-0.64951100
C	-2.38644200	0.82880100	1.14919400
C	-1.85509600	-1.08236700	-0.22824300
C	1.24733500	-2.60121000	1.25814800
C	1.76659400	-1.29865000	-0.70737300
C	2.58632900	3.30999500	0.64544300
H	2.38352900	1.79070400	2.14577200
C	1.02101100	3.18002600	-1.21186300
H	-0.37034000	1.55144400	-1.15773900
C	-3.70416600	0.79307700	0.71006700
H	-2.08973100	1.58864500	1.86788600
C	-3.17653500	-1.13588600	-0.66749900
H	-1.14522200	-1.81371100	-0.60021300
C	1.90276400	-3.70566900	0.71478100
H	0.80282300	-2.68382200	2.24680600
C	2.43596300	-2.39004100	-1.26069400
H	1.72734900	-0.36795200	-1.26476900
C	2.07991400	3.79739600	-0.55450100
H	3.40749400	3.82652500	1.13145000
H	0.65188200	3.59704900	-2.14329200
C	-4.11002800	-0.19567700	-0.20434300
H	-4.42617300	1.51735400	1.07358000
H	-3.48943400	-1.90001500	-1.37216900

C	2.48913200	-3.57851100	-0.53962600
H	1.97472100	-4.64726300	1.24913400
H	2.91365900	-2.33175400	-2.23340300
F	2.62611400	4.90485300	-1.09284600
F	3.13437800	-4.63544900	-1.06983500
C	-5.46928300	-0.24446200	-0.65733200
N	-6.57202400	-0.28259200	-1.02636400

P(*para*–F–phenyl)(*para*–CN–phenyl)$_2$

0 1

P	0.00000200	0.26828300	1.44211500
C	1.51047500	-0.49356700	0.68573600
C	-0.16361800	1.87869700	0.55177300
C	-1.36595300	-0.73541000	0.68949100
C	1.98744700	-1.68098400	1.27159600
C	2.23813600	0.07082500	-0.37327600
C	0.30601400	3.02413900	1.21768100
C	-0.73973800	2.03160700	-0.72106800
C	-2.64394800	-0.59067600	1.25904500
C	-1.20225400	-1.64164900	-0.37030700
C	3.13873300	-2.30243000	0.80152100
H	1.45273200	-2.12227100	2.10906000
C	3.40060800	-0.53540300	-0.84481300
H	1.89748400	0.99143500	-0.83545000
C	0.22468800	4.28599800	0.62990100
H	0.73637800	2.92970000	2.21132500
C	-0.83743500	3.28760500	-1.31872600
H	-1.12298200	1.16533900	-1.25176500
C	-3.73159900	-1.30948100	0.77586400
H	-2.78756300	0.09017400	2.09415500
C	-2.28198400	-2.37602800	-0.85601200
H	-0.22528600	-1.77952800	-0.82211800
C	3.85624300	-1.72912800	-0.26306400
H	3.49457400	-3.22115100	1.25664900
H	3.95704300	-0.09172000	-1.66438800
C	-0.34926700	4.39511700	-0.63196700
H	0.58552700	5.17573900	1.13517100

H	-1.28391400	3.41893400	-2.29902400
C	-3.55534700	-2.21158400	-0.28772400
H	-4.71431900	-1.18754200	1.21991800
H	-2.14646400	-3.07418400	-1.67601200
F	-0.44182600	5.60961600	-1.20458800
C	-4.66971500	-2.96356200	-0.78663400
N	-5.57434300	-3.57204400	-1.19235900
C	5.05016300	-2.35766100	-0.74841300
N	6.01767200	-2.86856600	-1.14357900

P(*para*–F–phenyl)$_2$(*para*–NO$_2$–phenyl)

0 1

P	0.62116000	0.01545300	1.41236500
C	1.31268900	1.49727200	0.54961200
C	-1.10425100	-0.04521400	0.73817100
C	1.45249700	-1.40373500	0.56733200
C	2.39106400	2.14970900	1.17199400
C	0.83090700	2.01271500	-0.66607600
C	-1.99618200	0.96572300	1.14793100
C	-1.59292500	-1.08433300	-0.07004900
C	1.55390300	-2.60321900	1.29353300
C	2.00755100	-1.35342000	-0.72222100
C	2.98855100	3.27029800	0.59647300
H	2.76621100	1.77970000	2.12269200
C	1.41071900	3.13889900	-1.25029100
H	-0.01064300	1.53850900	-1.16190500
C	-3.32732500	0.95665200	0.74840400
H	-1.64347900	1.77081900	1.78727300
C	-2.92792300	-1.11348600	-0.47077600
H	-0.92795800	-1.87742500	-0.39477300
C	2.16906800	-3.72991400	0.74826300
H	1.15087800	-2.65648200	2.30175500
C	2.63607200	-2.46715100	-1.27810000
H	1.95894700	-0.43481100	-1.29857000
C	2.48466900	3.74712100	-0.60871100
H	3.82184700	3.77934400	1.06950400
H	1.04434600	3.54723900	-2.18661400

C	-3.77638700	-0.08960800	-0.05840400
H	-4.01908000	1.73251800	1.05268500
H	-3.31479500	-1.90798900	-1.09728900
C	2.70257800	-3.64003500	-0.53253000
H	2.24992300	-4.66031200	1.30060400
H	3.07223700	-2.43842600	-2.27139600
F	3.04826200	4.83478100	-1.16828800
F	3.30859400	-4.71824200	-1.06542900
N	-5.18343600	-0.11190000	-0.48220300
O	-5.90814700	0.80872900	-0.10421900
O	-5.55249400	-1.04868600	-1.19051900

P(*para*–F–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

P	-0.00999800	0.59532100	1.50136800
C	1.48551500	-0.22522300	0.77880400
C	-0.13686100	2.18076800	0.56383000
C	-1.39811600	-0.39733600	0.77455700
C	1.89471900	-1.43879000	1.36490500
C	2.27075900	0.32713100	-0.24571200
C	0.31031000	3.34324800	1.21517200
C	-0.66374900	2.29818600	-0.73417400
C	-2.67766800	-0.18099400	1.31950400
C	-1.25025900	-1.35679000	-0.24068000
C	3.03763500	-2.09939400	0.92708800
H	1.31428000	-1.87031900	2.17638400
C	3.42625400	-0.31621400	-0.68680200
H	1.98132600	1.26569200	-0.70602000
C	0.25358200	4.58840300	0.58978400
H	0.70326800	3.27567800	2.22627000
C	-0.73562600	3.53674900	-1.36975300
H	-1.02803200	1.41776800	-1.25493500
C	-3.78489400	-0.88359300	0.85536000
H	-2.80778700	0.54263000	2.11986700
C	-2.34816300	-2.07684000	-0.70928500
H	-0.27329700	-1.54807500	-0.67188800
C	3.79007200	-1.52324800	-0.09602400

H	3.35856700	-3.03615800	1.36585500
H	4.04003800	0.09811500	-1.47736300
C	-0.27176800	4.66265400	-0.69547000
H	0.59711500	5.49148300	1.08323400
H	-1.14367900	3.64130000	-2.36978100
C	-3.60081800	-1.82617900	-0.15530700
H	-4.77480200	-0.72346500	1.26457600
H	-2.24884100	-2.81802100	-1.49300300
F	-0.33993300	5.86020500	-1.30479700
N	-4.76443900	-2.58088600	-0.64877200
O	-5.85780700	-2.33803200	-0.13963200
O	-4.57163600	-3.40622700	-1.54055100
N	5.00645300	-2.20909500	-0.56116700
O	5.65277000	-1.67504700	-1.46164300
O	5.30061800	-3.27490000	-0.02139500

P(*para*−F−phenyl)$_2$(*para*−OMe−phenyl)

0 1

P	0.33979600	-0.00251000	1.38961600
C	1.03900800	1.51043800	0.57892100
C	-1.32995500	-0.15936500	0.61529500
C	1.29178500	-1.36438400	0.56835700
C	2.18013600	2.08205400	1.16987400
C	0.48571200	2.14225300	-0.54606000
C	-2.41906700	0.36278800	1.32642500
C	-1.59211000	-0.78288500	-0.61951200
C	1.27560400	-2.62248900	1.19616600
C	2.04462800	-1.21776100	-0.60778000
C	2.76968200	3.23180600	0.64702500
H	2.61299800	1.62342700	2.05567900
C	1.05619100	3.30127600	-1.07593900
H	-0.40329700	1.73138100	-1.01420300
C	-3.72326500	0.29600300	0.83047700
H	-2.25154200	0.83110600	2.29363100
C	-2.88395600	-0.86615500	-1.12280400
H	-0.77581000	-1.21536900	-1.19063900
C	1.96655900	-3.70896200	0.66213900

H	0.71684500	-2.75428600	2.11951700
C	2.75186500	-2.29219300	-1.15055300
H	2.08649700	-0.25457700	-1.10683700
C	2.19286300	3.82457500	-0.47132900
H	3.65203400	3.67627200	1.09597700
H	0.63351400	3.79806700	-1.94346600
C	-3.96024600	-0.32335600	-0.40285600
H	-4.53633700	0.71505800	1.41231400
H	-3.08882800	-1.34992000	-2.07305800
C	2.69712500	-3.52266100	-0.50664700
H	1.95631000	-4.68331200	1.13983000
H	3.33870400	-2.18726200	-2.05755100
F	2.74921700	4.94412500	-0.97892800
F	3.37827400	-4.56512200	-1.02591600
O	-5.18612300	-0.45626100	-0.98230000
C	-6.31480000	0.06799000	-0.30036500
H	-7.17483300	-0.14491500	-0.93777200
H	-6.45759300	-0.41590800	0.67480500
H	-6.23057300	1.15311900	-0.15546600

P(*para*−F−phenyl)(*para*−OMe−phenyl)$_2$

0 1

P	-0.00201800	0.43629800	1.54279900
C	1.35371600	-0.61145500	0.84819500
C	0.17207000	2.00517900	0.56950600
C	-1.52505700	-0.32251800	0.81957400
C	1.78443600	-1.70710300	1.62233600
C	2.00383100	-0.38027800	-0.37028100
C	1.03870300	2.98591400	1.08392600
C	-0.52734700	2.29129200	-0.61361600
C	-2.75630800	-0.00928300	1.42905000
C	-1.54152300	-1.21263200	-0.26102300
C	2.80243700	-2.54462200	1.18813200
H	1.31420000	-1.90152100	2.58350400
C	3.03902000	-1.20742300	-0.81744600
H	1.70937800	0.46317900	-0.98789300
C	1.22450800	4.20446700	0.43291700

H	1.57420400	2.79551500	2.01090800
C	-0.36241600	3.51113000	-1.27288300
H	-1.21344900	1.55754400	-1.02513900
C	-3.95031100	-0.54274600	0.96441900
H	-2.77536400	0.66151000	2.28497400
C	-2.73433500	-1.76852700	-0.73431700
H	-0.60976900	-1.48963200	-0.74538800
C	3.44029000	-2.29882200	-0.03800300
H	3.13262800	-3.38971500	1.78436700
H	3.51976700	-0.99020100	-1.76480000
C	0.51551500	4.44671900	-0.73893000
H	1.89363800	4.96462900	0.82302400
H	-0.90180000	3.74225400	-2.18603500
C	-3.94755800	-1.43053300	-0.12311200
H	-4.89895500	-0.29910900	1.43282700
H	-2.70287300	-2.45814900	-1.57052000
F	0.68007400	5.62788400	-1.37156000
C	5.12631700	-2.96403000	-1.59417500
H	4.45097900	-3.03071900	-2.45758100
H	5.63616100	-1.99163400	-1.61082000
H	5.86911200	-3.76152200	-1.65575200
C	-5.22760400	-2.82082500	-1.58437400
H	-4.85172500	-2.36971900	-2.51238000
H	-4.65992300	-3.73700900	-1.37427700
H	-6.28296300	-3.07100900	-1.70746900
O	-5.16761200	-1.90944100	-0.49924600
O	4.43462100	-3.16975100	-0.37310900

P(*para*–F–phenyl)$_2$(*para*–Me–phenyl)

0 1

P	-0.03176800	0.00223200	1.38462800
C	-0.73988800	-1.50588900	0.57410700
C	1.63899700	0.13473500	0.59918900
C	-0.97498300	1.37343900	0.57063700
C	-1.84863600	-2.10560200	1.19722600
C	-0.22586900	-2.10274000	-0.58842200
C	2.70294400	-0.51807800	1.24485800

C	1.92185600	0.85725400	-0.56928600
C	-0.96826400	2.62217800	1.21692500
C	-1.71432200	1.24226600	-0.61595200
C	-2.44522600	-3.25036500	0.67095200
H	-2.24953500	-1.67362600	2.11091600
C	-0.80384700	-3.25566300	-1.12271600
H	0.63823800	-1.66883900	-1.08196200
C	3.99591300	-0.46710400	0.72843400
H	2.51590700	-1.07156400	2.16242800
C	3.22128700	0.91412500	-1.07633400
H	1.12506200	1.38140900	-1.08869500
C	-1.65550800	3.71513700	0.69100900
H	-0.42056800	2.74119200	2.14857700
C	-2.41769900	2.32291000	-1.15072000
H	-1.74847600	0.28631000	-1.12926700
C	-1.90813400	-3.80818400	-0.48436600
H	-3.30259600	-3.71724700	1.14480400
H	-0.41171300	-3.72617800	-2.01874600
C	4.28016100	0.25487500	-0.43947600
H	4.79951200	-0.98810600	1.24470600
H	3.41456400	1.48075200	-1.98490800
C	-2.37260500	3.54416500	-0.48827500
H	-1.65279300	4.68240300	1.18294200
H	-2.99466500	2.23012100	-2.06533100
F	-2.47113000	-4.92222100	-0.99601800
F	-3.05017100	4.59238900	-1.00006600
C	5.69047600	0.34344900	-0.97397700
H	6.25923800	1.13283400	-0.46430500
H	6.23616700	-0.59477900	-0.82447500
H	5.69998500	0.57488100	-2.04422300

P(*para*–F–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	0.00216800	0.03178700	1.39250500
C	1.50734700	-0.69551900	0.59666600
C	-0.12912700	1.68807700	0.57152700
C	-1.37633600	-0.91672100	0.59987100

C	2.10490500	-1.79222000	1.24090900
C	2.10598700	-0.21679200	-0.57792500
C	0.52012300	2.76594400	1.19892300
C	-0.85452700	1.94135300	-0.60380000
C	-2.63351100	-0.86623000	1.22588600
C	-1.24801000	-1.69993800	-0.55663500
C	3.24496800	-2.39885200	0.71798800
H	1.67189000	-2.17436200	2.16273600
C	3.25472000	-0.82123500	-1.09167900
H	1.67547300	0.63414500	-1.09748400
C	0.47088000	4.05306000	0.66548000
H	1.06962200	2.59733700	2.12184400
C	-0.92406800	3.22599200	-1.14574900
H	-1.37620900	1.12998200	-1.10182500
C	-3.72488300	-1.55597200	0.70213000
H	-2.75797400	-0.28039900	2.13397700
C	-2.34225400	-2.39787000	-1.07100900
H	-0.28822700	-1.76790800	-1.06020400
C	3.84462100	-1.92070500	-0.45575700
H	3.68223500	-3.25137500	1.23364000
H	3.69922400	-0.43122900	-2.00512300
C	-0.25546700	4.26078100	-0.50214400
H	0.97158600	4.88914100	1.14291000
H	-1.48494100	3.43195300	-2.05190100
C	-3.59797600	-2.33949300	-0.45373100
H	-4.68868900	-1.49307400	1.20314000
H	-2.21704300	-2.99777900	-1.97019100
F	-0.31876800	5.50492200	-1.02117300
C	-4.77243800	-3.12034300	-0.99569800
H	-4.88344900	-4.08220200	-0.47704900
H	-5.71288000	-2.57349200	-0.86525700
H	-4.65157500	-3.33794000	-2.06211800
C	5.10518800	-2.55331900	-0.99756500
H	5.99753600	-2.15129700	-0.49897800
H	5.10957000	-3.63773900	-0.84101800
H	5.21939100	-2.36485900	-2.07025000

P(*para*-F-phenyl)$_2$(*para*-NMe$_2$-phenyl)

0 1

P	-0.68817600	-0.02579200	1.44257300
C	-1.49180700	-1.44545700	0.56039300
C	1.02815500	-0.02251900	0.77403700
C	-1.45245100	1.43711000	0.59709700
C	-2.73989700	-1.87850600	1.04326800
C	-0.91680500	-2.14279000	-0.51348300
C	2.03000500	-0.63189400	1.54748000
C	1.42763700	0.56673200	-0.43629800
C	-1.34559600	2.67898300	1.24790900
C	-2.14825400	1.38377100	-0.62127700
C	-3.40946000	-2.95454200	0.46310700
H	-3.19476300	-1.36860300	1.88922800
C	-1.56780100	-3.23074100	-1.09901300
H	0.05233800	-1.83869900	-0.89637700
C	3.35571400	-0.67992900	1.13182900
H	1.76900200	-1.07567800	2.50581000
C	2.75055700	0.53690800	-0.86442000
H	0.69417900	1.07337200	-1.05753100
C	-1.89279800	3.83693300	0.69755300
H	-0.82898400	2.74114300	2.20260000
C	-2.71235200	2.53150700	-1.18188700
H	-2.25796800	0.43648200	-1.14003900
C	-2.80702100	-3.61576900	-0.60221700
H	-4.37422300	-3.29151600	0.82842400
H	-1.12914900	-3.77757600	-1.92771000
C	3.75344700	-0.10251100	-0.09706100
H	4.08434800	-1.15948400	1.77451400
H	3.00221100	1.01947500	-1.80151200
C	-2.57109900	3.74130800	-0.51289500
H	-1.81202300	4.79878700	1.19361500
H	-3.25427200	2.49853800	-2.12177200
F	-3.44200800	-4.66618200	-1.16417600
F	-3.11379700	4.85488900	-1.04922700
N	5.06872400	-0.16037500	-0.53137000
C	6.09820800	-0.65835100	0.36508000

C	5.47346600	0.60644700	-1.69746000
H	6.19880700	-0.05093100	1.27862000
H	5.89130700	-1.69219400	0.66744100
H	7.05797300	-0.65363400	-0.15519900
H	4.91172000	0.29774500	-2.58760000
H	5.33108800	1.69075900	-1.56518700
H	6.53115100	0.42301700	-1.89616600

P(*para*-F-phenyl)(*para*-NMe$_2$-phenyl)$_2$

0 1

P	0.01765600	0.66343900	-1.53033400
C	-1.43061700	-0.23416600	-0.82222900
C	-0.01685900	2.25697100	-0.57803500
C	1.46601300	-0.21808100	-0.80213200
C	-2.02644000	-1.23578600	-1.60568700
C	-2.00878300	0.01974800	0.43137800
C	-0.87296600	3.26954400	-1.04730700
C	0.78506100	2.53330000	0.54002300
C	2.70360200	-0.09183400	-1.45432000
C	1.42729200	-1.04175300	0.33338600
C	-3.12219400	-1.96725700	-1.16084200
H	-1.62815000	-1.44623200	-2.59596900
C	-3.11109800	-0.69529000	0.88988300
H	-1.60024600	0.80289000	1.06414700
C	-0.94899600	4.50891000	-0.41430500
H	-1.48948100	3.08674900	-1.92428500
C	0.73066800	3.77381200	1.18025700
H	1.46378100	1.77434500	0.91640800
C	3.85130400	-0.72464100	-0.98965800
H	2.77263000	0.51248700	-2.35646900
C	2.56302200	-1.69131200	0.80748600
H	0.48690900	-1.19339800	0.85579700
C	-3.69136200	-1.72323100	0.11068100
H	-3.54123300	-2.72314100	-1.81446100
H	-3.52173200	-0.44548400	1.86121800
C	-0.13986400	4.74045500	0.69333600
H	-1.61025000	5.29272900	-0.76981400

H	1.34931800	3.99568800	2.04423200
C	3.81479300	-1.53782800	0.16698400
H	4.77551900	-0.59249800	-1.53965000
H	2.46881100	-2.32505100	1.68156900
F	-0.19860900	5.94249100	1.30795600
N	4.95915800	-2.15751300	0.65392100
N	-4.77246100	-2.46234200	0.57504900
C	-5.46254900	-2.03475500	1.78003500
H	-4.78347200	-2.02937500	2.64103700
H	-5.90247200	-1.02840200	1.68865300
H	-6.26622100	-2.74035000	2.00064700
C	-5.47119400	-3.35154600	-0.33706600
H	-5.91824500	-2.82254200	-1.19439800
H	-4.79580600	-4.12093900	-0.72987900
H	-6.27052200	-3.86204000	0.20413100
C	4.83709700	-3.15549500	1.70279900
H	4.39032800	-2.72355200	2.60627300
H	4.22513600	-4.02147000	1.40233500
H	5.83254700	-3.51644500	1.96967600
C	6.16863700	-2.15307300	-0.15119600
H	6.04093000	-2.66070900	-1.12110700
H	6.50540900	-1.12831300	-0.34809000
H	6.96486800	-2.66010000	0.39778500

P(*para*–Cl–phenyl)$_2$(*para*–COOMe–phenyl)

0 1

P	-0.65913500	-0.01549100	1.63109400
C	-1.36911100	1.46248600	0.77050900
C	-1.45073400	-1.42762300	0.73181200
C	1.07880700	-0.07223500	0.99079100
C	-1.29592600	2.69009700	1.45008500
C	-1.99896700	1.43285000	-0.48317800
C	-2.65287000	-1.92742900	1.25997600
C	-0.92070600	-2.04204300	-0.41347500
C	1.95631300	-0.97910000	1.61401400
C	1.58055400	0.75582300	-0.02529900
C	-1.81235900	3.85933000	0.89307300

H	-0.83282100	2.73497200	2.43281600
C	-2.53158800	2.59178300	-1.04962300
H	-2.08244200	0.49716600	-1.02737900
C	-3.32197500	-2.99205400	0.65781000
H	-3.07234600	-1.48275400	2.15910600
C	-1.57235300	-3.11596800	-1.02184500
H	0.01343100	-1.68676600	-0.83766400
C	3.28595700	-1.07121200	1.21847700
H	1.59295200	-1.61435300	2.41829200
C	2.91686500	0.67476800	-0.41664600
H	0.92657300	1.46984700	-0.51552600
C	-2.42926300	3.79752900	-0.35639500
H	-1.74830800	4.80340900	1.42362800
H	-3.01979500	2.56093100	-2.01811100
C	-2.77160700	-3.57911800	-0.48160700
H	-4.25126800	-3.36964200	1.07099300
H	-1.15557000	-3.58796300	-1.90546100
C	3.77728500	-0.24202000	0.20024100
H	3.96472400	-1.77253700	1.69265100
H	3.29433300	1.31925800	-1.20283400
Cl	-3.59788500	-4.92940200	-1.24278700
Cl	-3.09637300	5.26046200	-1.06388400
C	5.21318700	-0.37579200	-0.17683200
O	5.98798200	-1.16008000	0.33577000
O	5.57046200	0.47737800	-1.16389100
C	6.94384500	0.39837000	-1.57359000
H	7.17533400	-0.60134100	-1.95096500
H	7.05660800	1.14257600	-2.36257700
H	7.60832800	0.62252300	-0.73479600

P(*para*–Cl–phenyl)(*para*–COOMe–phenyl)$_2$

0 1

P	-0.00813700	0.58003800	1.64319400
C	1.52895700	-0.11806200	0.88054000
C	-0.22076000	2.19135000	0.75683400
C	-1.33990700	-0.46291900	0.88597100
C	2.09711700	-1.23793200	1.51438800

C	2.17967600	0.42048000	-0.24109200
C	0.31227900	3.33446700	1.37534100
C	-0.89651500	2.34826300	-0.46343000
C	-2.61445700	-0.39014400	1.47579800
C	-1.15070500	-1.33342800	-0.19995400
C	3.26606500	-1.81926400	1.03158900
H	1.62021400	-1.65554100	2.39793900
C	3.35622700	-0.15131800	-0.72029000
H	1.76712200	1.28991100	-0.74280300
C	0.19670100	4.59530100	0.79105700
H	0.82176500	3.24136200	2.33127800
C	-1.03042200	3.60446100	-1.05602900
H	-1.32872700	1.48503400	-0.96021100
C	-3.67580900	-1.14598000	0.98566700
H	-2.77451200	0.26193000	2.33106400
C	-2.20785100	-2.09912100	-0.68669000
H	-0.17419500	-1.41491900	-0.66674300
C	3.90569200	-1.27542000	-0.09140600
H	3.69147700	-2.68561300	1.52557200
H	3.86374500	0.25961000	-1.58707700
C	-0.47812600	4.71801600	-0.42332300
H	0.61402400	5.47238600	1.27417700
H	-1.55570600	3.71908600	-1.99844800
C	-3.47682600	-2.00930500	-0.10097600
H	-4.65503100	-1.07849900	1.44625500
H	-2.06896800	-2.77294000	-1.52601600
C	5.16459600	-1.84388500	-0.65220500
O	5.74719800	-1.39946200	-1.62233200
O	5.59757400	-2.92246900	0.03970500
C	-4.56842100	-2.85187100	-0.66761500
O	-4.43347500	-3.61032700	-1.60818300
O	-5.74265400	-2.68171200	-0.01820900
C	-6.83680900	-3.46583700	-0.51649700
H	-6.61001500	-4.53276800	-0.44174900
H	-7.69012100	-3.20936800	0.11208100
H	-7.04077800	-3.21986000	-1.56209800
C	6.80754600	-3.51882100	-0.45076900

H	7.63007000	-2.79915300	-0.42053500
H	7.00850000	-4.36023600	0.21306700
H	6.67621300	-3.86305700	-1.48015500
Cl	-0.64303900	6.30233300	-1.16369400

P(*para*–Cl–phenyl)$_2$(*para*–CF$_3$–phenyl)

0 1

P	-0.57423800	-0.00017900	1.60026300
C	-1.40685400	1.42277400	0.75751900
C	-1.32591800	-1.46891100	0.75987300
C	1.13069000	0.03377000	0.87183000
C	-1.35903900	2.66539200	1.41179500
C	-2.10420700	1.33682000	-0.45725600
C	-2.46328500	-2.03392900	1.36086100
C	-0.82500600	-2.06477500	-0.40808500
C	2.09651000	-0.79016100	1.47630300
C	1.52387800	0.85087700	-0.19845600
C	-1.96571500	3.79585300	0.86609600
H	-0.84444400	2.75282600	2.36563100
C	-2.72702700	2.45625400	-1.01110400
H	-2.17039400	0.38776000	-0.98025200
C	-3.09864000	-3.14503300	0.80820700
H	-2.85782100	-1.60382000	2.27817200
C	-1.44283100	-3.18409700	-0.96790000
H	0.05971400	-1.65908100	-0.88921000
C	3.40939400	-0.81387700	1.01407200
H	1.81809400	-1.41891700	2.31846200
C	2.84139700	0.83985700	-0.65764300
H	0.80028400	1.50052600	-0.68017000
C	-2.64814200	3.67888700	-0.34489200
H	-1.92067400	4.75202500	1.37653800
H	-3.26699200	2.38194400	-1.94926700
C	-2.57873700	-3.71244900	-0.35528000
H	-3.97811600	-3.57294100	1.27753500
H	-1.04867600	-3.64112500	-1.86957200
C	3.78488500	0.00547500	-0.05504100
H	4.14197500	-1.46374300	1.48167200

H	3.13250100	1.47174300	-1.49054100
Cl	-3.36186200	-5.12016600	-1.05455800
Cl	-3.42841400	5.09187800	-1.03676300
C	5.21840100	0.03140000	-0.51271400
F	5.81881800	-1.16845400	-0.34938500
F	5.32464000	0.36584000	-1.81765900
F	5.94812900	0.93279500	0.18486500

P(*para*–Cl–phenyl)(*para*–CF_3–phenyl)$_2$

0 1

P	0.00041000	0.54802500	1.66685900
C	1.46237100	-0.29738200	0.90241400
C	-0.05065500	2.17133600	0.77903600
C	-1.42517700	-0.36191000	0.90690600
C	1.92850700	-1.45962700	1.54162300
C	2.15108100	0.16695000	-0.22809500
C	0.59533700	3.25511400	1.39694800
C	-0.70793700	2.39502000	-0.44089500
C	-2.68519400	-0.17584500	1.50142400
C	-1.32264400	-1.23605100	-0.18594600
C	3.03553900	-2.15014500	1.05551800
H	1.42093500	-1.82694500	2.43016600
C	3.26835200	-0.51429800	-0.71169400
H	1.81648200	1.06488000	-0.73743100
C	0.60752600	4.52065700	0.81170700
H	1.09284400	3.11198900	2.35300700
C	-0.71443600	3.65797300	-1.03422800
H	-1.22660100	1.58020000	-0.93671900
C	-3.81319000	-0.82713900	1.00906600
H	-2.78389000	0.48379500	2.35991400
C	-2.44768600	-1.89967000	-0.67578700
H	-0.36091600	-1.40249600	-0.66058700
C	3.70992400	-1.67510600	-0.07328700
H	3.37759900	-3.05293000	1.55103500
H	3.78982900	-0.14916700	-1.59059300
C	-0.05175200	4.71046900	-0.40275800
H	1.11131100	5.35129100	1.29444300

H	-1.22684200	3.82470500	-1.97593900
C	-3.69453300	-1.69383300	-0.08135900
H	-4.78225500	-0.66614300	1.47004800
H	-2.35787100	-2.56868700	-1.52555400
C	-4.89891800	-2.45111300	-0.57338600
C	4.94704500	-2.38070300	-0.56075400
F	-4.80614100	-2.74326100	-1.88935000
F	-6.04051700	-1.75158200	-0.39039900
F	-5.04923400	-3.62605600	0.08079100
F	5.13282000	-2.21118500	-1.88831000
F	6.05949100	-1.91713000	0.05458000
F	4.89272800	-3.70992000	-0.32305500
Cl	-0.05532200	6.30195000	-1.14421900

P(*para*–Cl–phenyl)$_2$(*para*–Ac–phenyl)

0 1

P	-0.27958200	-0.01741900	1.58468300
C	-1.12981800	1.40708200	0.76214900
C	-1.02882600	-1.48335400	0.73724800
C	1.41888000	0.03053900	0.84685500
C	-1.11408400	2.63626100	1.44251400
C	-1.80927800	1.33386600	-0.46363000
C	-2.15953600	-2.06015100	1.33934700
C	-0.53222200	-2.06439800	-0.44007200
C	2.37230100	-0.85896600	1.38014700
C	1.82662300	0.92611900	-0.15224100
C	-1.73492300	3.76670300	0.91228900
H	-0.61376600	2.71274500	2.40482800
C	-2.44582500	2.45267100	-1.00251300
H	-1.85055200	0.39478400	-1.00685400
C	-2.79287700	-3.16859600	0.77898300
H	-2.55026100	-1.64162900	2.26360300
C	-1.14797700	-3.18086100	-1.00770300
H	0.34808400	-1.64928700	-0.92125800
C	3.67997700	-0.86663000	0.91291100
H	2.08278100	-1.54769600	2.17053000
C	3.14454700	0.92679600	-0.61232600

H	1.11544900	1.62792700	-0.57590500
C	-2.39880300	3.66237400	-0.30990800
H	-1.71503000	4.71253400	1.44321700
H	-2.97211600	2.38812500	-1.94914900
C	-2.27753500	-3.72105600	-0.39363500
H	-3.66715700	-3.60593400	1.24933200
H	-0.75715900	-3.62679300	-1.91636300
C	4.08584900	0.02969000	-0.08980400
H	4.41623300	-1.55407800	1.31662700
H	3.42957200	1.63256700	-1.38681300
Cl	-3.05845400	-5.12509900	-1.10314200
Cl	-3.19635100	5.07504000	-0.98329100
C	5.51336000	-0.01611000	-0.54856200
O	6.29443800	-0.82166800	-0.06519400
C	5.97111500	0.95584700	-1.62417100
H	5.39468300	0.82367600	-2.54779600
H	5.83567400	1.99498400	-1.30078500
H	7.02778400	0.77674800	-1.82981500

P(*para*−Cl−phenyl)(*para*−Ac−phenyl)$_2$

0 1

P	-0.01251600	0.26152600	1.60203500
C	1.53593500	-0.39567700	0.82675200
C	-0.24797500	1.89072500	0.75570800
C	-1.32670600	-0.78264100	0.81638900
C	2.11565200	-1.52509500	1.43012600
C	2.18654400	0.18232800	-0.27639900
C	0.25340300	3.02768400	1.41082600
C	-0.91159800	2.06573000	-0.46884200
C	-2.60066000	-0.75009400	1.40844800
C	-1.12550300	-1.61867600	-0.29555700
C	3.29482200	-2.07572200	0.93355200
H	1.64135900	-1.97487500	2.29921900
C	3.37102500	-0.36117700	-0.76502500
H	1.76521300	1.06074300	-0.75494800
C	0.11857000	4.30089400	0.85827000
H	0.75290500	2.91984500	2.37045500

C	-1.06419700	3.33402500	-1.03007700
H	-1.31933100	1.20723700	-0.99378900
C	-3.64805200	-1.51155500	0.89463600
H	-2.77212100	-0.12660300	2.28263400
C	-2.16958300	-2.38678500	-0.80238100
H	-0.14828300	-1.66909400	-0.76568400
C	3.93946000	-1.49772400	-0.17068200
H	3.71354200	-2.95195400	1.41898300
H	3.87804600	0.07959800	-1.61744000
C	-0.54346300	4.44178100	-0.36115900
H	0.51142200	5.17331000	1.36952100
H	-1.57955500	3.46269000	-1.97615200
C	-3.44416000	-2.34235100	-0.21748200
H	-4.62153400	-1.46090800	1.37269700
H	-2.02194000	-3.03315000	-1.66171000
C	5.21618400	-2.03757800	-0.74586800
O	5.74024000	-1.49669200	-1.70766600
C	-4.52882000	-3.19263100	-0.81159400
O	-4.30065000	-3.90052400	-1.78067300
C	-5.91449300	-3.15686400	-0.18780400
H	-5.88298200	-3.47369000	0.86171200
H	-6.33207500	-2.14300600	-0.21027700
H	-6.56725100	-3.82853300	-0.74785000
C	5.84426800	-3.26818600	-0.11210900
H	6.09024400	-3.08758600	0.94133200
H	5.15841700	-4.12335400	-0.14526900
H	6.75615400	-3.51557500	-0.65814200
Cl	-0.73265500	6.04101700	-1.06161600

P(*para*–Cl–phenyl)$_2$(*para*–CN–phenyl)

0 1

P	-0.00136100	0.10741900	1.52843700
C	-1.49929200	-0.62972400	0.72984000
C	1.39180300	-0.81433000	0.73139700
C	0.12424900	1.76891300	0.71465500
C	-2.72487200	-0.45357500	1.39422200
C	-1.48769200	-1.37323800	-0.46039400

C	1.87935400	-1.94330200	1.41049200
C	2.00019600	-0.45168300	-0.48080400
C	1.10429400	2.64915400	1.20993200
C	-0.72709400	2.21992400	-0.30586700
C	-3.90954800	-0.98007700	0.88090000
H	-2.75621000	0.09864800	2.33031700
C	-2.66263500	-1.91687800	-0.98099400
H	-0.55422500	-1.53907500	-0.98924900
C	2.92716100	-2.70348300	0.89258600
H	1.43868700	-2.23210300	2.36146700
C	3.05679300	-1.19582900	-1.00718200
H	1.65429700	0.42306900	-1.02311100
C	1.24876300	3.93010400	0.69027000
H	1.76065300	2.32779400	2.01480100
C	-0.60013400	3.50605000	-0.82695600
H	-1.49648200	1.56420900	-0.70001200
C	-3.86603600	-1.71112000	-0.30633100
H	-4.85194000	-0.83634000	1.39861500
H	-2.64616300	-2.49347400	-1.89993200
C	3.50890200	-2.31972300	-0.31575100
H	3.29587300	-3.57531600	1.42244300
H	3.52418000	-0.90863000	-1.94326600
C	0.39185800	4.36878000	-0.33479600
H	2.01167900	4.59880100	1.07586200
H	-1.26280900	3.84566300	-1.61674600
Cl	4.83727200	-3.26084200	-0.97229700
Cl	-5.34794800	-2.39111300	-0.95672000
C	0.52800900	5.69155900	-0.87093900
N	0.63998500	6.76422600	-1.30716000

P(*para*–Cl–phenyl)(*para*–CN–phenyl)$_2$

0 1

P	-0.11576500	0.00075800	1.51346500
C	-1.10290700	-1.34316400	0.70505400
C	1.54706100	-0.16132600	0.72060400
C	-0.79014000	1.52711900	0.70532200
C	-2.37069600	-1.61608500	1.25098500

C	-0.64668900	-2.13373400	-0.36123000
C	2.51603400	-0.89845900	1.42146900
C	1.90699400	0.41746600	-0.50688000
C	-0.44497300	2.75806900	1.29194900
C	-1.63993800	1.53040200	-0.41229000
C	-3.17189700	-2.62895000	0.73579200
H	-2.73285700	-1.03141000	2.09293600
C	-1.43487000	-3.15982100	-0.87783800
H	0.33153300	-1.95050100	-0.79349400
C	3.80121300	-1.07435100	0.90976200
H	2.26715900	-1.33794100	2.38417400
C	3.19177200	0.25951200	-1.02696300
H	1.18379800	1.00345400	-1.06595000
C	-0.91319400	3.95881300	0.77001200
H	0.19439200	2.77575800	2.17086400
C	-2.12485100	2.72619900	-0.93748200
H	-1.92910100	0.59416400	-0.87863700
C	-2.70510500	-3.41120600	-0.33493200
H	-4.15052800	-2.82798200	1.16055700
H	-1.07422700	-3.76672600	-1.70229600
C	4.12815200	-0.48993600	-0.31386600
H	4.54303500	-1.64713800	1.45593300
H	3.46510900	0.71170100	-1.97453900
C	-1.76102400	3.94908100	-0.35113300
H	-0.63774100	4.90359000	1.22746900
H	-2.78129600	2.71983500	-1.80187900
C	-2.25588100	5.18214600	-0.89059900
N	-2.65565900	6.18263000	-1.32917000
C	-3.52025200	-4.46447200	-0.86642600
N	-4.18237900	-5.31757500	-1.29881200
Cl	5.74533000	-0.69278700	-0.96288900

P(*para*–Cl–phenyl)$_2$(*para*–NO$_2$–phenyl)

0 1

P	0.24082300	0.01450200	1.55945500
C	1.18302600	-1.35475700	0.74670300
C	0.90640400	1.53094800	0.73454900

C	-1.44286600	-0.12695500	0.79729100
C	1.26814400	-2.56984100	1.44679600
C	1.83725800	-1.25082900	-0.49073200
C	1.95143500	2.20400400	1.38888000
C	0.43203900	2.05558700	-0.47852000
C	-2.42094500	0.79142300	1.22667500
C	-1.81678000	-1.13486200	-0.10597400
C	1.96392200	-3.65970200	0.92416500
H	0.78907700	-2.66714500	2.41793900
C	2.54703100	-2.32790500	-1.02178600
H	1.80256400	-0.31997100	-1.04830800
C	2.52374900	3.35391700	0.84640400
H	2.32202300	1.82901100	2.33960400
C	0.98711900	3.21125000	-1.02912900
H	-0.38354100	1.56593200	-1.00203700
C	-3.72683900	0.72472800	0.75472300
H	-2.15719000	1.56785200	1.94014300
C	-3.12514200	-1.22212600	-0.57979700
H	-1.08376300	-1.85788100	-0.44733900
C	2.60043400	-3.52656600	-0.30967800
H	2.02207900	-4.59546100	1.46979900
H	3.05347800	-2.24028600	-1.97727800
C	2.03303200	3.84899200	-0.36179900
H	3.33189700	3.86630200	1.35740000
H	0.61427000	3.61282600	-1.96554700
C	-4.06113100	-0.28781200	-0.14492000
H	-4.48505900	1.42933400	1.07359300
H	-3.42497300	-1.99322300	-1.27902300
Cl	2.73638300	5.30253800	-1.04915600
Cl	3.49108900	-4.88549000	-0.97307700
N	-5.44140900	-0.37176700	-0.64533700
O	-6.24529800	0.46977600	-0.24474700
O	-5.70841500	-1.27717900	-1.43507200

P(*para*–Cl–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

P	-0.01050600	0.22884300	1.59146500

C	1.52602700	-0.45644300	0.81553800
C	-0.22670100	1.86047900	0.75065000
C	-1.34324600	-0.79409200	0.80645400
C	2.02949300	-1.65642500	1.35369300
C	2.24727400	0.17952400	-0.20759700
C	0.21473100	2.99804700	1.44628100
C	-0.81598900	2.03516400	-0.51202100
C	-2.62832200	-0.69315600	1.37144000
C	-1.14596800	-1.67358500	-0.27090200
C	3.20439500	-2.22332800	0.87099200
H	1.49861100	-2.15078300	2.16321900
C	3.43330300	-0.36927600	-0.69316400
H	1.88435300	1.10959300	-0.63170600
C	0.09262300	4.27399800	0.89660200
H	0.65540400	2.88898100	2.43400900
C	-0.95400500	3.30551800	-1.07063500
H	-1.17766900	1.17573800	-1.06848300
C	-3.69482100	-1.43060600	0.86728500
H	-2.79494900	-0.03365900	2.21904800
C	-2.20206400	-2.42757300	-0.78037800
H	-0.16311300	-1.77519100	-0.71890300
C	3.89181800	-1.56576500	-0.14852900
H	3.59852900	-3.14863500	1.27284800
H	3.99912300	0.10996400	-1.48281400
C	-0.49412700	4.41578900	-0.36074200
H	0.43786500	5.14773300	1.43884800
H	-1.41262300	3.43526200	-2.04524400
C	-3.46246500	-2.29143900	-0.20437200
H	-4.68889300	-1.35906700	1.29121800
H	-2.06493800	-3.10829200	-1.61178100
N	-4.58240400	-3.08273400	-0.74076900
O	-5.68362900	-2.94175500	-0.21087500
O	-4.34734800	-3.83405800	-1.68609000
N	5.14158900	-2.15182500	-0.66053000
O	5.72854800	-1.54760300	-1.55710400
O	5.52018900	-3.21024400	-0.16057500
Cl	-0.66483700	6.01564200	-1.05821000

P(*para*−Cl−phenyl)$_2$(*para*−OMe−phenyl)

0 1

P	-0.03414700	-0.02252800	1.50431600
C	1.14582000	-1.22386700	0.72813200
C	0.48249300	1.58158300	0.73199300
C	-1.62040700	-0.41711600	0.64751100
C	1.25565100	-2.48932400	1.32917200
C	1.95048200	-0.94785800	-0.38765000
C	1.55074200	2.26854200	1.33476400
C	-0.15142700	2.17720100	-0.36831400
C	-2.80879700	-0.10842600	1.32339900
C	-1.72413700	-1.02162700	-0.62023300
C	2.12106400	-3.45939200	0.82636400
H	0.65839600	-2.72171400	2.20762000
C	2.83095400	-1.90419300	-0.89743500
H	1.89766600	0.02436900	-0.86785600
C	1.99282300	3.49651700	0.84598100
H	2.04539200	1.84044600	2.20353600
C	0.27077000	3.41302000	-0.86309200
H	-0.98723000	1.67765400	-0.84805900
C	-4.06237100	-0.36508600	0.76299500
H	-2.76071600	0.33991600	2.31302800
C	-2.96226600	-1.29171900	-1.18759000
H	-0.82491300	-1.29128000	-1.16643200
C	2.90506000	-3.15484600	-0.28668400
H	2.19610500	-4.43469500	1.29560300
H	3.45085700	-1.68202300	-1.75985100
C	1.34371300	4.06011500	-0.25309600
H	2.82135600	4.01630400	1.31545500
H	-0.22629100	3.86743500	-1.71390300
C	-4.14249400	-0.96181500	-0.50130000
H	-4.95683100	-0.10844600	1.31903600
H	-3.04524600	-1.76141000	-2.16296100
Cl	1.88268500	5.61517500	-0.87131500
Cl	4.01026200	-4.36488900	-0.92282300
O	-5.30364100	-1.26686400	-1.14337600

C	-6.53163800	-0.96341600	-0.49911700
H	-6.63336100	0.11365700	-0.31218900
H	-7.31663400	-1.28620100	-1.18516500
H	-6.63355200	-1.50581200	0.44994200

P(*para*–Cl–phenyl)(*para*–OMe–phenyl)$_2$

0 1

P	0.01284300	-0.06481300	1.62830900
C	-0.40602000	1.56815600	0.87105900
C	-1.17196100	-1.20386400	0.76731200
C	1.63151300	-0.49028900	0.84465700
C	-0.02947000	2.72531900	1.58100700
C	-1.09053100	1.74023800	-0.33871200
C	-2.47143800	-1.29915300	1.29494900
C	-0.84528000	-2.00713000	-0.33496800
C	2.42474200	-1.46234900	1.48601800
C	2.14252800	0.10642700	-0.31442300
C	-0.30612500	3.99513000	1.09373100
H	0.48536700	2.62536900	2.53368300
C	-1.38715700	3.01204400	-0.83827200
H	-1.40970800	0.87171500	-0.90745200
C	-3.42403000	-2.14684300	0.73274700
H	-2.74517900	-0.70325700	2.16250400
C	-1.78389200	-2.87124800	-0.90364600
H	0.15351600	-1.96397400	-0.75803000
C	3.66111300	-1.83691100	0.97858300
H	2.06598800	-1.92847900	2.40082700
C	3.39115600	-0.25063300	-0.83235400
H	1.56576000	0.87121200	-0.82621500
C	-0.99071700	4.14806600	-0.12224500
H	-0.01451800	4.88655900	1.64050400
H	-1.92369600	3.10141000	-1.77626600
C	-3.06793000	-2.92960200	-0.36608900
H	-4.42558600	-2.20967000	1.14520700
H	-1.52183400	-3.49047200	-1.75539400
C	4.15547900	-1.23040300	-0.18698600
H	4.27104000	-2.58763800	1.47154700

H	3.75315700	0.23948100	-1.72926900
C	-1.92604400	5.65191800	-1.72582300
H	-1.38341100	5.23806300	-2.58613600
H	-2.93419100	5.21804000	-1.69368800
H	-2.00310400	6.73513700	-1.83594000
C	5.94088400	-1.07205300	-1.76660200
H	5.31439400	-1.25397600	-2.64992700
H	6.08698300	0.00945600	-1.64549000
H	6.91042400	-1.55325300	-1.90751700
O	5.38215800	-1.65672000	-0.60106200
O	-1.22498100	5.43311800	-0.51206500
Cl	-4.25743500	-4.01327200	-1.07777800

P(*para*–Cl–phenyl)$_2$(*para*–Me–phenyl)

P	-0.00189800	0.34774600	1.48848600
C	-1.41556400	-0.57805100	0.72685700
C	1.46863300	-0.48359100	0.72576900
C	-0.06181000	1.97066200	0.60326100
C	-2.67392000	-0.43308900	1.33533100
C	-1.30934600	-1.43110700	-0.38203400
C	1.97788800	-1.61514000	1.38569700
C	2.12677200	-0.03718800	-0.43001500
C	0.58582700	3.05680100	1.21530400
C	-0.72130400	2.19650300	-0.61457000
C	-3.79786000	-1.09650000	0.84576300
H	-2.77900800	0.20528200	2.20929400
C	-2.42258000	-2.11224100	-0.87811900
H	-0.34884300	-1.57335300	-0.86759100
C	3.09238400	-2.29784700	0.90109400
H	1.49992200	-1.96829300	2.29636800
C	3.25146700	-0.70226200	-0.92214600
H	1.76432800	0.84130500	-0.95475400
C	0.59045400	4.31706600	0.62026600
H	1.09069200	2.91387300	2.16805400
C	-0.72222700	3.46289400	-1.20050100
H	-1.23987400	1.38098700	-1.11011800
C	-3.65965800	-1.93479100	-0.26071300

H	-4.76584700	-0.97530500	1.32043600
H	-2.33158100	-2.77177300	-1.73492400
C	3.72194100	-1.83098600	-0.25305400
H	3.47565600	-3.17283300	1.41538700
H	3.75634600	-0.34961200	-1.81553200
C	-0.06817800	4.54456600	-0.59598900
H	1.10577100	5.13929700	1.11206900
H	-1.24008800	3.61263500	-2.14558100
Cl	5.13641200	-2.67450500	-0.86741700
Cl	-5.06632300	-2.78766400	-0.88007500
C	-0.09873900	5.92082500	-1.21821200
H	-0.93308600	6.51578200	-0.82292600
H	0.82191400	6.47633700	-1.00930100
H	-0.22442600	5.86721000	-2.30474100

P(*para*–Cl–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	-0.35411300	-0.00245800	1.43975800
C	-1.09410800	-1.47597800	0.59911000
C	1.35117200	0.04944600	0.71279800
C	-1.19274700	1.41773200	0.59991800
C	-2.22729300	-2.05193300	1.19751000
C	-0.59502700	-2.06746000	-0.57114000
C	2.34006800	-0.72591100	1.34224800
C	1.72654500	0.83652000	-0.38604700
C	-1.14545500	2.66392000	1.24740700
C	-1.89087900	1.33193600	-0.61385200
C	-2.84885100	-3.16505400	0.63489000
H	-2.62622100	-1.62375800	2.11438800
C	-1.21505800	-3.18872000	-1.12453600
H	0.28417300	-1.65297700	-1.05563800
C	3.65586700	-0.73830500	0.88256600
H	2.08053900	-1.32866500	2.20936200
C	3.04281300	0.84529700	-0.85239200
H	0.98773400	1.45433600	-0.88694600
C	-1.75548300	3.78613600	0.69026900
H	-0.62569000	2.75550100	2.19856900

C	-2.50937700	2.45675400	-1.16186500
H	-1.95458800	0.38159500	-1.13556500
C	-2.35070400	-3.75756900	-0.53384800
H	-3.72937300	-3.58646100	1.11537100
H	-0.80908800	-3.62824800	-2.03337100
C	3.99573600	0.05302100	-0.21495900
H	4.41093600	-1.34354500	1.37314500
H	3.32513100	1.45833700	-1.70209200
C	-2.45367100	3.70188900	-0.52247700
H	-1.69684900	4.74060200	1.20920900
H	-3.04410700	2.36471600	-2.10506400
C	-3.15089400	4.90976900	-1.10344800
H	-4.15640500	5.03035200	-0.67812700
H	-2.59862200	5.83214800	-0.89272700
H	-3.26565200	4.82311600	-2.18908400
C	-3.00030800	-4.98998100	-1.11847500
H	-2.61627900	-5.90367300	-0.64500100
H	-4.08561000	-4.98083700	-0.96939000
H	-2.80576200	-5.07458400	-2.19285400
Cl	5.65549200	0.05705000	-0.79721200

P(*para*−Cl−phenyl)$_2$(*para*−NMe$_2$−phenyl)

0 1

P	0.31474300	0.01826800	1.58873800
C	1.12966400	-1.43189500	0.76736300
C	1.14367900	1.44882600	0.74792900
C	-1.37034800	-0.00684200	0.85065500
C	0.97269300	-2.68535000	1.38307200
C	1.90695300	-1.36010300	-0.39848300
C	2.40351600	1.84148700	1.23309700
C	0.57049200	2.19959100	-0.28861700
C	-2.42262300	0.53459000	1.60753900
C	-1.69672000	-0.54069000	-0.40714900
C	1.55067800	-3.83541100	0.84832400
H	0.39134500	-2.76576300	2.29847100
C	2.50250900	-2.50044200	-0.94181300
H	2.05709600	-0.40518000	-0.89262100

C	3.08488400	2.92907000	0.68989200
H	2.86143600	1.29120300	2.05185300
C	1.23376000	3.30013600	-0.83600900
H	-0.40663600	1.92794400	-0.67558400
C	-3.73008800	0.56360400	1.13638800
H	-2.21523100	0.94535500	2.59321500
C	-2.99943800	-0.52859200	-0.89185900
H	-0.91919700	-0.98257400	-1.02435300
C	2.31490100	-3.73034900	-0.31406000
H	1.42061900	-4.79881500	1.33004100
H	3.10321700	-2.43528900	-1.84315000
C	2.48885500	3.65228700	-0.34394200
H	4.05913400	3.22050000	1.06810700
H	0.78224400	3.87637600	-1.63702900
C	-4.05810500	0.02275300	-0.12954900
H	-4.49887600	1.00085700	1.76227100
H	-3.19299700	-0.95485300	-1.86918700
Cl	3.33205600	5.03534600	-1.02959100
Cl	3.06013400	-5.17192500	-0.99240700
N	-5.35979300	0.02174200	-0.59831700
C	-5.64028600	-0.42314800	-1.95259700
C	-6.39720600	0.70945000	0.15098200
H	-5.13166300	0.19039800	-2.71229300
H	-5.33449000	-1.46678400	-2.10091000
H	-6.71512700	-0.36481900	-2.13319200
H	-6.50852100	0.28667700	1.15776400
H	-6.19749200	1.78708300	0.25606700
H	-7.35130200	0.58948100	-0.36534300

P(*para*–Cl–phenyl)(*para*–NMe$_2$–phenyl)$_2$

0 1

P	0.02179500	0.28942100	-1.61752800
C	-1.40084900	-0.60574500	-0.85919100
C	-0.07716800	1.93681500	-0.76578700
C	1.49818800	-0.49149400	-0.83544200
C	-1.98132000	-1.65349700	-1.59211400
C	-1.97080300	-0.31145700	0.38983800

C	-1.05948600	2.83976800	-1.20979700
C	0.80262500	2.36209600	0.23971200
C	2.72545400	-0.38987100	-1.51103900
C	1.49183100	-1.21605400	0.36666600
C	-3.05527200	-2.38941300	-1.10362800
H	-1.58849000	-1.89742700	-2.57680800
C	-3.05106000	-1.03062200	0.89131000
H	-1.57375000	0.50718700	0.98384400
C	-1.17929700	4.11399800	-0.65931500
H	-1.74495500	2.54355200	-2.00051500
C	0.70447200	3.64045000	0.79536100
H	1.57671800	1.69092500	0.59831800
C	3.89393700	-0.95157400	-1.00809400
H	2.76954400	0.13724700	-2.46181000
C	2.64830100	-1.79398200	0.88027900
H	0.56095200	-1.34664700	0.91128700
C	-3.61617300	-2.10378000	0.16299700
H	-3.46403700	-3.18188000	-1.71926900
H	-3.45659300	-0.74920400	1.85607800
C	-0.28964800	4.50413500	0.34261800
H	-1.94466000	4.80041700	-1.00637000
H	1.39038500	3.95984400	1.57335500
C	3.88961700	-1.66420600	0.21363700
H	4.80909500	-0.84349900	-1.57806200
H	2.57973400	-2.35307800	1.80614000
N	5.05323800	-2.21174200	0.73705900
N	-4.67479700	-2.84530500	0.67061900
C	-5.35764500	-2.38687800	1.86849700
H	-4.66786400	-2.33540900	2.71950900
H	-5.81912700	-1.39384400	1.74520400
H	-6.14394500	-3.09937600	2.12605300
C	-5.35793100	-3.79519300	-0.19079200
H	-5.82520400	-3.31941600	-1.06814500
H	-4.66645000	-4.56561700	-0.55257700
H	-6.13972600	-4.29845600	0.38173600
C	4.96993800	-3.11177400	1.87465300
H	4.52647000	-2.60918300	2.74266600

H	4.37392000	-4.01437800	1.66401000
H	5.97717600	-3.42550500	2.15621800
C	6.25823600	-2.23610500	-0.07441400
H	6.13957300	-2.82138200	-1.00056300
H	6.56493200	-1.22085700	-0.35333200
H	7.07116100	-2.67666500	0.50638100
Cl	-0.42332700	6.11629100	1.03882900

P(*para*–COOMe–phenyl)$_2$(*para*–CF$_3$–phenyl)

0 1

P	0.03485000	0.03531200	1.73109400
C	-0.98198100	-1.28818700	0.92691600
C	1.68990900	-0.18125000	0.92815500
C	-0.60848700	1.57618000	0.92586100
C	-2.21006900	-1.60109600	1.53633900
C	-0.59288800	-2.01145700	-0.21246400
C	2.57525600	-1.08575200	1.54100800
C	2.12317600	0.51609500	-0.21134900
C	-0.29210700	2.79643800	1.54721100
C	-1.40825100	1.59865800	-0.22700000
C	-3.03818600	-2.59085200	1.01374500
H	-2.51728100	-1.06704300	2.43227600
C	-1.41379000	-3.00990100	-0.73178700
H	0.35471700	-1.79530600	-0.69558600
C	3.84800400	-1.30667200	1.02165600
H	2.26523900	-1.61809300	2.43699300
C	3.39984100	0.30599500	-0.72741000
H	1.46230700	1.22651100	-0.69777700
C	-0.74437300	4.00553000	1.02448800
H	0.31215200	2.79991800	2.45092300
C	-1.87330600	2.80599700	-0.74790800
H	-1.67070500	0.67033900	-0.72422500
C	-2.64176300	-3.30439700	-0.12597100
H	-3.98494700	-2.82055300	1.48957100
H	-1.12003800	-3.57240000	-1.61215500
C	4.26912200	-0.60759100	-0.11809400
H	4.52041100	-2.00987700	1.50005700

H	3.74117400	0.84079100	-1.60786700
C	-1.53986700	4.01084300	-0.12481000
H	-0.48360000	4.94170900	1.50728700
H	-2.48584300	2.81229000	-1.64373200
C	-3.47737600	-4.38174800	-0.72987000
O	-3.16606300	-5.02106200	-1.71590600
O	-4.63486500	-4.57548500	-0.05800800
C	-5.48728200	-5.60081200	-0.58992800
H	-4.97625000	-6.56729900	-0.58180500
H	-6.36058200	-5.62224800	0.06264700
H	-5.77902100	-5.36321500	-1.61645900
C	5.62178500	-0.79091600	-0.71843000
O	6.02093800	-0.20260800	-1.70453600
O	6.36851400	-1.69355300	-0.04293400
C	7.68429900	-1.91773100	-0.57142600
H	8.26384000	-0.99069500	-0.56443100
H	8.13962200	-2.66070400	0.08404600
H	7.62735600	-2.29197700	-1.59710700
C	-2.08780600	5.30944900	-0.65306800
F	-2.29453900	5.26296400	-1.98752900
F	-3.27569800	5.61727300	-0.08192300
F	-1.25450100	6.34408800	-0.40534500

P(*para*–COOMe–phenyl)(*para*–CF_3–phenyl)$_2$

0 1

P	0.03402400	-0.03055600	1.74068800
C	0.27529500	1.62081100	0.93385200
C	-1.51683500	-0.64653000	0.93666600
C	1.34558000	-1.06449000	0.93705800
C	1.18086900	2.50157100	1.54998400
C	-0.40484300	2.05359500	-0.21474800
C	-2.73058900	-0.29500100	1.55359400
C	-1.55473400	-1.45807200	-0.20905100
C	1.64894200	-2.29154300	1.55177500
C	2.06841900	-0.69096000	-0.20614000
C	1.41615000	3.77012300	1.02558700
H	1.70495300	2.19237700	2.45086800

C	-0.18129500	3.32744000	-0.73714900
H	-1.11341100	1.39521500	-0.70709500
C	-3.94937500	-0.72097100	1.03220900
H	-2.71949700	0.31381500	2.45441600
C	-2.77164700	-1.89502500	-0.72731400
H	-0.63121500	-1.75162700	-0.69797900
C	2.63079000	-3.13070400	1.03104300
H	1.11283100	-2.59219200	2.44847000
C	3.06110000	-1.52239800	-0.72461600
H	1.85795900	0.25315300	-0.69826800
C	0.73130900	4.18592400	-0.11981400
H	2.12628900	4.43655200	1.50422300
H	-0.70806600	3.64985000	-1.62950100
C	-3.97592300	-1.52775800	-0.11379100
H	-4.87932800	-0.44045900	1.51384700
H	-2.80890100	-2.52203100	-1.61229700
C	3.34141100	-2.74431200	-0.10892100
H	2.84728300	-4.08089300	1.50827100
H	3.60978800	-1.22636900	-1.61289200
C	4.44992700	-3.61669900	-0.63463500
C	0.93193100	5.58057900	-0.64984400
F	4.61991200	-3.46599600	-1.96648300
F	4.21273100	-4.92595300	-0.39914600
F	5.63456400	-3.32110100	-0.05096600
F	0.72005600	5.64753700	-1.98259200
F	0.08089200	6.45957900	-0.07160000
F	2.18315800	6.03236000	-0.41258100
C	-5.24630400	-2.02476800	-0.71686300
O	-5.30711700	-2.72358600	-1.70965600
O	-6.33797100	-1.61003300	-0.03563400
C	-7.59613800	-2.05473900	-0.56547200
H	-7.64694500	-3.14682700	-0.56765900
H	-8.35564400	-1.63580500	0.09523400
H	-7.73180200	-1.69175700	-1.58778000

P(*para*–COOMe–phenyl)$_2$(*para*–Ac–phenyl)

0 1

P	0.00037800	0.32359500	1.68585300
C	-1.34863900	-0.67880600	0.90699600
C	1.52711500	-0.36998400	0.89849100
C	-0.17776200	1.96449000	0.84463200
C	-2.61424200	-0.61929800	1.51704000
C	-1.17998700	-1.51032700	-0.21225500
C	2.12637200	-1.46879400	1.53947200
C	2.13415600	0.14719500	-0.25770200
C	0.49318200	3.05191300	1.42932300
C	-0.95935700	2.19588300	-0.30039700
C	-3.68758300	-1.34990300	1.01443400
H	-2.75791800	0.00204600	2.39771200
C	-2.24860700	-2.25158800	-0.71106400
H	-0.21092600	-1.57992400	-0.69608300
C	3.28532900	-2.05029500	1.03229200
H	1.68245300	-1.86887700	2.44784400
C	3.29996000	-0.42473200	-0.76169900
H	1.69535300	0.99957900	-0.76662000
C	0.40550100	4.32774200	0.87644500
H	1.08534900	2.89864500	2.32832600
C	-1.05567600	3.47253400	-0.84580800
H	-1.49428100	1.37417600	-0.76626200
C	-3.50887500	-2.17487200	-0.10478600
H	-4.66011100	-1.29252900	1.49026900
H	-2.12585100	-2.89563500	-1.57585200
C	3.88174600	-1.52754100	-0.12362700
H	3.73593800	-2.90017200	1.53248900
H	3.77405600	-0.03103800	-1.65499600
C	-0.37360400	4.55419400	-0.26811300
H	0.93987900	5.14596900	1.34940100
H	-1.65639600	3.65842200	-1.73042600
C	-4.61373200	-2.99029600	-0.68581200
O	-4.49537800	-3.71854300	-1.65203700
O	-5.77885500	-2.83264100	-0.01734900
C	-6.88525700	-3.59076700	-0.52880700
H	-6.66680000	-4.66141800	-0.49204800
H	-7.72924300	-3.34826100	0.11764000

H	-7.09867000	-3.30838600	-1.56324400
C	5.12812100	-2.09674000	-0.71167000
O	5.67554700	-1.66772900	-1.70878900
O	5.59291300	-3.15609500	-0.01105600
C	-0.51592100	5.90597000	-0.90439600
O	-1.21000300	6.05326400	-1.89878500
C	6.79228400	-3.75251000	-0.52711300
H	7.60871200	-3.02539500	-0.53806400
H	7.02170600	-4.57790900	0.14749100
H	6.63156200	-4.11956600	-1.54435100
C	0.21877100	7.08705000	-0.29121000
H	-0.09823400	7.25408100	0.74535100
H	1.30178800	6.91480600	-0.27765500
H	0.00241000	7.97830400	-0.88261100

P(*para*–COOMe–phenyl)(*para*–Ac–phenyl)$_2$

0 1

P	-0.32969600	0.00083900	1.65941600
C	-0.98700300	-1.52679700	0.84361400
C	1.34674800	0.18101000	0.89243000
C	-1.29933800	1.34692700	0.83493700
C	-2.11915000	-2.11957000	1.42785900
C	-0.41236100	-2.14311600	-0.28127700
C	2.40867300	-0.48572500	1.52895400
C	1.62530600	0.95923400	-0.24309000
C	-1.28088400	2.60939800	1.45148100
C	-2.07013100	1.17991900	-0.32854900
C	-2.67534800	-3.27977700	0.89334400
H	-2.56590000	-1.67110000	2.31197500
C	-0.96156000	-3.30823400	-0.80800100
H	0.46767200	-1.70982200	-0.74620300
C	3.70811500	-0.39822200	1.03669100
H	2.21532600	-1.07504400	2.42203700
C	2.92593400	1.05857400	-0.73164700
H	0.82421600	1.48973500	-0.74792200
C	-1.99221100	3.67928500	0.91229100
H	-0.70838300	2.75416400	2.36450200

C	-2.78942900	2.24584200	-0.86040000
H	-2.10726200	0.21247900	-0.81958900
C	-2.10047500	-3.89055400	-0.23125300
H	-3.55328000	-3.71023200	1.36523600
H	-0.52395800	-3.78902700	-1.67707600
C	3.97474200	0.37949700	-0.09870300
H	4.51830800	-0.92055100	1.53295800
H	3.14859000	1.65738500	-1.60890900
C	-2.75861300	3.50915000	-0.25037400
H	-1.95354200	4.64340200	1.41001700
H	-3.38583600	2.12467500	-1.75906300
C	-2.64613000	-5.14582800	-0.84714700
O	-2.10609600	-5.64239600	-1.82384300
C	-3.55443600	4.61882700	-0.87338100
O	-4.21174000	4.41864100	-1.88334500
C	-3.52735100	5.99426700	-0.22693900
H	-3.90356500	5.95385200	0.80248000
H	-2.50598100	6.39160300	-0.18589300
H	-4.15369400	6.66841500	-0.81354100
C	-3.88131300	-5.78683500	-0.23566600
H	-3.70358300	-6.06804700	0.80941900
H	-4.73235900	-5.09520400	-0.24748400
H	-4.13323100	-6.67903100	-0.81134600
C	5.34463900	0.52342400	-0.66984800
O	5.61405000	1.19301800	-1.64808100
O	6.26946700	-0.17932300	0.02273500
C	7.61148600	-0.08459100	-0.47798500
H	7.95581000	0.95293500	-0.45954400
H	8.21574400	-0.70202100	0.18732400
H	7.66542800	-0.45728600	-1.50438600

P(*para*–COOMe–phenyl)$_2$(*para*–CN–phenyl)

0 1

P	-0.01138000	0.68127300	1.62031600
C	-1.37858300	-0.31570800	0.86789500
C	1.50593600	-0.06355400	0.86360600
C	-0.14955400	2.29783900	0.72308300

C	-2.63634100	-0.23659700	1.49160000
C	-1.23058300	-1.15939800	-0.24527300
C	2.10932800	-1.11910900	1.56947300
C	2.09782300	0.37089500	-0.33400400
C	0.60984300	3.37008700	1.22603100
C	-0.99060600	2.52896900	-0.37677600
C	-3.72308500	-0.96035700	1.00733900
H	-2.76318500	0.39361100	2.36852400
C	-2.31268700	-1.89311200	-0.72566800
H	-0.26710100	-1.24540300	-0.73762600
C	3.25871700	-1.73938600	1.08630700
H	1.67706500	-1.45390600	2.50923800
C	3.25333600	-0.24016400	-0.81489400
H	1.65645200	1.19000000	-0.89306900
C	0.55162900	4.62941000	0.63984400
H	1.25118900	3.21730900	2.09037100
C	-1.06693500	3.78935900	-0.96547100
H	-1.59200100	1.72064000	-0.77968400
C	-3.56531400	-1.79670600	-0.10629000
H	-4.68951300	-0.88877200	1.49351200
H	-2.20653700	-2.54700400	-1.58523100
C	3.83951400	-1.29988000	-0.11108300
H	3.71365600	-2.55512300	1.63679600
H	3.71626400	0.08934100	-1.73945100
C	-0.29318300	4.84745300	-0.46248400
H	1.14517200	5.44872900	1.03258700
H	-1.71970600	3.95901400	-1.81595000
C	-4.68573500	-2.60527200	-0.66860800
O	-4.58506000	-3.34009900	-1.63165000
O	-5.84001900	-2.43224100	0.01332400
C	-6.96053900	-3.18371500	-0.47822300
H	-6.75094800	-4.25590000	-0.43706500
H	-7.79323700	-2.92911700	0.17800700
H	-7.18505500	-2.90593900	-1.51150300
C	5.07490600	-1.91487700	-0.67761800
O	5.60480200	-1.56030000	-1.71248900
O	5.54821700	-2.92230700	0.08941900

C	6.73764100	-3.55941100	-0.40175200
H	7.55535500	-2.83784900	-0.47860600
H	6.97587400	-4.33449400	0.32718400
H	6.55868200	-3.99847900	-1.38684600
C	-0.36828000	6.14601700	-1.06611900
N	-0.42839200	7.19958800	-1.55574800

P(*para*–COOMe–phenyl)(*para*–CN–phenyl)$_2$

0 1

P	0.72336800	0.01848600	1.55323900
C	1.40197500	1.51992000	0.70441400
C	-0.97481400	-0.12751300	0.83094400
C	1.63681500	-1.35954600	0.71507800
C	2.57858200	2.07418300	1.24013500
C	0.79754700	2.15588400	-0.39160700
C	-2.01513100	0.50618500	1.53272800
C	-1.28683600	-0.84305700	-0.33705900
C	1.56032100	-2.62726800	1.31962100
C	2.42137800	-1.21204500	-0.43978400
C	3.15108400	3.21514100	0.68820800
H	3.04868500	1.60985300	2.10332200
C	1.35482600	3.30599900	-0.94578100
H	-0.11582100	1.75325600	-0.81726600
C	-3.32854000	0.44720800	1.07282300
H	-1.79467800	1.04508300	2.45090100
C	-2.60061700	-0.91238500	-0.79410700
H	-0.50269300	-1.35010400	-0.89060400
C	2.22678700	-3.72178500	0.77974600
H	0.97565200	-2.75748800	2.22670900
C	3.10344400	-2.29827600	-0.98335600
H	2.50374900	-0.24315700	-0.92148500
C	2.53806800	3.84089800	-0.41095900
H	4.06147700	3.63279500	1.10593500
H	0.88133100	3.79205300	-1.79293900
C	-3.62842500	-0.26621400	-0.09540600
H	-4.12320200	0.94214200	1.61957900
H	-2.85058100	-1.46294700	-1.69524500

C	3.00732000	-3.56173200	-0.37816600
H	2.15783600	-4.69686700	1.25111000
H	3.70795500	-2.17571900	-1.87646700
C	3.70686500	-4.68261500	-0.93556100
N	4.27337100	-5.59232500	-1.38791900
C	3.11533400	5.02379600	-0.98022900
N	3.58438800	5.98244300	-1.44294800
C	-5.01513100	-0.37559800	-0.63645500
O	-5.30913800	-0.98329300	-1.64705600
O	-5.91831500	0.28103900	0.12397900
C	-7.27555100	0.21571700	-0.34203900
H	-7.61845400	-0.82165800	-0.37824800
H	-7.85923900	0.78910300	0.37851500
H	-7.35902500	0.65217800	-1.34084200

P(*para*−COOMe−phenyl)$_2$(*para*−NO$_2$−phenyl)

0 1

P	0.00179600	0.34286200	1.67453600
C	-1.35077400	-0.65434700	0.89726200
C	1.53058700	-0.34711400	0.89060600
C	-0.16366700	1.98581000	0.83202500
C	-2.59506000	-0.65037900	1.55183400
C	-1.20284500	-1.42867000	-0.26529200
C	2.17395200	-1.39202800	1.57625300
C	2.09017400	0.11465400	-0.31262500
C	0.66513400	3.02525100	1.29638800
C	-1.09834800	2.26878200	-0.17708700
C	-3.67045600	-1.38003000	1.05053200
H	-2.72013600	-0.07504200	2.46589700
C	-2.27276300	-2.16830800	-0.76297100
H	-0.24880500	-1.45636400	-0.78217300
C	3.33226900	-1.97539600	1.06852000
H	1.76635600	-1.74737400	2.51941500
C	3.25390000	-0.45959600	-0.81806400
H	1.61735300	0.92647700	-0.85650400
C	0.58322700	4.30510800	0.75886400
H	1.38099600	2.83100800	2.09088500

C	-1.20113600	3.54960300	-0.71782900
H	-1.75116200	1.48607200	-0.54835200
C	-3.51295500	-2.14676100	-0.11186100
H	-4.62699300	-1.36680300	1.56071500
H	-2.16691900	-2.76940400	-1.66026100
C	3.88063800	-1.50892900	-0.13373800
H	3.81876600	-2.78304000	1.60372700
H	3.69221200	-0.10921800	-1.74691900
C	-0.35571400	4.54902100	-0.24324100
H	1.21904100	5.11083700	1.10459700
H	-1.91619100	3.78046000	-1.49806500
C	-4.62108200	-2.95831900	-0.69471200
O	-4.51946300	-3.63592100	-1.69863100
O	-5.76433800	-2.85828400	0.01919400
C	-6.87296900	-3.61609700	-0.48968600
H	-6.63112400	-4.68204200	-0.51096400
H	-7.69815500	-3.42248900	0.19615700
H	-7.12793800	-3.29012200	-1.50156800
C	5.12326800	-2.08409900	-0.72636200
O	5.62568300	-1.70474500	-1.76605800
O	5.63708800	-3.08442400	0.02329400
C	6.83587200	-3.68335100	-0.49293800
H	7.63158600	-2.93828300	-0.57594500
H	7.10750900	-4.45795300	0.22470600
H	6.65313900	-4.11829000	-1.47914800
N	-0.45811600	5.90183500	-0.81183200
O	0.30350700	6.76359500	-0.37365500
O	-1.29837600	6.08939900	-1.69122700

P(*para*–COOMe–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

P	-0.35416200	0.00038300	1.65010300
C	-1.05288200	-1.50942100	0.83327000
C	1.32300800	0.15260600	0.88345600
C	-1.29391100	1.37011300	0.82690000
C	-2.25152000	-2.02065800	1.36588000
C	-0.43644300	-2.19601400	-0.22541000

C	2.39490300	-0.41544000	1.59320000
C	1.58818700	0.80950200	-0.33000900
C	-1.17542100	2.64869000	1.40312100
C	-2.13362400	1.20592800	-0.28698400
C	-2.83599200	-3.17101900	0.84547800
H	-2.72994000	-1.51615100	2.20133500
C	-1.00305600	-3.35683000	-0.74952400
H	0.49186200	-1.82536100	-0.64689100
C	3.69553800	-0.34911600	1.09814600
H	2.20966800	-0.90799500	2.54447800
C	2.88833600	0.88563700	-0.82265700
H	0.77814500	1.26524200	-0.89097900
C	-1.85668700	3.74067000	0.87495700
H	-0.54687000	2.79023000	2.27837000
C	-2.83191700	2.28786000	-0.82083800
H	-2.24658900	0.22914200	-0.74534100
C	-2.19736700	-3.82463100	-0.20738900
H	-3.76019800	-3.57170100	1.24334700
H	-0.53950100	-3.89615600	-1.56659200
C	3.94868100	0.30517200	-0.11450300
H	4.51555900	-0.79290800	1.65126500
H	3.10299100	1.39086200	-1.75874200
C	-2.67970300	3.54063800	-0.23227400
H	-1.77075100	4.73012800	1.30690000
H	-3.48160900	2.17639500	-1.68040400
N	-3.41296000	4.68759300	-0.79356300
O	-3.25880800	5.78141500	-0.25206800
O	-4.13295200	4.48079000	-1.76935400
N	-2.80161500	-5.04889200	-0.75921300
O	-2.21381600	-5.60677300	-1.68473600
O	-3.85739400	-5.43666100	-0.26081900
C	5.31938000	0.41868500	-0.69546200
O	5.57251200	0.97699000	-1.74471600
O	6.25654400	-0.17252900	0.07664800
C	7.60058800	-0.10032400	-0.42602900
H	7.91573000	0.94148700	-0.52741800
H	8.21538500	-0.61868900	0.31010400

H	7.67129700	-0.58933400	-1.40114900

P(*para*−COOMe−phenyl)$_2$(*para*−OMe−phenyl)

0 1

P	0.00745100	0.55156900	1.69324700
C	-1.28296100	-0.53040800	0.91610400
C	1.56671200	-0.06724600	0.90667000
C	-0.29093300	2.17073700	0.86175000
C	-2.56176300	-0.51143200	1.50134200
C	-1.06193000	-1.37639600	-0.18318300
C	2.11353000	-1.25962000	1.41656700
C	2.26748800	0.61245900	-0.10201200
C	0.06788700	3.33654900	1.56582900
C	-0.86553700	2.32328600	-0.40734300
C	-3.59478600	-1.29535400	0.99606000
H	-2.74701400	0.12221600	2.36532900
C	-2.09060300	-2.16991600	-0.68629100
H	-0.08186000	-1.41729500	-0.64775800
C	3.30735300	-1.77272300	0.91912300
H	1.59822200	-1.79035300	2.21378400
C	3.46973400	0.10878600	-0.59416400
H	1.87159400	1.53891100	-0.50513000
C	-0.12221000	4.59804800	1.01815500
H	0.49926000	3.25048700	2.56019200
C	-1.07200800	3.58547200	-0.96873600
H	-1.16627800	1.44667300	-0.97385900
C	-3.36375300	-2.13402600	-0.10393500
H	-4.57695400	-1.26903700	1.45470500
H	-1.92587700	-2.82407600	-1.53650200
C	3.99678500	-1.08731600	-0.09217100
H	3.71405200	-2.69622100	1.31591200
H	4.01479800	0.62977500	-1.37477500
C	-0.69616800	4.73192700	-0.25571900
H	0.15566800	5.49718700	1.55917700
H	-1.52311700	3.66166000	-1.95164600
C	-4.42355200	-3.00346800	-0.68731800
O	-4.26272500	-3.74059800	-1.64105000

O	-5.60496600	-2.88648500	-0.03721900
C	-6.66877300	-3.70054900	-0.55122100
H	-6.40427300	-4.75995600	-0.49442500
H	-7.53209000	-3.48605200	0.07958500
H	-6.88014800	-3.44464900	-1.59305600
C	5.28329600	-1.57741000	-0.66103800
O	5.90983600	-1.01185900	-1.53655800
O	5.69069100	-2.73767800	-0.09536000
C	6.92593700	-3.26368600	-0.60121600
H	7.74161000	-2.55395500	-0.43837000
H	7.10146800	-4.18469700	-0.04427900
H	6.84618900	-3.47060800	-1.67191500
O	-0.85007000	6.00818000	-0.70378800
C	-1.42862100	6.21053000	-1.98427200
H	-0.82543500	5.74857700	-2.77675100
H	-2.45147700	5.81455100	-2.03161800
H	-1.45297500	7.29139600	-2.13338000

P(*para*−COOMe−phenyl)(*para*−OMe−phenyl)$_2$

0 1

P	0.59181500	-0.00392500	1.67579400
C	1.11341700	1.57545100	0.87187100
C	-1.07467600	-0.28292000	0.91087900
C	1.65045900	-1.27504600	0.85390900
C	2.07908600	2.35449100	1.53865900
C	0.60777400	2.06164800	-0.34096900
C	-2.14017500	0.50889600	1.37924100
C	-1.35023300	-1.27512600	-0.04325300
C	1.84197200	-2.49366000	1.53442200
C	2.30109700	-1.10499200	-0.37444600
C	2.53230500	3.55449500	1.00807700
H	2.47685400	2.01375100	2.49160700
C	1.04572900	3.27304800	-0.88396900
H	-0.14872200	1.49543000	-0.87659200
C	-3.43273400	0.33354500	0.89674800
H	-1.95258500	1.27141300	2.13160500
C	-2.64553000	-1.46096000	-0.52248300

H	-0.54791100	-1.90415600	-0.41513000
C	2.62915500	-3.50472100	1.00019400
H	1.36764200	-2.64787600	2.50084300
C	3.10643000	-2.10790800	-0.92100400
H	2.18970800	-0.17219800	-0.91935200
C	2.01631900	4.02440500	-0.20977900
H	3.27723400	4.15435200	1.52175600
H	0.62540500	3.61618200	-1.82271600
C	-3.69561600	-0.65821700	-0.06077100
H	-4.24273000	0.95470600	1.26275900
H	-2.86192700	-2.22520200	-1.26219700
C	3.27012900	-3.31768900	-0.23438800
H	2.77441800	-4.44483600	1.52329300
H	3.59688600	-1.93481700	-1.87239400
C	2.02463000	5.74838500	-1.86382100
H	2.23300100	5.07976800	-2.70958900
H	0.94468800	5.94057100	-1.81451300
H	2.55232900	6.69224100	-2.01241100
C	4.70704300	-4.23078000	-1.91073000
H	4.00497700	-4.07894500	-2.74124000
H	5.42675500	-3.40174000	-1.89131900
H	5.24301300	-5.16995800	-2.05931600
O	4.02879500	-4.36200300	-0.67153300
O	2.51600800	5.21582300	-0.64413500
C	-5.05651500	-0.90114400	-0.61231400
O	-5.32420900	-1.74556700	-1.44599600
O	-5.98630500	-0.06988700	-0.08346800
C	-7.32101700	-0.25594700	-0.57399700
H	-7.67296300	-1.26858800	-0.35860500
H	-7.93071300	0.48142800	-0.05051800
H	-7.36117900	-0.09111200	-1.65428600

P(*para*−COOMe−phenyl)$_2$(*para*−Me−phenyl)

0 1

P	-0.01340600	0.90994000	1.55170500
C	-1.36855400	-0.13785500	0.84173800
C	1.50609600	0.13002700	0.83374800

C	-0.18551200	2.47886300	0.58987300
C	-2.64493500	0.00382700	1.41495600
C	-1.19841800	-1.07179600	-0.19347600
C	1.98572900	-1.03303800	1.46419500
C	2.23622600	0.65770800	-0.24301000
C	0.29951000	3.65325500	1.18720400
C	-0.77632900	2.57758200	-0.68001400
C	-3.72452000	-0.74685400	0.95846900
H	-2.79172200	0.70709200	2.23115800
C	-2.27401500	-1.83231400	-0.64666300
H	-0.22165900	-1.20679200	-0.64707000
C	3.14283700	-1.66558500	1.02004000
H	1.44712200	-1.44543300	2.31420800
C	3.40219700	0.03450200	-0.68273500
H	1.89224800	1.55848300	-0.74081400
C	0.21304800	4.88024200	0.53003600
H	0.74862300	3.60660000	2.17658000
C	-0.86864600	3.80863300	-1.32811300
H	-1.16766000	1.68895300	-1.16672200
C	-3.54392900	-1.67443400	-0.07750400
H	-4.70440700	-0.62582500	1.40661700
H	-2.14899100	-2.55439500	-1.44718700
C	3.86224100	-1.13178700	-0.05924000
H	3.49799000	-2.56504600	1.51041900
H	3.96983600	0.43737600	-1.51540400
C	-0.37708500	4.98096300	-0.73644600
H	0.60286800	5.77424200	1.01181100
H	-1.32922000	3.85993600	-2.31251100
C	-4.65531500	-2.51481900	-0.60543400
O	-4.53828300	-3.32764400	-1.50224000
O	-5.82890000	-2.27632300	0.02501600
C	-6.94105900	-3.05569500	-0.43815000
H	-6.74510300	-4.12298900	-0.30401900
H	-7.79090900	-2.74203600	0.16896400
H	-7.13204900	-2.86190400	-1.49716500
C	5.11272100	-1.75449300	-0.57708200
O	5.76455500	-1.32055100	-1.50744000

O	5.45453700	-2.87269400	0.10449100
C	6.65170200	-3.52199800	-0.34707700
H	7.50990500	-2.85010400	-0.25997200
H	6.77607100	-4.38983200	0.30147100
H	6.55057800	-3.83258400	-1.39055400
C	-0.50875800	6.31585400	-1.43127500
H	-0.45305300	6.20860200	-2.51993200
H	-1.47308500	6.78856300	-1.20098800
H	0.27702900	7.01094700	-1.11732100

P(*para*–COOMe–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	0.96405800	0.02964000	1.45550200
C	1.56052000	1.54745400	0.58144100
C	-0.76034900	-0.13874300	0.79523900
C	1.87238000	-1.33499800	0.59826300
C	2.63996000	2.23719900	1.15724200
C	1.00539200	2.06081200	-0.60119200
C	-1.73873000	0.72006500	1.33020700
C	-1.15958500	-1.10358400	-0.14320500
C	1.98367700	-2.55741200	1.28122700
C	2.47468700	-1.22783700	-0.66454100
C	3.15640800	3.38718200	0.56233000
H	3.07968200	1.86984400	2.08169800
C	1.51991900	3.21782900	-1.18699100
H	0.16476300	1.55630600	-1.06858800
C	-3.06735900	0.63580700	0.92705800
H	-1.45457800	1.46225800	2.07254400
C	-2.49140700	-1.19866400	-0.54188400
H	-0.42639000	-1.78262400	-0.56621800
C	2.65432900	-3.63926700	0.71247200
H	1.54051800	-2.66287800	2.26896500
C	3.15439200	-2.30989700	-1.22402300
H	2.41503400	-0.29382500	-1.21531000
C	2.60241000	3.90165300	-0.61768200
H	3.99735700	3.89842000	1.02612800
H	1.07315800	3.59491400	-2.10471300

C	-3.45442000	-0.32995200	-0.01433200
H	-3.80956400	1.30777200	1.34348200
H	-2.80398100	-1.94161900	-1.26872800
C	3.25679600	-3.53340900	-0.54824700
H	2.71852800	-4.57733200	1.25974300
H	3.61207300	-2.20242400	-2.20535700
C	4.02049800	-4.69180800	-1.14605100
H	5.07580300	-4.67029500	-0.84204500
H	3.60958000	-5.65380000	-0.82136600
H	3.99807600	-4.66480500	-2.24075200
C	3.13529000	5.17177500	-1.23850400
H	2.63893000	6.05721000	-0.81876000
H	4.20947600	5.28696200	-1.05769000
H	2.96904600	5.18967400	-2.32089300
C	-4.86036700	-0.47788300	-0.48114300
O	-5.23519500	-1.30045500	-1.29496900
O	-5.69653000	0.41385700	0.10189800
C	-7.06841100	0.32182400	-0.30628600
H	-7.47588900	-0.66443200	-0.06766700
H	-7.59249000	1.09865800	0.25165000
H	-7.16236000	0.49131700	-1.38247200

P(*para*−COOMe−phenyl)$_2$(*para*−NMe$_2$−phenyl)

0 1

P	0.01205400	0.28877400	1.69157900
C	-1.15306300	-0.93067700	0.91786200
C	1.62828000	-0.16169500	0.90442700
C	-0.46625900	1.86053000	0.86659100
C	-2.42477600	-1.05276600	1.50621100
C	-0.84569400	-1.74483300	-0.18478400
C	2.27738600	-1.31915700	1.37393800
C	2.27903400	0.62451900	-0.05938600
C	-0.31104200	3.05391300	1.59060700
C	-0.99800900	1.96296600	-0.43003600
C	-3.36789200	-1.94334400	1.00215500
H	-2.67532300	-0.44438400	2.37189400
C	-1.78332700	-2.64431300	-0.68733800

H	0.13135100	-1.67739900	-0.65254100
C	3.52224800	-1.69568400	0.88011300
H	1.80124600	-1.93149100	2.13632000
C	3.53138800	0.25787700	-0.54781500
H	1.80318600	1.52647900	-0.43039000
C	-0.64406400	4.29113600	1.05082100
H	0.07524200	3.01570600	2.60666900
C	-1.34386300	3.18963700	-0.98340400
H	-1.15667200	1.06512400	-1.02115600
C	-3.05088500	-2.74932600	-0.10102600
H	-4.34554300	-2.02528900	1.46396200
H	-1.55113900	-3.27383700	-1.54042700
C	4.16101900	-0.90469800	-0.08680900
H	4.00736900	-2.59402000	1.24538500
H	4.03727100	0.86166600	-1.29446800
C	-1.16409100	4.39488500	-0.26097900
H	-0.50654400	5.17731900	1.65874500
H	-1.75933800	3.20792300	-1.98401500
C	-4.01120000	-3.72730100	-0.68324100
O	-3.77528800	-4.44092400	-1.63942300
O	-5.19679400	-3.74161700	-0.02911500
C	-6.16637600	-4.66556800	-0.54263800
H	-5.78759900	-5.68996900	-0.49002400
H	-7.04621100	-4.54876300	0.09110800
H	-6.40788700	-4.43173000	-1.58315900
C	5.49665700	-1.24672900	-0.64890200
O	6.08369000	-0.58686200	-1.48518500
O	6.00152800	-2.38936800	-0.12607700
C	7.28857200	-2.77458100	-0.62845300
H	8.03177700	-2.00081800	-0.41717700
H	7.54018300	-3.70019200	-0.10948500
H	7.24703600	-2.93837200	-1.70879100
N	-1.48408300	5.62163700	-0.81612800
C	-1.43211900	6.81919300	0.00511400
C	-2.16556300	5.67762100	-2.09848500
H	-2.12966200	6.78021500	0.85642700
H	-0.42258700	6.98352900	0.40213000

H	-1.69060500	7.68473500	-0.60766400
H	-1.56560000	5.20734200	-2.88758800
H	-3.14850800	5.18170600	-2.07791500
H	-2.31693100	6.72197800	-2.37750300

P(*para*–COOMe–phenyl)(*para*–NMe_2–phenyl)$_2$

0 1

P	-0.31004000	0.00206100	-1.66567600
C	-0.63560100	1.63356300	-0.87245600
C	1.31765600	-0.46450600	-0.90837600
C	-1.50139700	-1.14038300	-0.84535400
C	-1.44079500	2.55088200	-1.56657200
C	-0.13291500	2.04381800	0.37331200
C	2.44658400	0.30680800	-1.24591600
C	1.50484900	-1.59855400	-0.10192700
C	-1.91039500	-2.27887900	-1.55844900
C	-2.06263800	-0.95032900	0.42733700
C	-1.75282000	3.80160100	-1.04486600
H	-1.82968400	2.28411100	-2.54680000
C	-0.42710000	3.29398000	0.90753800
H	0.51706900	1.38041100	0.93727100
C	3.71298100	-0.02805400	-0.77998800
H	2.32843900	1.18326400	-1.87861400
C	2.77326200	-1.94300100	0.36049700
H	0.65219000	-2.21252200	0.16973400
C	-2.80856500	-3.19916100	-1.02808100
H	-1.52151800	-2.44941200	-2.56009000
C	-2.96969500	-1.85345000	0.97017600
H	-1.79895500	-0.06965000	1.00611700
C	-1.26101600	4.20575800	0.21808500
H	-2.37340000	4.46842600	-1.63163900
H	-0.00047100	3.55950300	1.86770200
C	3.88716400	-1.16174400	0.02961500
H	4.57131200	0.58016000	-1.04351100
H	2.91911500	-2.81679800	0.98770700
C	-3.35787200	-3.01607700	0.26206900
H	-3.08943400	-4.05612500	-1.62870200

H	-3.37952600	-1.64812200	1.95218500
N	-4.23892600	-3.93680200	0.81136700
N	-1.58307400	5.44298300	0.75907300
C	-0.89231000	5.90292300	1.95175500
H	-1.06117300	5.21978800	2.79293800
H	0.19565100	5.99933200	1.80601400
H	-1.28638600	6.88007900	2.23820700
C	-2.26918600	6.42486100	-0.06315100
H	-1.68864300	6.72025200	-0.95200700
H	-3.23892500	6.04316400	-0.40461600
H	-2.45980800	7.31953200	0.53304800
C	-4.93515500	-3.61355200	2.04493000
H	-4.22632500	-3.43689200	2.86298000
H	-5.57659000	-2.72233400	1.95316700
H	-5.56400200	-4.45868800	2.33204900
C	-4.76306000	-5.00756400	-0.01899600
H	-5.34386400	-4.63692800	-0.87893500
H	-3.95329900	-5.63850500	-0.40504400
H	-5.41454600	-5.64214700	0.58517600
C	5.21448500	-1.57637600	0.55566300
O	5.40880900	-2.54911700	1.26042400
O	6.21146300	-0.74422100	0.16497000
C	7.51783600	-1.09363200	0.63982400
H	7.80551700	-2.08667900	0.28334100
H	8.18885300	-0.33325600	0.23810200
H	7.54502500	-1.09101900	1.73313000

P(*para*–CF_3–phenyl)$_2$(*para*–Ac–phenyl)

0 1

P	-0.01485700	0.29713900	-1.71182700
C	-1.38426800	-0.67090200	-0.92196100
C	-0.14988100	1.94083900	-0.86857300
C	1.49722500	-0.43626200	-0.93051700
C	-1.77988400	-1.85403900	-1.56921000
C	-2.06287800	-0.28545000	0.24434700
C	-1.00340900	2.88681600	-1.46093500
C	0.56189800	2.30940000	0.28606700

C	2.72854200	-0.15146100	-1.54547500
C	1.48809900	-1.27332600	0.19561100
C	-2.80965000	-2.64043400	-1.05836400
H	-1.27878000	-2.16143600	-2.48366400
C	-3.10229700	-1.06368700	0.75362800
H	-1.78070100	0.62628300	0.76116400
C	-1.15990300	4.15529600	-0.90590100
H	-1.54579400	2.62965500	-2.36758600
C	0.41285600	3.57979300	0.83425600
H	1.23587300	1.60050500	0.75693500
C	3.91847000	-0.67024100	-1.04107300
H	2.75607000	0.48067900	-2.42950000
C	2.67588000	-1.80496000	0.69755500
H	0.55083000	-1.51350800	0.68722300
C	-3.47497700	-2.24325200	0.10492400
H	-3.09819500	-3.55767900	-1.56123000
H	-3.61607000	-0.75981200	1.65997700
C	-0.45088200	4.51793600	0.24890200
H	-1.83022300	4.86222500	-1.38503500
H	0.95821200	3.87132000	1.72619400
C	3.89246100	-1.50185700	0.08205300
H	4.86388300	-0.43328500	-1.51804900
H	2.65808700	-2.44617300	1.57290400
C	5.16822600	-2.11978900	0.58910800
C	-4.63301300	-3.05427400	0.62230800
F	5.11507600	-2.36507400	1.91660700
F	6.23589000	-1.32299400	0.36362000
F	5.42420800	-3.30112400	-0.01936500
F	-4.77019400	-2.93733100	1.96131100
F	-5.80337500	-2.65753100	0.07081900
F	-4.49161400	-4.36798300	0.33977900
C	-0.56993700	5.87066400	0.88968600
O	0.06646100	6.13564900	1.89791100
C	-1.49501500	6.90100500	0.26332000
H	-1.19462200	7.12629900	-0.76713600
H	-2.52851600	6.53548100	0.22963300
H	-1.45479000	7.81459600	0.85879000

P(*para*−CF_3−phenyl)(*para*−Ac−phenyl)$_2$

0 1

P	-0.30498700	0.01674900	1.67352900
C	1.37611400	-0.12960000	0.90673700
C	-0.99235700	1.52396300	0.84405800
C	-1.24509000	-1.35528100	0.85874200
C	2.30163800	-0.96008900	1.56148900
C	1.78734700	0.55254000	-0.24863800
C	-0.73855700	2.75919000	1.46363800
C	-1.76853400	1.50783400	-0.32779400
C	-2.47912600	-1.70373200	1.43366800
C	-0.79373900	-2.08543500	-0.25405100
C	3.59444100	-1.12065800	1.06875700
H	2.00826400	-1.48431100	2.46754200
C	3.08425500	0.40400400	-0.73963300
H	1.09362000	1.20314600	-0.77151900
C	-1.22576600	3.94575900	0.91928000
H	-0.15916900	2.79119600	2.38319600
C	-2.26339700	2.69216200	-0.86540200
H	-1.98662200	0.56525100	-0.82028500
C	-3.25084700	-2.73406800	0.90094000
H	-2.83648200	-1.16655100	2.30895900
C	-1.55977200	-3.12204200	-0.77882400
H	0.16026100	-1.84274600	-0.71153500
C	3.98839200	-0.43454700	-0.08341800
H	4.29625500	-1.77375100	1.57709200
H	3.38991300	0.93086300	-1.63781700
C	-1.99716600	3.92593300	-0.25223400
H	-1.00882000	4.88448700	1.41970700
H	-2.86218700	2.68796300	-1.77062000
C	-2.79835100	-3.45841200	-0.21205500
H	-4.20217300	-2.97539100	1.36506400
H	-1.21808400	-3.68949000	-1.63859500
C	-2.55771300	5.16806600	-0.88215300
O	-3.22550700	5.09743800	-1.90244200
C	-3.57842200	-4.58457700	-0.82602300

O	-3.13923700	-5.18631000	-1.79397500
C	-2.27914500	6.51215900	-0.22961800
H	-2.67019400	6.54213600	0.79461000
H	-1.20159900	6.70848900	-0.17348700
H	-2.75803400	7.29393100	-0.82152400
C	-4.92203800	-4.96112300	-0.22356700
H	-4.81341300	-5.26342900	0.82509400
H	-5.61785300	-4.11377000	-0.24874900
H	-5.34175100	-5.78988600	-0.79614900
C	5.40480100	-0.55088000	-0.57989000
F	6.20918100	0.37589200	-0.00889900
F	5.93814100	-1.75983000	-0.29762100
F	5.48590400	-0.37110400	-1.91643800

P(*para*–CF_3–phenyl)$_2$(*para*–CN–phenyl)

0 1

P	-0.00020100	0.65266400	1.64923400
C	0.00673000	2.27230500	0.74754400
C	-1.44637500	-0.22518000	0.89410100
C	1.44763000	-0.22356400	0.89447300
C	0.85011700	3.27685700	1.25618100
C	-0.79996500	2.57091100	-0.36180300
C	-2.69232200	-0.04468800	1.51888500
C	-1.37154800	-1.07189200	-0.22248000
C	1.95769000	-1.32618400	1.60072800
C	2.07382100	0.15483600	-0.30321900
C	0.90725900	4.53421100	0.66536200
H	1.46606200	3.07313900	2.12844500
C	-0.76065100	3.83079800	-0.95515600
H	-1.46587200	1.81672600	-0.76826900
C	-3.83530800	-0.67482200	1.03237000
H	-2.76829000	0.59244300	2.39643900
C	-2.51110100	-1.71428400	-0.70608300
H	-0.42056400	-1.23397300	-0.71974000
C	3.04980600	-2.04295700	1.11732500
H	1.49780200	-1.62483000	2.53934200
C	3.17457200	-0.55291500	-0.78543400

H	1.70369500	1.00620100	-0.86560600
C	0.09687800	4.81980700	-0.44718900
H	1.56485800	5.30076300	1.06250900
H	-1.38780500	4.05335600	-1.81264900
C	-3.74439100	-1.51404700	-0.08149300
H	-4.79376400	-0.51868200	1.51648100
H	-2.44362600	-2.36272800	-1.57361900
C	3.66178300	-1.65408200	-0.07742900
H	3.42786700	-2.89931100	1.66606600
H	3.64799300	-0.25580400	-1.71562000
C	-4.96444200	-2.25011900	-0.56913400
C	4.88379000	-2.38478800	-0.56817300
F	6.01785400	-1.85311600	-0.05723300
F	4.99439700	-2.33040800	-1.91336700
F	4.86487300	-3.68774200	-0.21196000
F	-5.10718200	-3.44158500	0.05515200
F	-4.90046900	-2.50474900	-1.89422300
F	-6.09646500	-1.54873600	-0.34195200
C	0.14204600	6.11675400	-1.05725900
N	0.18020900	7.16828900	-1.55325200

P(*para*−CF_3−phenyl)(*para*−CN−phenyl)$_2$

0 1

P	-0.69886400	0.00044600	1.56753400
C	-1.49941600	-1.44002800	0.72011500
C	1.00966800	-0.00055400	0.85221400
C	-1.48499200	1.44920100	0.71983900
C	-2.72537800	-1.88363600	1.24829500
C	-0.94437200	-2.13491200	-0.36610100
C	1.98968300	-0.71928900	1.55760500
C	1.38657400	0.68330800	-0.31411300
C	-1.30874200	2.70683000	1.32451700
C	-2.26590900	1.36613900	-0.44395500
C	-3.39237500	-2.97273900	0.69781100
H	-3.15992900	-1.37364700	2.10431900
C	-1.59690600	-3.23479100	-0.91838200
H	0.00512700	-1.81880100	-0.78564200

C	3.30544700	-0.77040600	1.10280300
H	1.72177500	-1.24079900	2.47297800
C	2.70495700	0.64415400	-0.76692100
H	0.65067600	1.25130600	-0.87443800
C	-1.87397100	3.85281900	0.77578100
H	-0.72622800	2.78872400	2.23861000
C	-2.84717300	2.50520000	-0.99648500
H	-2.42500400	0.40658100	-0.92517300
C	-2.82789800	-3.65820500	-0.39168600
H	-4.33999800	-3.30470700	1.10952600
H	-1.16089800	-3.76724800	-1.75770700
C	3.66478400	-0.08496500	-0.06071700
H	4.05129600	-1.33756400	1.64992500
H	2.98549000	1.17157700	-1.67287000
C	-2.65125400	3.75713600	-0.39134700
H	-1.72864100	4.81939100	1.24727900
H	-3.44977500	2.43258000	-1.89631000
C	-3.24584300	4.93226200	-0.95887100
N	-3.72652200	5.88580400	-1.42011600
C	-3.50352600	-4.78854600	-0.95952400
N	-4.05249100	-5.70420000	-1.42131500
C	5.09987200	-0.08205600	-0.51868400
F	5.79501500	0.93548200	0.03841700
F	5.19787300	0.05997300	-1.85829300
F	5.73519900	-1.22510400	-0.18086500

P(*para*–CF_3–phenyl)$_2$(*para*–NO_2–phenyl)

0 1

P	0.00733500	0.31686300	1.70514000
C	0.08459700	1.96412500	0.85833200
C	-1.47490000	-0.47577600	0.92698500
C	1.41953900	-0.58902500	0.91975000
C	1.04082200	2.87944400	1.33838900
C	-0.78007700	2.36946200	-0.17118400
C	-2.70660100	-0.28747000	1.57698700
C	-1.44045800	-1.26731300	-0.23131400
C	1.91169200	-1.71102400	1.60744600

C	2.03209200	-0.21877200	-0.28785300
C	1.15089700	4.15506500	0.79536300
H	1.70447300	2.59171900	2.14967700
C	-0.69028500	3.64886200	-0.71784500
H	-1.52969700	1.68486900	-0.55343200
C	-3.87524500	-0.85584500	1.07495100
H	-2.75131800	0.30660600	2.48629100
C	-2.60567500	-1.84817700	-0.73073000
H	-0.50115800	-1.43475000	-0.74856100
C	2.97395600	-2.45393400	1.09711700
H	1.46180900	-2.00411500	2.55255700
C	3.10258400	-0.95311100	-0.79714000
H	1.67498000	0.64704200	-0.83652900
C	0.27746300	4.52183800	-0.22803800
H	1.88566400	4.86588600	1.15294800
H	-1.34965500	3.97386400	-1.51345400
C	-3.82443800	-1.64049700	-0.08024500
H	-4.82233300	-0.69390500	1.57907400
H	-2.56958800	-2.45421000	-1.63018900
C	3.57268800	-2.07285500	-0.10659200
H	3.33878900	-3.32466200	1.63195900
H	3.56554500	-0.66235500	-1.73455800
C	-5.07329100	-2.31259400	-0.58760400
C	4.76404200	-2.83328700	-0.62730800
F	5.92230800	-2.33369100	-0.13918500
F	4.84619300	-2.77513200	-1.97428500
F	4.71838300	-4.13682200	-0.27625300
F	-5.24546900	-3.52923600	-0.02228100
F	-5.03345100	-2.50107800	-1.92450300
F	-6.17944300	-1.58895000	-0.30941600
N	0.37946000	5.87219500	-0.80437400
O	-0.40587500	6.16889000	-1.70388400
O	1.24501800	6.62050900	-0.35183600

P(*para*–CF_3–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

P	-0.33257300	0.01048100	1.66557900

C	-1.22806000	-1.39055300	0.84774600
C	1.35325900	-0.06976600	0.90459100
C	-1.07147500	1.49443800	0.83577000
C	-2.49046400	-1.72624100	1.37261400
C	-0.70594300	-2.16182300	-0.20325700
C	2.33089500	-0.79115800	1.61001800
C	1.71507700	0.55519300	-0.29926900
C	-0.80050100	2.74407700	1.42348900
C	-1.90116100	1.44504300	-0.29658300
C	-3.22634900	-2.78584400	0.85165700
H	-2.89990200	-1.15587900	2.20233600
C	-1.42568000	-3.23437400	-0.72769400
H	0.26851100	-1.92783500	-0.61857500
C	3.63046300	-0.90195100	1.11964300
H	2.07452400	-1.26727400	2.55293500
C	3.01704500	0.45594100	-0.78797500
H	0.98035900	1.12370200	-0.86071600
C	-1.32265200	3.91762400	0.88848500
H	-0.17867300	2.79889500	2.31313500
C	-2.44100300	2.61077700	-0.83771600
H	-2.13081000	0.49282500	-0.76307200
C	-2.67776000	-3.52738700	-0.19362900
H	-4.20052600	-3.05128600	1.24348600
H	-1.03604300	-3.83747500	-1.53875800
C	3.97493500	-0.27491300	-0.08034500
H	4.37479300	-1.47039100	1.66737800
H	3.28631100	0.93758600	-1.72237400
C	-2.13980700	3.83062200	-0.23741400
H	-1.11880200	4.88574600	1.32915400
H	-3.08115700	2.58838700	-1.71126800
N	-2.70467700	5.06588500	-0.80707500
O	-2.42145200	6.12788800	-0.25485900
O	-3.42270400	4.95805200	-1.79996500
N	-3.44382300	-4.65739400	-0.74629500
O	-2.93325400	-5.29559400	-1.66557500
O	-4.54691200	-4.89097800	-0.25463100
C	5.39496100	-0.33523800	-0.58057400

F	5.45390000	-0.26376600	-1.92788100
F	6.13261400	0.68991800	-0.09751900
F	6.01008800	-1.47675100	-0.20358500

P(*para*–CF_3–phenyl)$_2$(*para*–OMe–phenyl)

0 1

P	-0.00915000	0.51143100	-1.71286800
C	0.16383800	2.14993700	-0.88456600
C	1.36118800	-0.46849000	-0.93533900
C	-1.51352200	-0.22440900	-0.91616900
C	-0.31802700	3.27764900	-1.57787400
C	0.75754500	2.35618300	0.36798600
C	2.63318500	-0.35755100	-1.52366800
C	1.20759300	-1.32318900	0.16676300
C	-2.00657700	-1.42299000	-1.46241100
C	-2.21837500	0.36643900	0.14254900
C	-0.22796400	4.55176200	-1.03461500
H	-0.76603900	3.15181200	-2.56059300
C	0.86495700	3.63308500	0.92419300
H	1.15321700	1.51196200	0.92530900
C	3.72194700	-1.06231800	-1.01783200
H	2.77184000	0.28706300	-2.38803900
C	2.29293000	-2.04054800	0.67090300
H	0.23622400	-1.43226900	0.63831900
C	-3.15357300	-2.02534600	-0.95333900
H	-1.48722200	-1.88950400	-2.29605700
C	-3.37606300	-0.22612100	0.64805500
H	-1.86264900	1.29467800	0.57773100
C	0.36714900	4.73960100	0.22295300
H	-0.60022300	5.42116100	-1.56740700
H	1.33583300	3.75168100	1.89350700
C	3.55213000	-1.90894100	0.08201600
H	4.70060900	-0.95850700	-1.47520400
H	2.16274900	-2.69336600	1.52807100
C	-3.84332900	-1.42423700	0.10442800
H	-3.51524000	-2.95730900	-1.37574000
H	-3.90953900	0.23746900	1.47165200

C	4.71215200	-2.72197700	0.58899800
C	-5.12036500	-2.03734500	0.61131300
F	-6.19490600	-1.60505900	-0.08930200
F	-5.34822600	-1.72940800	1.90755700
F	-5.10502500	-3.38536000	0.51013900
F	4.81576400	-3.90465100	-0.06123700
F	4.59135200	-3.00747900	1.90458900
F	5.88892600	-2.07855600	0.41888700
O	0.41768000	6.02487500	0.66677200
C	1.01678600	6.28297400	1.92804200
H	0.48329300	5.77136400	2.73972600
H	2.07204900	5.98082900	1.94201400
H	0.94829000	7.36208100	2.07553000

P(*para*–CF_3–phenyl)(*para*–OMe–phenyl)$_2$

0 1

P	-0.55190700	-0.01011600	-1.68246100
C	-1.21811200	1.51685700	-0.88496800
C	1.12947900	-0.13727100	-0.90664100
C	-1.49285000	-1.37116200	-0.86164200
C	-2.24680100	2.20286400	-1.55993100
C	-0.76536700	2.05124400	0.32848700
C	2.12411000	0.74260000	-1.37166300
C	1.48519600	-1.09411700	0.05476800
C	-1.56551000	-2.60514700	-1.53765500
C	-2.16499600	-1.25713900	0.36165900
C	-2.80966600	3.35871100	-1.03664900
H	-2.60672500	1.82428900	-2.51364200
C	-1.31399900	3.22008700	0.86413600
H	0.03642700	1.55849500	0.87084800
C	3.42381800	0.68303200	-0.87915800
H	1.87636100	1.48486900	-2.12658800
C	2.79049400	-1.16646400	0.54387600
H	0.73883100	-1.78713200	0.42920400
C	-2.25898700	-3.68271300	-1.00367100
H	-1.07266800	-2.71855700	-2.50046300
C	-2.87758400	-2.32822600	0.90766300

H	-2.14496700	-0.31553900	0.90243300
C	-2.34486700	3.87813000	0.18183700
H	-3.60285800	3.88684900	-1.55672300
H	-0.93138700	3.60353900	1.80339000
C	3.76133800	-0.27658500	0.08174900
H	4.17665700	1.37774200	-1.23798400
H	3.04994400	-1.90742900	1.29329700
C	-2.92344900	-3.55088000	0.22573600
H	-2.31302100	-4.63426900	-1.52343000
H	-3.38921200	-2.19733300	1.85463100
C	-2.51628400	5.60213600	1.82706500
H	-2.66761800	4.92195500	2.67569100
H	-1.45787000	5.89047000	1.78077800
H	-3.12750800	6.49536600	1.96797100
C	-4.28584000	-4.58491400	1.89413700
H	-3.60981100	-4.36503000	2.73098700
H	-5.07849800	-3.82583600	1.86213700
H	-4.73453100	-5.56876800	2.04252000
O	-3.58482900	-4.65907200	0.66269300
O	-2.95226100	5.02089800	0.60826800
C	5.18046000	-0.38353700	0.56615700
F	5.25389800	-0.91644000	1.80672700
F	5.93001400	-1.17029300	-0.24221400
F	5.79056400	0.82322200	0.60686700

P(*para*–CF_3–phenyl)$_2$(*para*–Me–phenyl)

0 1

P	0.00029800	0.87494000	-1.57567100
C	0.05518100	2.44994300	-0.61062900
C	1.42488800	-0.07605900	-0.86349400
C	-1.46003300	-0.01335200	-0.85681500
C	-0.54091700	3.57883900	-1.19594900
C	0.66031700	2.59862400	0.64736400
C	2.68859500	0.15286600	-1.43493500
C	1.32003700	-1.01807700	0.17113600
C	-1.89393600	-1.17271600	-1.52397300
C	-2.18358600	0.42390100	0.26245600

C	-0.54764300	4.80796200	-0.53787300
H	-1.00311300	3.49482500	-2.17681600
C	0.65918700	3.83308000	1.29625900
H	1.13744600	1.74750000	1.12444700
C	3.81642500	-0.52290500	-0.97684300
H	2.79003800	0.86675200	-2.24856000
C	2.44489500	-1.70631900	0.62633300
H	0.35615400	-1.21833500	0.62793500
C	-3.00203900	-1.88634100	-1.07574900
H	-1.35927500	-1.51988400	-2.40478100
C	-3.30250000	-0.28037800	0.70818200
H	-1.87337000	1.31860900	0.79239000
C	0.05691100	4.95878600	0.71715900
H	-1.02210400	5.66528400	-1.01020700
H	1.13398500	3.92361600	2.27095500
C	3.69495700	-1.45773100	0.05563300
H	4.78785700	-0.32830200	-1.41966600
H	2.35238200	-2.42782900	1.43176400
C	-3.71129600	-1.43795100	0.04289100
H	-3.31819900	-2.78672300	-1.59253400
H	-3.85067500	0.06422100	1.57914900
C	4.89923700	-2.23878600	0.50720600
C	-4.94888000	-2.16858600	0.48863700
F	-6.05269100	-1.71846900	-0.15270700
F	-5.17530800	-2.01614100	1.81231200
F	-4.86618900	-3.49470600	0.24000400
F	5.06243900	-3.36899400	-0.21961700
F	4.79896200	-2.61622500	1.80107600
F	6.03911600	-1.52366300	0.37901700
C	0.08739500	6.30035300	1.41077900
H	0.98415200	6.86954600	1.13125900
H	-0.78114200	6.91090800	1.14214700
H	0.10124600	6.18856900	2.50016500

P(*para*–CF_3–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	-0.93303100	-0.00186200	1.46647900

C	-1.64524100	-1.47293200	0.59982700
C	0.80026700	0.02911800	0.80467900
C	-1.72871100	1.42548600	0.59941900
C	-2.77691100	-2.07101700	1.17811200
C	-1.13015700	-2.03751200	-0.57745800
C	1.71829500	-0.87592400	1.36745400
C	1.26241300	0.92860400	-0.16705500
C	-1.73675600	2.65885000	1.27192200
C	-2.34292900	1.35696600	-0.66029000
C	-3.38136800	-3.18099300	0.59039400
H	-3.18802100	-1.66336000	2.09883400
C	-1.73319400	-3.15485200	-1.15593100
H	-0.25143700	-1.60503200	-1.04702900
C	3.04858900	-0.89669100	0.95981900
H	1.38675800	-1.57324100	2.13300700
C	2.59823200	0.92046200	-0.57099600
H	0.57652500	1.63948400	-0.61615000
C	-2.31916700	3.78680500	0.69588200
H	-1.28284500	2.73618800	2.25738400
C	-2.93414700	2.48631900	-1.22718100
H	-2.36281100	0.41626500	-1.20251600
C	-2.86737500	-3.74670100	-0.58436000
H	-4.26091100	-3.62063900	1.05593200
H	-1.31551300	-3.57323500	-2.06939200
C	3.49286100	0.00631500	-0.01188100
H	3.74232000	-1.60975500	1.39369500
H	2.94124500	1.61714100	-1.32922600
C	-2.93359100	3.71972600	-0.56191200
H	-2.30465200	4.73152200	1.23520500
H	-3.40364200	2.40805100	-2.20566500
C	-3.60322900	4.93151500	-1.16652400
H	-4.65139300	5.00599700	-0.84669600
H	-3.10560200	5.85872700	-0.86254400
H	-3.60058900	4.88721900	-2.26083500
C	-3.49766600	-4.97555800	-1.19677000
H	-3.08144700	-5.89382000	-0.76084500
H	-4.57959000	-4.99863900	-1.02718400

H	-3.32183100	-5.02070000	-2.27679100
C	4.94406800	0.02972000	-0.40504700
F	5.67278100	0.82646400	0.41243700
F	5.12057400	0.49461300	-1.66228100
F	5.50144600	-1.20113000	-0.34559800

P(*para*–CF_3–phenyl)$_2$(*para*–NMe_2–phenyl)

0 1

P	-0.00720200	0.24981000	-1.70872800
C	0.30911600	1.86319100	-0.88750800
C	1.27916500	-0.84296700	-0.93566500
C	-1.56454200	-0.36450100	-0.90979900
C	0.02294800	3.03241100	-1.61151500
C	0.83822800	2.02369000	0.40445300
C	2.55714300	-0.82894000	-1.52146400
C	1.05918100	-1.68750400	0.16306100
C	-2.11431500	-1.56331000	-1.39945800
C	-2.26298800	0.32983100	0.08848100
C	0.22865300	4.29858700	-1.07600100
H	-0.36543600	2.95200200	-2.62430200
C	1.05767500	3.28090400	0.95369200
H	1.09677300	1.14881900	0.99486000
C	3.58725400	-1.61819200	-1.01796600
H	2.74670800	-0.19234600	-2.38212400
C	2.08492300	-2.48890800	0.66548100
H	0.08185800	-1.72314400	0.63355100
C	-3.30934000	-2.06527400	-0.89265200
H	-1.60054300	-2.11058500	-2.18623500
C	-3.46834400	-0.16193200	0.59103500
H	-1.86347100	1.26006800	0.47907600
C	0.74632100	4.45934000	0.23129500
H	-0.00592500	5.16416900	-1.68382400
H	1.47863400	3.34483800	1.95008400
C	3.35125800	-2.45361400	0.07839000
H	4.57158900	-1.58868800	-1.47411600
H	1.90341600	-3.13238000	1.52043400
C	-3.99171000	-1.36156600	0.10536100

H	-3.71412100	-2.99885900	-1.27013700
H	-3.99550500	0.38161300	1.36859000
C	4.44355500	-3.35633000	0.58262000
C	-5.31656100	-1.86722800	0.60637200
F	-6.34362800	-1.42180900	-0.15544600
F	-5.56567900	-1.46403000	1.87245200
F	-5.37788100	-3.21798500	0.59087900
F	4.45704300	-4.54093000	-0.07311800
F	4.29944200	-3.63866900	1.89674700
F	5.66754200	-2.80588300	0.41732400
N	0.94107600	5.71349000	0.78126200
C	1.61858900	5.84415900	2.06052600
C	0.75523000	6.89760300	-0.04068100
H	1.07489400	5.31543500	2.85341000
H	2.64805600	5.45449200	2.03601500
H	1.66056200	6.89929700	2.33658700
H	1.44398200	6.92913900	-0.89917600
H	-0.27018500	6.95501700	-0.42671800
H	0.92903700	7.78659400	0.56821900

P(*para*−CF_3−phenyl)(*para*−NMe_2−phenyl)$_2$

0 1

P	-0.27127200	-0.00351100	-1.66849700
C	-0.86400100	1.55306800	-0.88021700
C	1.40540200	-0.19729300	-0.89451200
C	-1.26329400	-1.32604600	-0.85352800
C	-1.79816800	2.32899600	-1.58527400
C	-0.44759000	2.03947000	0.37002600
C	2.40206000	0.73410800	-1.24115900
C	1.76051400	-1.26769700	-0.06091100
C	-1.46771200	-2.51994100	-1.56431900
C	-1.86366300	-1.22731100	0.41169200
C	-2.31233100	3.51384500	-1.07016200
H	-2.12834500	2.00275600	-2.56904200
C	-0.94389800	3.22678500	0.89782200
H	0.29357100	1.48926300	0.94332600
C	3.70073400	0.61153700	-0.75870400

H	2.15503800	1.56961600	-1.89153900
C	3.06456600	-1.40166000	0.41830500
H	1.01221800	-2.00052300	0.22297100
C	-2.20573200	-3.57515800	-1.03849600
H	-1.04433700	-2.62696500	-2.56076600
C	-2.61329900	-2.26730000	0.94992400
H	-1.75843200	-0.31231400	0.98775900
C	-1.90530600	3.99289600	0.19690900
H	-3.02514900	4.07212100	-1.66536100
H	-0.57575000	3.55814700	1.86169400
C	4.03723000	-0.46172400	0.07439600
H	4.45387100	1.34683200	-1.02426400
H	3.32140800	-2.23062000	1.07024100
C	-2.79345000	-3.48126900	0.24445200
H	-2.33279500	-4.46920600	-1.63728800
H	-3.06405900	-2.12911600	1.92571600
N	-3.51493100	-4.53381600	0.78920400
N	-2.42633700	5.16310800	0.73054900
C	-1.83349000	5.72772400	1.93103900
H	-1.90241300	5.02684400	2.77178700
H	-0.77306800	5.99607700	1.79884400
H	-2.38175800	6.62982600	2.20979700
C	-3.25502300	6.02007100	-0.10009800
H	-2.72201700	6.40352700	-0.98498700
H	-4.14763200	5.48639900	-0.44818900
H	-3.59226700	6.87337000	0.49173500
C	-4.26934500	-4.32668700	2.01365100
H	-3.60911800	-4.03198700	2.83833200
H	-5.04882700	-3.55484500	1.91036100
H	-4.75226600	-5.26361900	2.29830900
C	-3.84450100	-5.67976500	-0.04107000
H	-4.46899300	-5.41359700	-0.90894500
H	-2.93691800	-6.16884200	-0.41510300
H	-4.38839700	-6.41160300	0.55949700
C	5.45434400	-0.62869200	0.54408000
F	6.20904100	-1.30436300	-0.35625700
F	5.52750100	-1.31684300	1.70631100

F	6.06458000	0.56324200	0.74119500

P(*para*−Ac−phenyl)$_2$(*para*−CN−phenyl)

0 1

P	-0.01364300	0.36901000	1.58431800
C	-0.11586500	2.00917200	0.72622800
C	-1.39805200	-0.58165300	0.80396100
C	1.48989900	-0.38991700	0.81460700
C	0.64747900	3.05823400	1.26997900
C	-0.93281300	2.27839100	-0.38320700
C	-2.65278000	-0.50160500	1.43107600
C	-1.26727200	-1.39340000	-0.33618600
C	2.06308100	-1.47938100	1.49144300
C	2.10229500	0.06499600	-0.36611400
C	0.61638000	4.33252700	0.71451400
H	1.27010300	2.87561100	2.14216200
C	-0.98170500	3.55377000	-0.94152800
H	-1.53654300	1.48825400	-0.81757300
C	-3.75097300	-1.19347600	0.92356300
H	-2.76924400	0.10264400	2.32751200
C	-2.36180600	-2.09214700	-0.83624500
H	-0.30582600	-1.47982200	-0.83286800
C	3.20139800	-2.11094400	0.99411300
H	1.61747800	-1.83253700	2.41822100
C	3.24504700	-0.55940600	-0.85644500
H	1.68456600	0.91096500	-0.90317900
C	-0.20438200	4.58894300	-0.39750200
H	1.21264700	5.13392300	1.13880300
H	-1.61562600	3.75320800	-1.79975000
C	-3.61732300	-1.99990300	-0.21624700
H	-4.70826900	-1.10793400	1.42841400
H	-2.26941600	-2.72035900	-1.71644600
C	3.80785500	-1.65603800	-0.18591400
H	3.61803400	-2.95318500	1.53782400
H	3.72326600	-0.21488300	-1.76777500
C	-4.75926600	-2.77731800	-0.80568700
O	-4.58975100	-3.46609100	-1.79981600

C	5.04022200	-2.28779500	-0.76726700
O	5.53076900	-1.85191200	-1.79717400
C	-6.12509400	-2.69067000	-0.14522500
H	-6.08370200	-3.03896000	0.89393000
H	-6.49132100	-1.65702100	-0.12882400
H	-6.82470200	-3.31236700	-0.70633800
C	5.66262000	-3.47608700	-0.05324600
H	5.96494600	-3.20943800	0.96674200
H	4.95159000	-4.30755600	0.02361200
H	6.53922500	-3.80178900	-0.61564900
C	-0.25247000	5.90302800	-0.96945400
N	-0.29136600	6.96916800	-1.43328200

P(*para*–Ac–phenyl)(*para*–CN–phenyl)$_2$

0 1

P	-0.38313200	-0.01730800	1.54067200
C	-1.11026800	-1.50185400	0.70236100
C	1.30482600	0.09062300	0.78817900
C	-1.27882300	1.38303200	0.72086500
C	-2.28074700	-2.03935000	1.26755300
C	-0.54821200	-2.14032300	-0.41463300
C	2.34295700	-0.56477300	1.47088200
C	1.61365000	0.79836200	-0.38661600
C	-1.15762900	2.64850700	1.32282400
C	-2.09169200	1.25491800	-0.41655900
C	-2.88819800	-3.16667200	0.72482300
H	-2.71816600	-1.57287500	2.14659900
C	-1.14076000	-3.27678600	-0.96020600
H	0.35944000	-1.75027200	-0.86367000
C	3.64882500	-0.53338000	0.98454500
H	2.12834400	-1.09835700	2.39356200
C	2.91923300	0.83693000	-0.86621700
H	0.83101100	1.32265900	-0.92638200
C	-1.80798100	3.75926400	0.79666500
H	-0.55055200	2.76430300	2.21706400
C	-2.75795700	2.35781600	-0.94599200
H	-2.20884400	0.28836200	-0.89570300

C	-2.31735200	-3.79520300	-0.39517700
H	-3.79347900	-3.57158700	1.16555500
H	-0.70015600	-3.76487000	-1.82378200
C	3.95239600	0.17031600	-0.18988900
H	4.42902700	-1.05251300	1.53252200
H	3.16644900	1.38023400	-1.77264100
C	-2.61713700	3.61856800	-0.34397100
H	-1.70446200	4.73239900	1.26570500
H	-3.38457100	2.25024500	-1.82568700
C	-3.30048600	4.75647300	-0.88679500
N	-3.85398600	5.67991900	-1.32722600
C	-2.93046000	-4.96449200	-0.95505800
N	-3.42835800	-5.91226900	-1.40992300
C	5.34036100	0.24872200	-0.76058800
O	5.54899300	0.87125200	-1.79000900
C	6.47327200	-0.45850000	-0.03638600
H	6.58977100	-0.07409500	0.98418500
H	6.28208300	-1.53574100	0.04017800
H	7.39864300	-0.29503400	-0.59111300

P(*para*−Ac−phenyl)$_2$(*para*−NO$_2$−phenyl)

0 1

P	0.00209200	0.02377900	1.62925800
C	-0.20531000	1.68070600	0.82445100
C	-1.32422700	-0.99005600	0.82856100
C	1.54707700	-0.61028800	0.83020500
C	0.58379900	2.73372300	1.32555900
C	-1.13407600	1.95848300	-0.19155400
C	-2.56314000	-1.04536100	1.48848000
C	-1.16161600	-1.72349200	-0.35959100
C	2.21161100	-1.65931700	1.48660200
C	2.10132900	-0.10242000	-0.35796600
C	0.46918900	4.02309500	0.81724200
H	1.29387500	2.54280700	2.12602300
C	-1.26946500	3.24813500	-0.70333000
H	-1.75638500	1.16494900	-0.59121600
C	-3.61760000	-1.79345500	0.96726100

H	-2.70130700	-0.50345100	2.42091500
C	-2.21122200	-2.47839400	-0.87352100
H	-0.21030900	-1.70525400	-0.88229200
C	3.38418700	-2.20085900	0.96279400
H	1.81083900	-2.05137900	2.41812300
C	3.27742000	-0.63675600	-0.87475000
H	1.61230600	0.71445400	-0.87981600
C	-0.46280300	4.26157200	-0.19244500
H	1.07427000	4.83974700	1.19133600
H	-1.98018400	3.47550200	-1.48854100
C	-3.45244000	-2.52150300	-0.21987600
H	-4.56426200	-1.81307900	1.49832200
H	-2.09438600	-3.04735500	-1.79032100
C	3.93245100	-1.69356700	-0.22410600
H	3.87239000	-3.01366800	1.49153600
H	3.71134800	-0.25128200	-1.79181400
C	-4.54575000	-3.35434100	-0.82660000
O	-4.34901400	-3.97189000	-1.86151600
C	5.19705900	-2.22765700	-0.83427700
O	5.63334700	-1.74820600	-1.86911100
C	-5.89574200	-3.41314400	-0.13174800
H	-5.79916700	-3.81393600	0.88457700
H	-6.34101000	-2.41437500	-0.04802900
H	-6.55952600	-4.05659900	-0.71152400
C	5.91964000	-3.37175500	-0.14317200
H	6.22107100	-3.09131300	0.87337500
H	5.27391400	-4.25439600	-0.06074900
H	6.80693100	-3.62688600	-0.72489800
N	-0.60042900	5.62432800	-0.72983700
O	0.12773000	6.49822900	-0.26030400
O	-1.43468900	5.80667200	-1.61585900

P(*para*–Ac–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

P	-0.02574300	-0.00068600	1.63018700
C	-0.77879600	-1.49146800	0.82661500
C	1.63904700	0.10880700	0.82986100

C	-0.94600700	1.39365800	0.82674400
C	-1.97180500	-1.98035000	1.39167500
C	-0.20887100	-2.18409500	-0.25401400
C	2.70950800	-0.48742400	1.51612000
C	1.89886900	0.76093700	-0.38850400
C	-0.78436600	2.66784600	1.40208600
C	-1.81085600	1.25222600	-0.27087700
C	-2.59582100	-3.11490900	0.88243100
H	-2.41430700	-1.47099500	2.24380000
C	-0.81543900	-3.32930200	-0.76762700
H	0.71405500	-1.83032100	-0.70111200
C	4.00108300	-0.45233800	0.99211500
H	2.53199500	-0.97698100	2.47045300
C	3.18949200	0.80305600	-0.90591600
H	1.08975400	1.23894300	-0.93233200
C	-1.44807700	3.77741400	0.88834100
H	-0.13587500	2.79219100	2.26532200
C	-2.49193800	2.35217600	-0.78993100
H	-1.95708400	0.27931800	-0.72806600
C	-2.00271100	-3.77521100	-0.19255400
H	-3.51612900	-3.49852000	1.30538800
H	-0.38819500	-3.87307500	-1.60138400
C	4.25576800	0.19554000	-0.22483100
H	4.80773300	-0.92483100	1.54390500
H	3.39975700	1.30346000	-1.84571300
C	-2.29699500	3.59976200	-0.20298000
H	-1.32911400	4.76373800	1.31961300
H	-3.16072200	2.25841100	-1.63687300
N	-3.01220100	4.76569900	-0.74859900
O	-2.82017400	5.85433700	-0.20888000
O	-3.75601700	4.57839600	-1.71028000
N	-2.64879000	-4.98335100	-0.73277300
O	-2.10004800	-5.54817900	-1.67779900
O	-3.69754500	-5.35146800	-0.20562800
C	5.62609600	0.27495300	-0.83817800
O	5.79096200	0.84892200	-1.90292200
C	6.79418900	-0.36982900	-0.11213600

H	6.92967400	0.06827800	0.88414800
H	6.62986900	-1.44568100	0.02353000
H	7.70004900	-0.21482600	-0.70043400

P(*para*–Ac–phenyl)$_2$(*para*–OMe–phenyl)

0 1

P	0.00851400	0.22811200	1.64677800
C	-0.39268500	1.84885500	0.86383000
C	-1.21319800	-0.91041900	0.84009000
C	1.60036400	-0.27048900	0.84080900
C	-0.11278500	3.01301700	1.60548300
C	-0.97166200	2.00308400	-0.40315000
C	-2.48083000	-1.00720600	1.43896600
C	-0.95050700	-1.69228800	-0.29825600
C	2.21759800	-1.44392000	1.30972600
C	2.26023000	0.48268400	-0.14444000
C	-0.38246000	4.27589100	1.09578700
H	0.32005100	2.92433200	2.59896400
C	-1.25740700	3.26598800	-0.92665500
H	-1.21297400	1.12701500	-0.99824100
C	-3.46202700	-1.84149400	0.90864400
H	-2.69881700	-0.42631000	2.33192400
C	-1.92798100	-2.53259000	-0.82307300
H	0.02361700	-1.64362600	-0.77490700
C	3.43983000	-1.86601800	0.79346700
H	1.73679900	-2.03191300	2.08815400
C	3.48801400	0.06702000	-0.65179800
H	1.80977600	1.39739800	-0.51624300
C	-0.95912400	4.41182700	-0.17669700
H	-0.16516000	5.17392300	1.66557400
H	-1.70858200	3.34333700	-1.90942300
C	-3.19673900	-2.61771500	-0.23003500
H	-4.43208200	-1.89055200	1.39394500
H	-1.73184500	-3.13653300	-1.70337700
C	4.09334400	-1.11287600	-0.19473400
H	3.88528100	-2.78081500	1.17246600
H	4.00113600	0.64409400	-1.41454200

C	-4.20821000	-3.53949900	-0.84316400
O	-3.93157600	-4.19346900	-1.83768400
C	5.41390900	-1.50984000	-0.78341500
O	5.94468300	-0.82119400	-1.64217500
C	-5.58514600	-3.64616200	-0.20695800
H	-5.51441400	-3.99106300	0.83171800
H	-6.09094800	-2.67313300	-0.19373500
H	-6.18204700	-4.35542700	-0.78283600
C	6.08195700	-2.78523800	-0.29429700
H	6.28125200	-2.73818400	0.78315200
H	5.44255200	-3.65879500	-0.46996200
H	7.02391000	-2.91385800	-0.83017500
O	-1.19348800	5.68839300	-0.58625100
C	-1.77640400	5.89312900	-1.86460300
H	-1.14014600	5.49543000	-2.66594300
H	-2.77153100	5.43440900	-1.93189300
H	-1.86896700	6.97432600	-1.98058300

P(*para*−Ac−phenyl)(*para*−OMe−phenyl)$_2$

0 1

P	-0.24591500	-0.00291300	-1.65455900
C	-0.67205600	1.61320400	-0.86784700
C	1.37495400	-0.39922800	-0.84501900
C	-1.41505800	-1.19159200	-0.86032300
C	-1.55355200	2.46167700	-1.56574100
C	-0.17144000	2.06209500	0.36143200
C	2.50745500	0.30772900	-1.28821600
C	1.55365400	-1.40347500	0.12104500
C	-1.67366200	-2.39623300	-1.54356600
C	-2.08608400	-0.97059100	0.34881800
C	-1.93194900	3.69354100	-1.04972700
H	-1.94442500	2.15003800	-2.53140200
C	-0.53441600	3.30402500	0.89049000
H	0.52165500	1.44118600	0.92174700
C	3.77018900	0.03765900	-0.76917800
H	2.39755700	1.07734900	-2.04870600
C	2.81802200	-1.67983700	0.63415700

H	0.69761400	-1.96953700	0.47433600
C	-2.54533000	-3.34658200	-1.02958900
H	-1.18462400	-2.58776500	-2.49587400
C	-2.97565900	-1.91150200	0.87452800
H	-1.92395100	-0.04587900	0.89473300
C	-1.42265500	4.12535300	0.18494300
H	-2.61215200	4.34692100	-1.58733200
H	-0.12112000	3.61602400	1.84312100
C	3.94332900	-0.96346900	0.20064100
H	4.62183400	0.60651300	-1.13019700
H	2.95960100	-2.45243300	1.38336100
C	-3.20562200	-3.10946300	0.18610800
H	-2.74233700	-4.27618100	-1.55452400
H	-3.47899000	-1.70021500	1.81135600
C	-1.35782000	5.84714400	1.84016600
H	-1.64488700	5.19676800	2.67702200
H	-0.26546900	5.95793800	1.82857100
H	-1.81821300	6.82798600	1.97188800
C	-4.74930900	-3.91207300	1.82367800
H	-4.06119200	-3.80729300	2.67288600
H	-5.40773300	-3.03432000	1.78295200
H	-5.35424400	-4.81046500	1.95895100
O	-4.04832900	-4.09542800	0.60378700
O	-1.84514100	5.35168900	0.60324400
C	5.27633300	-1.30365300	0.79257300
O	5.37859300	-2.17628600	1.64271900
C	6.50568100	-0.54330200	0.31841500
H	6.65712300	-0.67090700	-0.76026000
H	6.40324300	0.53203700	0.50812100
H	7.37841400	-0.92243900	0.85291900

P(*para*–Ac–phenyl)$_2$(*para*–Me–phenyl)

0 1

P	-0.01516300	0.59841900	1.52431500
C	-0.15231900	2.19363300	0.60159300
C	-1.38770800	-0.40499100	0.78454000
C	1.49103600	-0.19443200	0.79337500

C	0.34705600	3.34388100	1.23301600
C	-0.72966100	2.33444400	-0.67058500
C	-2.66022900	-0.26147500	1.36314300
C	-1.23557200	-1.30933800	-0.28082000
C	1.94129800	-1.38445900	1.39205500
C	2.24182500	0.34745600	-0.26325400
C	0.28762500	4.58839900	0.60644700
H	0.78622800	3.26448400	2.22475100
C	-0.79483900	3.58282000	-1.28794000
H	-1.13130700	1.46530100	-1.18340600
C	-3.75120500	-0.98157600	0.88198600
H	-2.79592200	0.41745200	2.20159200
C	-2.32357300	-2.03600700	-0.75520600
H	-0.26147400	-1.44542500	-0.74024000
C	3.08889400	-2.02681800	0.93452700
H	1.38889500	-1.81064400	2.22631100
C	3.39585400	-0.28829800	-0.71222500
H	1.92086900	1.26971800	-0.73681700
C	-0.28872500	4.73119100	-0.66229300
H	0.68828800	5.46302800	1.11411200
H	-1.24489000	3.66689200	-2.27492500
C	-3.59560200	-1.88133200	-0.18354700
H	-4.72171100	-0.84471300	1.34919100
H	-2.21300800	-2.73407500	-1.57896800
C	3.83384900	-1.48414000	-0.12419600
H	3.40520400	-2.94794400	1.41446900
H	3.97884900	0.12478900	-1.52925300
C	-4.72876600	-2.69116800	-0.73992600
O	-4.54382500	-3.46299800	-1.66896300
C	5.08246600	-2.12287600	-0.65510300
O	5.69931400	-1.61069100	-1.57724300
C	-6.11224200	-2.53477200	-0.12889400
H	-6.10512200	-2.79612100	0.93622900
H	-6.46465200	-1.49926600	-0.20833600
H	-6.80394200	-3.19306300	-0.65725600
C	5.56776600	-3.41973900	-0.02696800
H	5.77891300	-3.28620900	1.04094200

H	4.81072700	-4.20850100	-0.11376000
H	6.47871300	-3.73595200	-0.53800600
C	-0.39057400	6.08506000	-1.32457700
H	-0.32093100	6.00449100	-2.41472300
H	-1.35101000	6.56631200	-1.09574500
H	0.40089500	6.75988900	-0.98210900

P(*para*–Ac–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	0.62188500	0.02633700	1.44724200
C	1.26965800	1.52737900	0.58100000
C	-1.09505000	-0.10022400	0.75920100
C	1.50965300	-1.36253200	0.60819200
C	2.35323900	2.19410600	1.17580400
C	0.74985900	2.04910300	-0.61401100
C	-2.05991300	0.78373900	1.27468100
C	-1.50512800	-1.05813700	-0.18323500
C	1.58050700	-2.58494800	1.29648400
C	2.13376800	-1.27414000	-0.64544400
C	2.90762600	3.32978600	0.58757100
H	2.76626500	1.81991900	2.10976900
C	1.30239000	3.19181400	-1.19321800
H	-0.09258300	1.56218800	-1.09663000
C	-3.38362800	0.72874200	0.84777300
H	-1.77059400	1.52167700	2.01930700
C	-2.83109400	-1.11977500	-0.60276700
H	-0.78227400	-1.75698800	-0.59193400
C	2.23316400	-3.68470900	0.74128800
H	1.11985200	-2.67631600	2.27759500
C	2.79521200	-2.37431500	-1.19119100
H	2.10568900	-0.34076200	-1.19977400
C	2.38900300	3.85259500	-0.60479800
H	3.75094800	3.82311000	1.06619700
H	0.88290000	3.57550400	-2.12101400
C	-3.78833300	-0.22763000	-0.09745500
H	-4.10136900	1.43026900	1.26231900
H	-3.15170300	-1.85614800	-1.33294100

C	2.85722400	-3.59776100	-0.51032700
H	2.26598500	-4.62222800	1.29223000
H	3.27035200	-2.28130200	-2.16565900
C	3.60124500	-4.77644900	-1.09302700
H	4.65232000	-4.77897500	-0.77403000
H	3.16273700	-5.72700100	-0.77081200
H	3.59499400	-4.75317500	-2.18801400
C	2.96346800	5.10759900	-1.21920100
H	2.48115300	6.00601500	-0.81082900
H	4.03666600	5.19743100	-1.01922800
H	2.81729900	5.12613900	-2.30445500
C	-5.19859500	-0.34142000	-0.59019300
O	-5.50457500	-1.18748500	-1.41773300
C	-6.24664900	0.61581500	-0.04340100
H	-6.34140500	0.51781800	1.04481400
H	-5.97875500	1.65811000	-0.25476700
H	-7.20589800	0.38771700	-0.51126000

P(*para*−Ac−phenyl)$_2$(*para*−NMe$_2$−phenyl)

0 1

P	0.06826300	-0.00653200	-1.64404600
C	-1.48561700	-0.60933600	-0.86975000
C	0.29006500	1.65046600	-0.83911100
C	1.39854200	-1.01409700	-0.83899100
C	-2.32110800	-1.43886800	-1.63539000
C	-1.91238300	-0.29617500	0.43212000
C	-0.37778400	2.73604400	-1.43140900
C	1.08640000	1.89502900	0.29328300
C	2.72443100	-0.78892000	-1.25144500
C	1.15376600	-2.04626000	0.08198400
C	-3.51352600	-1.94749800	-1.13306300
H	-2.03199700	-1.69596400	-2.65193100
C	-3.10403800	-0.78887100	0.94885500
H	-1.30381400	0.34966700	1.05927100
C	-0.27107500	4.01950100	-0.90159200
H	-0.98473000	2.57311600	-2.31877300
C	1.20047700	3.17910200	0.81778900

H	1.62047100	1.07664500	0.76595600
C	3.77296400	-1.54953200	-0.74157100
H	2.93763800	-0.00990500	-1.97988300
C	2.20076400	-2.81480400	0.58266700
H	0.13835500	-2.24594600	0.40901400
C	-3.94409700	-1.62907600	0.17676400
H	-4.11333400	-2.58921600	-1.76730200
H	-3.38262200	-0.51663100	1.96003000
C	0.52287500	4.25851700	0.23092800
H	-0.80304900	4.83492800	-1.38236900
H	1.81157900	3.37252600	1.69377800
C	3.52405400	-2.57670000	0.18294400
H	4.78543000	-1.34351800	-1.07555600
H	2.01666700	-3.61149100	1.29650200
C	0.68330000	5.61719600	0.84287600
O	1.38551200	5.77728100	1.83038100
C	4.60815100	-3.43482800	0.76050600
O	4.34334800	-4.32029400	1.56051600
C	-0.04421500	6.79580800	0.21469700
H	0.26622500	6.94165600	-0.82701500
H	-1.12903700	6.63482800	0.21216000
H	0.18608100	7.69475200	0.78907000
C	6.04688200	-3.18532300	0.33505900
H	6.16569200	-3.31028900	-0.74803500
H	6.36052600	-2.16378800	0.58178500
H	6.69265900	-3.89628300	0.85328700
N	-5.13961800	-2.10903600	0.67972800
C	-5.48600100	-1.87297000	2.07117000
C	-5.91086600	-3.07158000	-0.08835300
H	-4.75833600	-2.31648500	2.76810900
H	-5.55207200	-0.79930700	2.28875300
H	-6.46385700	-2.31240800	2.27591200
H	-6.21250000	-2.65670400	-1.05868000
H	-5.35535600	-4.00343200	-0.27565600
H	-6.81988800	-3.32236600	0.46118700

P(*para*–Ac–phenyl)(*para*–NMe$_2$–phenyl)$_2$

0 1

P	0.03170000	0.04405000	-1.63548600
C	-1.15559800	-1.13303000	-0.86014800
C	-0.45037000	1.64591400	-0.83526800
C	1.64598700	-0.35715300	-0.84235300
C	-1.50010100	-2.28688300	-1.58237700
C	-1.75636200	-0.96761100	0.39879300
C	-1.72002600	2.17630100	-1.13093600
C	0.41711300	2.41016200	-0.03651600
C	2.81593300	-0.08201800	-1.56855200
C	1.80461300	-0.94657400	0.42201800
C	-2.37582700	-3.24085200	-1.07565700
H	-1.07785200	-2.44188200	-2.57278100
C	-2.64115600	-1.90660300	0.91863000
H	-1.54295800	-0.07810900	0.98525200
C	-2.11586300	3.41294200	-0.63147200
H	-2.40696000	1.61046700	-1.75575200
C	0.02420700	3.65083300	0.45730800
H	1.40369100	2.02661400	0.20360700
C	4.08185600	-0.35043900	-1.05835300
H	2.73695200	0.34882800	-2.56438100
C	3.06085200	-1.23134600	0.94482000
H	0.92826800	-1.20452000	1.00992800
C	-2.96514200	-3.08188300	0.20021500
H	-2.60810200	-4.10709100	-1.68370200
H	-3.08238600	-1.71921400	1.89056300
C	-1.24677300	4.17105800	0.17120100
H	-3.10585700	3.78738900	-0.87485300
H	0.69096700	4.24006300	1.07908400
C	4.24023400	-0.92574600	0.22372800
H	4.94727600	-0.11989700	-1.66819500
H	3.12161200	-1.69784000	1.92109700
N	5.49720300	-1.17927800	0.75311400
N	-3.82344100	-4.03751100	0.72588100
C	-4.56561700	-3.74195300	1.93950800
H	-3.88713600	-3.53913700	2.77700600
H	-5.23762000	-2.87564600	1.82972300

H	-5.16971700	-4.61052600	2.20924800
C	-4.28448000	-5.12584600	-0.11901200
H	-4.85832100	-4.77636700	-0.99241300
H	-3.44120700	-5.72333600	-0.48596400
H	-4.92499300	-5.78717200	0.46796500
C	5.61641100	-1.94717700	1.98072300
H	5.09817200	-1.44925700	2.80923500
H	5.20839400	-2.96651800	1.88867800
H	6.67105500	-2.02497700	2.25231700
C	6.67116500	-1.03320900	-0.09023300
H	6.66018700	-1.71074100	-0.95906600
H	6.76235100	-0.00607900	-0.46393200
H	7.56418700	-1.24894200	0.49970800
C	-1.61435500	5.50746300	0.73342500
O	-0.82946500	6.13255600	1.43299700
C	-2.98864900	6.08226100	0.42101900
H	-3.12920500	6.20493300	-0.65970500
H	-3.78545800	5.41962400	0.77998800
H	-3.07977100	7.05398400	0.90961800

P(*para*−CN−phenyl)$_2$(*para*−NO$_2$−phenyl)

0 1

P	0.35809600	0.01580200	1.53859200
C	-1.33338300	-0.06696100	0.78547700
C	1.23877100	-1.39324400	0.71954800
C	1.09229100	1.49598000	0.70068600
C	-2.32700700	0.73520500	1.37745500
C	-1.68822500	-0.90351300	-0.28535600
C	1.16645400	-2.64185500	1.36258400
C	1.99451800	-1.28486800	-0.45884400
C	2.23553800	2.05662500	1.29732700
C	0.56769700	2.10229000	-0.45223900
C	-3.63520900	0.72413100	0.90381000
H	-2.07578700	1.37131300	2.22216600
C	-2.99739400	-0.93465700	-0.76348900
H	-0.94178700	-1.53704300	-0.75273400
C	1.80903000	-3.75790400	0.83663900

H	0.60583300	-2.74004300	2.28864200
C	2.65216200	-2.39247200	-0.98856400
H	2.07450100	-0.33012800	-0.96852600
C	2.85344300	3.17687000	0.75114200
H	2.64279400	1.61483500	2.20307800
C	1.17097900	3.23096300	-1.00186000
H	-0.31937900	1.69464800	-0.92631400
C	-3.95041200	-0.11642400	-0.16263200
H	-4.40802000	1.33958200	1.34766800
H	-3.28568100	-1.57394600	-1.58908000
C	2.55986800	-3.63748900	-0.34503200
H	1.74433500	-4.71846100	1.33737400
H	3.23540600	-2.30115200	-1.89931200
C	2.32074600	3.77303800	-0.40444800
H	3.73748900	3.60071400	1.21634100
H	0.75961400	3.69481400	-1.89270600
C	3.23428300	-4.78044300	-0.88886300
N	3.77982600	-5.70779400	-1.33070400
C	2.94576600	4.93390400	-0.96894200
N	3.45381300	5.87421400	-1.42777400
N	-5.33446400	-0.14267000	-0.66633400
O	-6.15354700	0.59122700	-0.11556200
O	-5.58326200	-0.89541000	-1.60671200

P(*para*–CN–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

P	-0.01216500	0.34458900	1.58241800
C	1.47574300	-0.44658600	0.81140600
C	-0.09520500	1.98508900	0.72632500
C	-1.41179900	-0.58468100	0.79974100
C	1.96703500	-1.60769800	1.43689800
C	2.15888300	0.06168400	-0.30550100
C	0.57641900	3.05428900	1.34506400
C	-0.80357700	2.23017200	-0.46118700
C	-2.68055600	-0.42267100	1.38647300
C	-1.27767800	-1.45525100	-0.29440900
C	3.09565300	-2.26147600	0.95181400

H	1.46500400	-2.00123600	2.31687000
C	3.29782000	-0.57511400	-0.79591700
H	1.80404300	0.96024500	-0.79911000
C	0.56251800	4.32874200	0.78730400
H	1.11074800	2.88867300	2.27696900
C	-0.83419100	3.50418000	-1.02292900
H	-1.33818900	1.42373700	-0.95279300
C	-3.79342800	-1.09185800	0.88612100
H	-2.79804000	0.22907200	2.24820100
C	-2.38083000	-2.14137500	-0.79983100
H	-0.30808500	-1.60273000	-0.75836100
C	3.74621400	-1.73015000	-0.16042300
H	3.48174900	-3.15796600	1.42113000
H	3.83496800	-0.19562400	-1.65664500
C	-0.14743800	4.56098200	-0.40276700
H	1.08661400	5.14746300	1.26956500
H	-1.38438700	3.68687500	-1.94045300
C	-3.62334300	-1.94545900	-0.20240900
H	-4.77602100	-0.97346400	1.32601700
H	-2.29346100	-2.81528900	-1.64339400
N	-4.79337500	-2.66567700	-0.73479300
O	-5.87697200	-2.47287300	-0.18600200
O	-4.61251700	-3.41250800	-1.69504400
N	4.94773000	-2.40900800	-0.67669700
O	5.50175400	-1.91603200	-1.65780900
O	5.31942800	-3.42658100	-0.09450100
C	-0.17546700	5.87389300	-0.97944300
N	-0.19673500	6.93826900	-1.44785100

P(*para*–CN–phenyl)$_2$(*para*–OMe–phenyl)

0 1

P	-0.17049800	0.01685500	1.54923800
C	1.37086400	-0.68690200	0.82647100
C	-0.26921500	1.67501900	0.72295200
C	-1.52683900	-0.92186000	0.70339000
C	2.07988600	-1.62324000	1.60450700
C	1.89649800	-0.34346800	-0.42692000

C	0.46509200	2.71968500	1.31335000
C	-1.04124200	1.95894500	-0.41484700
C	-2.84430200	-0.67900000	1.13517100
C	-1.31291800	-1.90736800	-0.27250200
C	3.25244000	-2.20411800	1.14187800
H	1.70678900	-1.89519000	2.58886000
C	3.07992700	-0.91190300	-0.90253500
H	1.38436800	0.38546500	-1.04853500
C	0.44930700	4.00232300	0.77750500
H	1.05387700	2.52559500	2.20623900
C	-1.07422400	3.24273900	-0.95518100
H	-1.62398300	1.17407100	-0.88593700
C	-3.91857100	-1.37549300	0.59369900
H	-3.03077900	0.06277900	1.90790200
C	-2.37981400	-2.62166400	-0.81346300
H	-0.30514400	-2.12018900	-0.61359800
C	3.76347700	-1.85095400	-0.11735900
H	3.79934500	-2.92654200	1.73948900
H	3.45725500	-0.61657300	-1.87495700
C	-0.32540900	4.27286200	-0.36409600
H	1.02273100	4.79986700	1.23903900
H	-1.67334300	3.45231300	-1.83577800
C	-3.69104700	-2.35704600	-0.38719300
H	-4.93115300	-1.17560100	0.92932800
H	-2.20471600	-3.38212100	-1.56801800
C	-0.35311000	5.59441000	-0.91958600
N	-0.37318300	6.66619400	-1.37161300
C	-4.79165100	-3.08720900	-0.94511400
N	-5.68461200	-3.67831400	-1.39974600
O	4.92048300	-2.46607400	-0.47854200
C	5.49680100	-2.14492100	-1.73685200
H	4.82344600	-2.40149200	-2.56487500
H	5.75918400	-1.08097000	-1.79907900
H	6.40460000	-2.74581300	-1.81047000

P(*para*−CN−phenyl)(*para*−OMe−phenyl)$_2$

0 1

P	-0.00593300	0.15592700	1.59946300
C	1.13766400	-1.08880500	0.85789300
C	0.51319100	1.70857300	0.72688700
C	-1.63905400	-0.22961400	0.82979700
C	1.41711100	-2.24239800	1.61640500
C	1.75573400	-0.96556900	-0.39391700
C	1.77098000	2.25144900	1.05303800
C	-0.30793400	2.41838400	-0.16286300
C	-2.79292200	0.19513500	1.51771300
C	-1.81519900	-0.93818500	-0.36544800
C	2.26103200	-3.23511100	1.13789800
H	0.96774800	-2.35857900	2.59967800
C	2.61599200	-1.95093000	-0.88594200
H	1.57650700	-0.08316700	-1.00152000
C	2.20613300	3.44711500	0.49571300
H	2.41876100	1.72776400	1.75156500
C	0.11237800	3.62416800	-0.72065100
H	-1.28422000	2.02520100	-0.42659600
C	-4.06460100	-0.05650400	1.02072000
H	-2.68950200	0.72784600	2.46016300
C	-3.08799600	-1.21044200	-0.87322500
H	-0.94880100	-1.29718200	-0.91303700
C	2.86954300	-3.09567200	-0.11945000
H	2.47617900	-4.12424500	1.72237200
H	3.07825600	-1.81485400	-1.85718300
C	1.37499000	4.14606500	-0.39887000
H	3.18092700	3.85134400	0.75000800
H	-0.53036400	4.16284400	-1.41009500
C	-4.22167200	-0.76472400	-0.18099000
H	-4.95383000	0.27262800	1.54928200
H	-3.18206900	-1.76715200	-1.79884800
C	4.34359800	-4.02787400	-1.75286400
H	3.62445700	-3.98172300	-2.58124400
H	5.00601900	-3.15368000	-1.80098100
H	4.93973200	-4.93756500	-1.84347200
C	-5.73202400	-1.69156100	-1.78414700
H	-5.29153200	-1.17958400	-2.64979100

H	-5.32973600	-2.71136100	-1.72478300
H	-6.81562500	-1.73776400	-1.90585800
O	-5.50650800	-0.97146700	-0.58200100
O	3.68778200	-4.11655500	-0.49719700
C	1.81434700	5.38223300	-0.97601000
N	2.17259100	6.38430000	-1.44687900

P(*para*–CN–phenyl)$_2$(*para*–Me–phenyl)

0 1

P	-0.00169300	0.23286300	1.45407600
C	-0.17285800	1.85189500	0.58332700
C	-1.36173600	-0.77091200	0.69029500
C	1.51272400	-0.51261200	0.68838700
C	0.29605500	2.99174300	1.25579700
C	-0.74693400	2.02028700	-0.68734600
C	-2.64264100	-0.63152800	1.25481800
C	-1.19227700	-1.67222400	-0.37272900
C	1.99511300	-1.70738400	1.25453900
C	2.23926800	0.07362900	-0.35958400
C	0.20980700	4.25429800	0.66977600
H	0.73110700	2.89054200	2.24728500
C	-0.83864900	3.28628000	-1.26357200
H	-1.12691900	1.15986600	-1.23065400
C	-3.72677400	-1.35043600	0.76427100
H	-2.79114800	0.04600700	2.09177900
C	-2.26832100	-2.40695200	-0.86595900
H	-0.21347200	-1.80526100	-0.82193300
C	3.15056800	-2.31464100	0.77619700
H	1.46111800	-2.16567000	2.08330500
C	3.40578900	-0.51826200	-0.83911200
H	1.89319900	0.99990500	-0.80618500
C	-0.36342300	4.42512100	-0.59695900
H	0.58599000	5.12093100	1.20859200
H	-1.28681200	3.39248900	-2.24914600
C	-3.54443000	-2.24782500	-0.30237700
H	-4.71162900	-1.23222600	1.20467000
H	-2.12791200	-3.10095100	-1.68870300

C	3.86701400	-1.71932600	-0.27702200
H	3.51051500	-3.23916100	1.21618000
H	3.96125600	-0.05785700	-1.65012800
C	-4.65522000	-2.99968700	-0.80915900
N	-5.55718900	-3.60795800	-1.22127100
C	5.06523600	-2.33283300	-0.77077300
N	6.03642500	-2.83136100	-1.17285100
C	-0.49549800	5.79707300	-1.21456500
H	-0.40505600	5.75641700	-2.30535700
H	-1.47454400	6.23949900	-0.98685400
H	0.26818100	6.48352000	-0.83463900

P(*para*–CN–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	-0.24328100	-0.00222100	1.41432400
C	-0.93330600	-1.50396400	0.58517900
C	1.45817200	0.08758700	0.68175700
C	-1.12508300	1.39423400	0.58287600
C	-1.98844300	-2.16491700	1.23478900
C	-0.47600100	-2.02969000	-0.63381600
C	2.39590700	-0.87569600	1.10038100
C	1.88702200	1.10124600	-0.18902900
C	-1.19209500	2.61260200	1.27827800
C	-1.74618200	1.31530900	-0.67326800
C	-2.57589500	-3.29944300	0.67697000
H	-2.35259800	-1.78763300	2.18756200
C	-1.06118200	-3.17090500	-1.18242100
H	0.34402100	-1.54858600	-1.15912300
C	3.70996300	-0.84478800	0.65053600
H	2.09126700	-1.66135500	1.78725500
C	3.20503700	1.14986800	-0.63859300
H	1.18611700	1.85894500	-0.52334900
C	-1.83901100	3.71849900	0.72750100
H	-0.73414300	2.69601000	2.26131100
C	-2.40132200	2.42106500	-1.21416400
H	-1.72232300	0.38437900	-1.23190800
C	-2.11972800	-3.82625200	-0.53878400

H	-3.39584100	-3.78869100	1.19827000
H	-0.68983900	-3.55813900	-2.12896200
C	4.12594700	0.17460800	-0.22508700
H	4.42169700	-1.59719200	0.97534700
H	3.52508900	1.93713600	-1.31409300
C	-2.46004900	3.64112600	-0.52593100
H	-1.86996600	4.65270300	1.28396400
H	-2.87506700	2.33556500	-2.18995000
C	-3.19867500	4.82524100	-1.10419600
H	-4.25947600	4.80710600	-0.82004000
H	-2.78267900	5.77241400	-0.74490100
H	-3.15699400	4.82867100	-2.19871100
C	-2.72853700	-5.08004800	-1.12138800
H	-2.21995500	-5.97843600	-0.74637000
H	-3.78716100	-5.17273000	-0.85628800
H	-2.64878200	-5.09465900	-2.21355800
C	5.48134800	0.21813200	-0.68939800
N	6.58121900	0.25213000	-1.06778000

P(*para*−CN−phenyl)$_2$(*para*−NMe$_2$−phenyl)

0 1

P	0.44515200	0.01966000	1.53851400
C	-1.23629700	0.10526600	0.80769800
C	1.14945300	-1.49317900	0.72545900
C	1.37924200	1.38229600	0.69699900
C	-2.26791900	0.63503200	1.60091200
C	-1.58108300	-0.33824100	-0.48105000
C	0.82845100	-2.73123400	1.31161200
C	1.98884800	-1.48438900	-0.40001200
C	2.71196900	1.60001000	1.09505300
C	0.80833100	2.26135800	-0.23612800
C	-3.57285900	0.74103000	1.13488900
H	-2.04698200	0.96860000	2.61225800
C	-2.88093900	-0.24699000	-0.96138000
H	-0.82162600	-0.77511100	-1.12397300
C	1.30997600	-3.92395600	0.78475800
H	0.19447600	-2.75949000	2.19415300

C	2.48670400	-2.67206600	-0.93176800
H	2.25961300	-0.54385900	-0.86861200
C	3.46171100	2.64162700	0.56135700
H	3.16777300	0.94639800	1.83483500
C	1.54504200	3.31706800	-0.76888200
H	-0.22061700	2.12012300	-0.55019400
C	-3.91687000	0.30745200	-0.16820200
H	-4.32790500	1.15394900	1.79288800
H	-3.09238700	-0.61398100	-1.95866000
C	2.14740600	-3.90132700	-0.34448100
H	1.05256900	-4.87327600	1.24361000
H	3.13360400	-2.65436700	-1.80333000
C	2.87910100	3.51191100	-0.37731000
H	4.49068300	2.79556600	0.87050800
H	1.09475500	3.99101500	-1.49100500
C	2.65411500	-5.12618000	-0.89077100
N	3.06303800	-6.12071500	-1.33500400
C	3.64127800	4.59464000	-0.92696200
N	4.25989700	5.47236400	-1.37486500
N	-5.20736900	0.41777500	-0.64713500
C	-6.26892400	0.87884100	0.23238000
C	-5.55345700	-0.15284500	-1.93868600
H	-6.41642100	0.21432800	1.09726200
H	-6.06196600	1.88785500	0.61122800
H	-7.20470800	0.92068500	-0.32743200
H	-4.96126400	0.29761800	-2.74546700
H	-5.40023800	-1.24215700	-1.97136400
H	-6.60528300	0.04848800	-2.14830900

P(*para*–CN–phenyl)(*para*–NMe$_2$–phenyl)$_2$

0 1

P	0.01976700	0.39706000	-1.57948800
C	-1.43483000	-0.45503000	-0.83887100
C	-0.03301000	2.04104000	-0.72097400
C	1.47742000	-0.42809800	-0.81270500
C	-2.08500500	-1.42975300	-1.61307800
C	-1.95781600	-0.20600500	0.44128000

C	-1.14795600	2.87287600	-0.94232100
C	1.02937000	2.54542200	0.04582400
C	2.67769700	-0.44110000	-1.54185300
C	1.48117300	-1.07544600	0.43339300
C	-3.18234200	-2.13870100	-1.13728900
H	-1.72857400	-1.63627000	-2.61975100
C	-3.05948900	-0.89875100	0.93119500
H	-1.50725200	0.55765500	1.06949800
C	-1.21221700	4.15157200	-0.40388900
H	-1.97983500	2.50936500	-1.54008400
C	0.98111400	3.82919400	0.58460600
H	1.90148100	1.92624900	0.22909700
C	3.83304000	-1.04003100	-1.05072600
H	2.71021500	0.02395300	-2.52480800
C	2.62277300	-1.68829700	0.93641400
H	0.56869700	-1.11822100	1.02129100
C	-3.69653200	-1.89928800	0.15866400
H	-3.64581900	-2.87360200	-1.78463600
H	-3.42575700	-0.65495900	1.92150500
C	-0.14229100	4.64246200	0.36712500
H	-2.08118600	4.77904000	-0.57630600
H	1.80748500	4.20526100	1.18001700
C	3.84017400	-1.67480300	0.21320300
H	4.72756900	-1.02207900	-1.66180100
H	2.56324200	-2.18404000	1.89821600
N	4.98943400	-2.25879900	0.72303500
N	-4.77774600	-2.61338100	0.65150200
C	-5.39516400	-2.20783700	1.90295300
H	-4.67743600	-2.25522100	2.73107700
H	-5.80337700	-1.18537300	1.86544800
H	-6.21240800	-2.89293000	2.13659000
C	-5.51694100	-3.49644100	-0.23458100
H	-5.97777300	-2.96318200	-1.08129400
H	-4.86683400	-4.28026700	-0.64206100
H	-6.31040800	-3.98826000	0.33142600
C	4.91080500	-3.06355700	1.93043300
H	4.54357800	-2.47057100	2.77695000

H	4.25155300	-3.93885200	1.81738100
H	5.91008500	-3.42007000	2.18772800
C	6.16331000	-2.38815500	-0.12359700
H	5.98015400	-3.00964700	-1.01454800
H	6.51487200	-1.40611100	-0.46281600
H	6.97037300	-2.84579100	0.45178700
C	-0.19965500	5.96105300	0.92502800
N	-0.24753500	7.03133400	1.37989300

P(*para*–NO_2–phenyl)$_2$(*para*–OMe–phenyl)

0 1

P	0.01338300	0.18860100	1.63346000
C	-0.39317800	1.80838200	0.85906800
C	-1.21483200	-0.94624900	0.83001200
C	1.60329900	-0.31185900	0.82410500
C	-0.15594500	2.96814000	1.62274000
C	-0.93682200	1.96613200	-0.42374400
C	-2.50347700	-0.97851300	1.39577800
C	-0.93882800	-1.78233200	-0.26454400
C	2.20054400	-1.51101500	1.25947900
C	2.28424800	0.47623100	-0.11751400
C	-0.43400500	4.23122900	1.11905500
H	0.24851900	2.87575400	2.62764100
C	-1.22987000	3.22909200	-0.94106400
H	-1.14500400	1.09319600	-1.03593800
C	-3.49656600	-1.80279300	0.87757500
H	-2.73031900	-0.35278000	2.25492100
C	-1.92012200	-2.62200200	-0.78931700
H	0.04807200	-1.78207100	-0.71501200
C	3.42621500	-1.92968900	0.75312300
H	1.70185300	-2.12321100	2.00663100
C	3.51973400	0.07708000	-0.62498400
H	1.84801300	1.40862200	-0.45949900
C	-0.97565800	4.37173900	-0.16878000
H	-0.25100600	5.12623100	1.70517100
H	-1.65387400	3.31019100	-1.93542200
C	-3.18704700	-2.61695400	-0.21147700

H	-4.49214800	-1.83316600	1.30291900
H	-1.72085800	-3.26934100	-1.63471200
C	4.07081000	-1.12357100	-0.18511500
H	3.89140300	-2.85309400	1.07560100
H	4.05434700	0.67489300	-1.35313000
N	5.37176700	-1.55226800	-0.72146300
O	5.83236000	-2.61873200	-0.31524500
O	5.91924700	-0.81927700	-1.54462600
N	-4.22825900	-3.49712500	-0.76426300
O	-5.33804200	-3.47051000	-0.23308200
O	-3.92648600	-4.20442000	-1.72504900
O	-1.22127800	5.64625700	-0.56978200
C	-1.77891300	5.85847300	-1.85961400
H	-1.11584600	5.48500200	-2.65052400
H	-2.76283100	5.38170900	-1.95528200
H	-1.88953600	6.93913300	-1.96158600

P(*para*–NO_2–phenyl)(*para*–OMe–phenyl)$_2$

0 1

P	0.21701600	0.00256500	1.63752300
C	0.70040500	1.60544200	0.86249500
C	-1.41536700	-0.33275700	0.82527000
C	1.33997100	-1.23295900	0.85104200
C	1.57180000	2.43826600	1.59138800
C	0.26092600	2.05721400	-0.38956000
C	-2.48504100	0.53844600	1.11399600
C	-1.66826600	-1.46146500	0.02837700
C	1.58872500	-2.42330300	1.56238800
C	1.98351700	-1.06131700	-0.38120100
C	1.99815400	3.65800100	1.08438700
H	1.91581700	2.12426700	2.57382900
C	0.67247100	3.28705000	-0.90980700
H	-0.42378000	1.44996800	-0.97467600
C	-3.75885400	0.30823400	0.60896900
H	-2.31591200	1.41086600	1.73962500
C	-2.94232100	-1.71197800	-0.47827400
H	-0.86266900	-2.14968700	-0.20438700

C	2.42424800	-3.40834700	1.05307900
H	1.12158100	-2.57572100	2.53251800
C	2.83644600	-2.03709500	-0.90222100
H	1.83066400	-0.14766300	-0.94798800
C	1.54951100	4.09327300	-0.17256200
H	2.66983500	4.29973900	1.64600500
H	0.30518100	3.60234300	-1.87992800
C	-3.97120000	-0.82070000	-0.18423000
H	-4.58478300	0.97645200	0.81982200
H	-3.14619600	-2.57674300	-1.09802100
C	3.05698000	-3.22107800	-0.18577800
H	2.61432600	-4.32687400	1.59947800
H	3.32015300	-1.86409900	-1.85699400
C	1.58707500	5.80796500	-1.83645000
H	1.89282900	5.14848700	-2.65925900
H	0.49793700	5.94237300	-1.86699100
H	2.07368800	6.77794800	-1.95211100
C	4.54005600	-4.10471500	-1.83826700
H	3.83400200	-4.00718600	-2.67333800
H	5.21966800	-3.24250100	-1.83723900
H	5.11995700	-5.02097800	-1.96172800
O	3.86430000	-4.23719800	-0.59693900
O	2.01519700	5.30606500	-0.57945200
N	-5.31329500	-1.07424100	-0.72174400
O	-6.20168700	-0.26582800	-0.44860200
O	-5.47279700	-2.07914400	-1.41594400

P(*para*–NO_2–phenyl)$_2$(*para*–Me–phenyl)

0 1

P	-0.01127800	0.56026300	1.51617500
C	-0.13829500	2.15572100	0.59807700
C	-1.39845700	-0.42585900	0.77842300
C	1.48507700	-0.25102100	0.78421400
C	0.31223400	3.31068200	1.25674000
C	-0.66100300	2.29099900	-0.69875700
C	-2.68101900	-0.20303000	1.31396800
C	-1.24891000	-1.38672000	-0.23518700

C	1.89583300	-1.47280600	1.35195000
C	2.27097500	0.31848200	-0.23053600
C	0.25698100	4.55689600	0.63275700
H	0.70823100	3.23445400	2.26657000
C	-0.72118400	3.54042700	-1.31310700
H	-1.02480200	1.41762000	-1.23249400
C	-3.78844300	-0.90023800	0.84281300
H	-2.81315300	0.52244500	2.11233200
C	-2.34698100	-2.10177500	-0.71081900
H	-0.27027700	-1.58227600	-0.66052700
C	3.04056100	-2.12462100	0.90582100
H	1.31489400	-1.91769000	2.15583800
C	3.42824500	-0.31587100	-0.67961400
H	1.97917700	1.26326600	-0.67642000
C	-0.26488900	4.69500700	-0.65974300
H	0.61773300	5.43617100	1.16140900
H	-1.12915500	3.62157700	-2.31825000
C	-3.60239400	-1.84477400	-0.16591800
H	-4.78033900	-0.73450900	1.24491400
H	-2.24577400	-2.84356300	-1.49372100
C	3.79369500	-1.53135700	-0.10709200
H	3.36247300	-3.06750100	1.33055100
H	4.04232600	0.11163100	-1.46289500
N	5.01171500	-2.20740900	-0.58069600
O	5.30734500	-3.28132400	-0.05762800
O	5.65919000	-1.65833600	-1.47154700
N	-4.76591100	-2.59338300	-0.66696400
O	-5.86217700	-2.34429000	-0.16653500
O	-4.57161000	-3.42110500	-1.55650400
C	-0.36313200	6.04950000	-1.32048900
H	-0.22339100	5.97811900	-2.40443800
H	-1.34988300	6.50032700	-1.14990200
H	0.38512500	6.74411700	-0.92526500

P(*para*–NO_2–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	-0.59637900	-0.01339300	1.43025100

C	-1.30795400	-1.49057200	0.57745600
C	1.12376800	0.03322600	0.74179300
C	-1.41825300	1.41528600	0.59304900
C	-2.38021900	-2.13889900	1.21116900
C	-0.85477800	-2.00705200	-0.64745000
C	1.99816000	-1.01418100	1.09461800
C	1.62918000	1.10010200	-0.01913300
C	-1.49060900	2.62052600	1.30993900
C	-1.98817800	1.37299100	-0.68908500
C	-2.98784400	-3.25253000	0.63278100
H	-2.74193900	-1.76852800	2.16749900
C	-1.46031800	-3.12709900	-1.21648500
H	-0.02150700	-1.53586400	-1.16076600
C	3.32640800	-1.01253200	0.68627700
H	1.63247800	-1.84338100	1.69452000
C	2.96145000	1.12169700	-0.42820100
H	0.97748700	1.92030000	-0.30062000
C	-2.09260800	3.75003600	0.75524600
H	-1.07251500	2.67542400	2.31250000
C	-2.59855300	2.50171600	-1.23375600
H	-1.96016700	0.45264200	-1.26475400
C	-2.53602400	-3.76997800	-0.58836500
H	-3.82054200	-3.73252600	1.14221600
H	-1.09188000	-3.50745700	-2.16690900
C	3.79231900	0.06228400	-0.07255400
H	4.00365200	-1.81662400	0.94681800
H	3.35987200	1.93736800	-1.01927900
C	-2.66192600	3.70949700	-0.52383700
H	-2.12868300	4.67361200	1.32876200
H	-3.03294500	2.44482300	-2.22971400
C	-3.35190200	4.91900700	-1.10946700
H	-4.43057100	4.89722200	-0.90384900
H	-2.95891100	5.84938900	-0.68645300
H	-3.23117900	4.96215800	-2.19734500
C	-3.16713800	-5.00156200	-1.19399300
H	-2.66313400	-5.91460900	-0.84951600
H	-4.22282300	-5.08935300	-0.91623800

H	-3.10274000	-4.98902700	-2.28724400
N	5.19516400	0.07629700	-0.50579300
O	5.90443300	-0.87621300	-0.17935300
O	5.58002700	1.03864800	-1.17100400

P(*para*–NO_2–phenyl)$_2$(*para*–NMe_2–phenyl)

0 1

P	0.10422900	0.01552000	1.62280300
C	-1.47022800	0.55015700	0.84958500
C	0.38655300	-1.63798200	0.82872500
C	1.39834200	1.06850000	0.81588400
C	-2.35273400	1.32060900	1.62540600
C	-1.87500700	0.23196300	-0.45900400
C	-0.32174800	-2.72500500	1.37577600
C	1.26469200	-1.87845900	-0.24099800
C	2.73334000	0.89528100	1.23130600
C	1.10686000	2.09220300	-0.09998500
C	-3.56798400	1.77176600	1.12495500
H	-2.08569100	1.57043600	2.64963700
C	-3.08825300	0.66829100	-0.97393300
H	-1.23428700	-0.37778800	-1.09047500
C	-0.17717500	-4.00986300	0.86453700
H	-0.99353900	-2.56202100	2.21438800
C	1.42881100	-3.16229500	-0.75883200
H	1.82718600	-1.06048100	-0.67835100
C	3.75330900	1.69661700	0.73008800
H	2.97735500	0.12525000	1.95884200
C	2.11578700	2.91239900	-0.60219500
H	0.08413700	2.24976200	-0.42548900
C	-3.96978100	1.46220500	-0.19706700
H	-4.20990400	2.35944300	1.76999300
H	-3.35402200	0.38634800	-1.98575100
C	0.70202500	-4.21022000	-0.19964200
H	-0.71984600	-4.85192200	1.27621200
H	2.10038500	-3.35923700	-1.58567600
C	3.42655900	2.69962500	-0.18285600
H	4.78381000	1.56729400	1.03739500

H	1.90402400	3.70355300	-1.31116400
N	4.49549400	3.55870700	-0.71298000
O	5.64435500	3.34473200	-0.32628300
O	4.17749300	4.43912700	-1.51239000
N	0.86693300	-5.56565100	-0.74478100
O	0.21018400	-6.47122400	-0.23099900
O	1.65007800	-5.71297700	-1.68294300
N	-5.16966000	1.91191800	-0.70875600
C	-5.60209400	1.48647800	-2.03007500
C	-6.09542400	2.63827100	0.14484300
H	-4.88660800	1.79383200	-2.80374700
H	-5.72890700	0.39566800	-2.09752600
H	-6.56070700	1.95400000	-2.26049600
H	-6.43874000	2.03485000	0.99852300
H	-5.63929800	3.55558200	0.53902000
H	-6.97013100	2.92732000	-0.43992900

P(*para*–NO_2–phenyl)(*para*–NMe_2–phenyl)$_2$

0 1

P	0.02137100	0.05111500	-1.61924900
C	-1.39467500	-0.84015200	-0.85297900
C	-0.10508700	1.71841800	-0.81822200
C	1.51771600	-0.68004100	-0.83347700
C	-2.01491600	-1.85087500	-1.60536100
C	-1.91521000	-0.58980000	0.42823800
C	0.96002400	2.31655800	-0.12355100
C	-1.28087300	2.47035600	-1.01658100
C	2.71240400	-0.66840600	-1.57196200
C	1.55850300	-1.27751200	0.43662200
C	-3.08072900	-2.59220000	-1.10796700
H	-1.66015700	-2.06019100	-2.61200100
C	-2.98511100	-1.31535800	0.93965700
H	-1.48856400	0.20056600	1.03988800
C	0.85781200	3.61519800	0.37049400
H	1.87597000	1.75839700	0.04004600
C	-1.40203200	3.76358600	-0.52381500
H	-2.11484300	2.03189100	-1.55785800

C	3.89654600	-1.19593700	-1.06783500
H	2.71762900	-0.24053900	-2.57214700
C	2.72944700	-1.81910900	0.95312100
H	0.65304200	-1.33757300	1.03369700
C	-3.59110500	-2.35181200	0.18936300
H	-3.52300600	-3.35354200	-1.73928500
H	-3.35154300	-1.06972000	1.92938600
C	-0.32495500	4.32277800	0.16689400
H	1.67150600	4.08101600	0.91314000
H	-2.30522500	4.34466300	-0.66471500
C	3.94031300	-1.78044300	0.21946700
H	4.78530600	-1.16203200	-1.68658900
H	2.69821600	-2.27842400	1.93410000
N	5.11706500	-2.29345900	0.74120900
N	-4.63889200	-3.09801200	0.70461200
C	-5.25559200	-2.70014100	1.95902800
H	-4.52660600	-2.71079100	2.77862400
H	-5.70173200	-1.69408000	1.91411900
H	-6.04406600	-3.41187300	2.21091100
C	-5.34854100	-4.02862600	-0.15663700
H	-5.84263400	-3.53149600	-1.00651200
H	-4.66902500	-4.79007300	-0.55853100
H	-6.11283600	-4.54491400	0.42746100
C	5.08488900	-3.04563300	1.98407000
H	4.69939300	-2.43178500	2.80730100
H	4.46418300	-3.95320800	1.91719100
H	6.10118400	-3.34624700	2.24586700
C	6.29091300	-2.40185400	-0.10851200
H	6.13028200	-3.06414400	-0.97392200
H	6.59635100	-1.41869800	-0.48704600
H	7.12101400	-2.80110700	0.47738500
N	-0.44303600	5.68658900	0.69133300
O	0.52462600	6.15808600	1.29136400
O	-1.50447600	6.28408500	0.50336500

P(*para*−OMe−phenyl)$_2$(*para*−Me−phenyl)

0 1

P	0.00020500	0.40393800	1.55600000
C	1.33314500	-0.66748500	0.85178700
C	0.21299800	1.97891700	0.60308800
C	-1.53680100	-0.31546700	0.82057100
C	1.72829800	-1.79019000	1.60567800
C	1.99914900	-0.42826000	-0.35647200
C	1.10772100	2.93024300	1.12295300
C	-0.47738600	2.30161900	-0.57387200
C	-2.76270200	0.01600000	1.43092800
C	-1.56966700	-1.19245700	-0.27018100
C	2.72723900	-2.64554300	1.16169800
H	1.24508300	-1.99204800	2.55887400
C	3.01569900	-1.27344900	-0.81303900
H	1.73143600	0.43567000	-0.95771800
C	1.31823000	4.14693900	0.47821900
H	1.64481000	2.71427300	2.04402200
C	-0.27120200	3.52737600	-1.21056500
H	-1.18261800	1.59284700	-0.99771300
C	-3.96663000	-0.48756800	0.95823400
H	-2.76963000	0.67768300	2.29410900
C	-2.77266600	-1.71863700	-0.75183700
H	-0.64290200	-1.48211100	-0.75666600
C	3.38129200	-2.39124400	-0.05397100
H	3.02983100	-3.51156100	1.74242400
H	3.50968500	-1.04947800	-1.75202800
C	0.62773600	4.47072600	-0.69879800
H	2.02237000	4.86166200	0.89959400
H	-0.81936400	3.75304700	-2.12321400
C	-3.97980400	-1.36292000	-0.13901500
H	-4.91106400	-0.22963300	1.42759000
H	-2.75362400	-2.39888800	-1.59610600
C	5.06049300	-3.06944800	-1.61176600
H	4.38985300	-3.09934500	-2.48096600
H	5.59664000	-2.11108900	-1.60479700
H	5.78198400	-3.88533600	-1.68574300
C	-5.28462600	-2.71051600	-1.61802600
H	-4.89775200	-2.25687300	-2.54034900

H	-4.73552100	-3.64012500	-1.41735500
H	-6.34443400	-2.93865400	-1.74630900
O	-5.20922400	-1.81286100	-0.52294300
O	4.35512700	-3.28188600	-0.40015500
C	0.82690900	5.80844300	-1.37264400
H	0.23046100	6.59210400	-0.88619300
H	1.87424400	6.12818300	-1.32950700
H	0.52564800	5.77609500	-2.42498500

P(*para*–OMe–phenyl)(*para*–Me–phenyl)$_2$

0 1

P	0.31238000	0.00006400	1.40843800
C	-1.35242700	-0.15765300	0.62057100
C	1.26580900	-1.36513800	0.59582100
C	1.01804700	1.51177400	0.60289100
C	-2.44819200	0.36713700	1.31892600
C	-1.60316700	-0.78517500	-0.61441700
C	1.22128700	-2.63121400	1.20432100
C	2.04522900	-1.21931500	-0.56090300
C	2.16397300	2.07577100	1.19022300
C	0.47300400	2.15209100	-0.51901600
C	-3.74802300	0.29862300	0.81106700
H	-2.28942700	0.83914200	2.28584600
C	-2.89039900	-0.87033900	-1.12963800
H	-0.78052100	-1.21849300	-1.17568100
C	1.91285500	-3.71309300	0.66410100
H	0.63761800	-2.77011900	2.11175000
C	2.74524300	-2.30444500	-1.09232500
H	2.10834700	-0.25280500	-1.05208000
C	2.75305600	3.22199300	0.66163500
H	2.59935800	1.61055900	2.07202800
C	1.06057600	3.30770000	-1.03824500
H	-0.41653300	1.74852100	-0.99334400
C	-3.97316200	-0.32513700	-0.42193300
H	-4.56656400	0.71985400	1.38374300
H	-3.08627700	-1.35697100	-2.08042400
C	2.69267000	-3.56837800	-0.49238300

H	1.85416900	-4.68391400	1.15214800
H	3.34155000	-2.16515100	-1.99191000
C	2.20846100	3.86309600	-0.46053700
H	3.64454800	3.63170900	1.13231700
H	0.61835900	3.78442300	-1.91083800
C	3.47419600	-4.73383800	-1.05280300
H	4.42483300	-4.86919000	-0.51937100
H	2.91683000	-5.67280700	-0.96035600
H	3.71308600	-4.58447700	-2.11102100
C	2.82580900	5.12939100	-1.00693300
H	2.50791800	6.00852400	-0.43020300
H	3.92025200	5.09432600	-0.96260300
H	2.53432900	5.30031000	-2.04856000
O	-5.19487900	-0.46014800	-1.01287400
C	-6.32821400	0.06691800	-0.34249300
H	-6.47957300	-0.41272700	0.63366000
H	-6.24513500	1.15268200	-0.20050400
H	-7.18361600	-0.14779200	-0.98576000

P(*para*−OMe−phenyl)$_2$(*para*−NMe$_2$−phenyl)

0 1

P	-0.34369200	-0.00790400	1.51726100
C	-1.06470100	1.47269700	0.67111000
C	-1.19241300	-1.41072200	0.65644900
C	1.36812400	-0.07285300	0.83057300
C	-0.96062300	2.70584500	1.32914200
C	-1.73272500	1.44873800	-0.56714300
C	-2.39242400	-1.87755100	1.21038100
C	-0.70518800	-2.06493600	-0.48990500
C	2.33629500	-0.78655900	1.55567500
C	1.79307100	0.55290300	-0.35153400
C	-1.47478600	3.88246700	0.77882200
H	-0.46869900	2.75473000	2.29807600
C	-2.25904200	2.60811500	-1.12475900
H	-1.84805200	0.50901400	-1.09914200
C	-3.10504000	-2.93663900	0.64294200
H	-2.78457800	-1.40796400	2.10986900

C	-1.39601200	-3.12700100	-1.06170600
H	0.23064800	-1.74221100	-0.93645900
C	3.65324600	-0.89348700	1.12255000
H	2.05393100	-1.27558900	2.48570100
C	3.10901300	0.46545700	-0.79604200
H	1.08416000	1.12662300	-0.94201700
C	-2.13040900	3.83532800	-0.45740100
H	-1.36890600	4.81502400	1.32175500
H	-2.77703400	2.58968900	-2.07907400
C	-2.60410200	-3.56847900	-0.50175600
H	-4.03112400	-3.26265500	1.10306200
H	-1.01933700	-3.63420800	-1.94502600
C	4.08085800	-0.25797500	-0.06639400
H	4.35162400	-1.46690200	1.72063800
H	3.37751500	0.96715800	-1.71844700
C	-4.42762300	-5.10737000	-0.61357800
H	-5.20962600	-4.33620800	-0.61977300
H	-4.72671100	-5.92833800	-1.26815200
C	-2.58419700	6.18046400	-0.45721500
H	-3.09232000	6.18719400	0.51643100
H	-1.53831200	6.48542900	-0.31785200
H	-3.07903800	6.88732600	-1.12609200
O	-2.67992900	4.91453500	-1.08789400
O	-3.20530700	-4.61648100	-1.13758200
H	-4.30609200	-5.48656500	0.40998000
N	5.40200800	-0.32788800	-0.49029700
C	5.75379900	0.16337500	-1.81129700
C	6.31439800	-1.24559600	0.16988300
H	5.23037900	-0.37062100	-2.62096500
H	5.52415900	1.23141500	-1.90823600
H	6.82860000	0.04375900	-1.96248300
H	6.41829100	-1.00068900	1.23390300
H	5.99378700	-2.29725500	0.09391000
H	7.30283200	-1.15613800	-0.28543900

P(*para*−OMe−phenyl)(*para*−NMe$_2$−phenyl)$_2$

0 1

P	0.00454500	0.26296200	-1.66352400
C	-1.49505500	-0.46451600	-0.86849500
C	0.10173900	1.93210900	-0.86538200
C	1.39085600	-0.65659000	-0.86160300
C	-2.14551800	-1.51611300	-1.53407100
C	-2.06330100	-0.02961200	0.33857200
C	-0.64058400	2.97738500	-1.45032100
C	0.89239800	2.24236800	0.24678600
C	2.63097300	-0.67704700	-1.52044100
C	1.29836000	-1.37617600	0.33935500
C	-3.28456400	-2.12467700	-1.01813900
H	-1.75614900	-1.86579300	-2.48794400
C	-3.20845000	-0.61976500	0.86588900
H	-1.61160900	0.79870300	0.87740900
C	-0.61135500	4.26521400	-0.93370400
H	-1.24983700	2.77519800	-2.32849500
C	0.94305400	3.53799500	0.77357000
H	1.48871900	1.46554700	0.71610100
C	3.73169300	-1.35131300	-1.00294900
H	2.73937900	-0.15755000	-2.47030500
C	2.38611600	-2.06571000	0.86768400
H	0.35225100	-1.41284700	0.87213400
C	-3.84436100	-1.69792200	0.20831500
H	-3.74443400	-2.92753200	-1.58223300
H	-3.60835500	-0.23179500	1.79551600
C	0.18522200	4.55577900	0.18497300
H	-1.18639900	5.06872900	-1.38402000
H	1.57218700	3.73568600	1.63453400
C	3.64186300	-2.05946100	0.21776700
H	4.66007600	-1.33429800	-1.56159400
H	2.25006700	-2.61486400	1.79213000
N	4.74173700	-2.71887500	0.75682800
N	-4.97004500	-2.31359700	0.74565400
C	-5.64638500	-1.69576800	1.87330500
H	-4.97646900	-1.61723000	2.73777200
H	-6.02701400	-0.68642100	1.64647400
H	-6.49112000	-2.32145700	2.16930300

C	-5.72138200	-3.25357100	-0.06841400
H	-6.13442600	-2.79719100	-0.98292100
H	-5.09400200	-4.10133700	-0.36807000
H	-6.55093000	-3.65170000	0.51986600
C	4.54750100	-3.62424100	1.87635700
H	4.13300300	-3.09443700	2.74222300
H	3.87443800	-4.46431000	1.63881000
H	5.51439600	-4.03453500	2.17548800
C	5.93760900	-2.88199700	-0.05198400
H	5.75975100	-3.46338300	-0.97152500
H	6.34994600	-1.90858400	-0.34270500
H	6.69918900	-3.39771000	0.53686900
O	0.15590400	5.85292300	0.61303800
C	0.95098500	6.20686800	1.73126000
H	0.65527000	5.65086700	2.63128400
H	2.01885300	6.03537000	1.53970500
H	0.78148000	7.27291400	1.89540200

P(*para*−Me−phenyl)$_2$(*para*−NMe$_2$−phenyl)

0 1

P	0.67067700	-0.02421300	-1.47116500
C	-1.04769700	0.04361400	-0.80690600
C	1.48280300	1.40825400	-0.61980200
C	1.41779700	-1.47571400	-0.59331400
C	-2.07089600	-0.53009100	-1.57889300
C	-1.42428700	0.64191900	0.40604500
C	1.39662500	2.66310000	-1.24696400
C	2.19518200	1.32492700	0.58525600
C	2.65794300	-1.94428600	-1.06163300
C	0.81502700	-2.16529600	0.46782700
C	-3.39800500	-0.52865100	-1.16353300
H	-1.82464600	-0.99257600	-2.53232100
C	-2.74776500	0.66153900	0.83395800
H	-0.66956300	1.10846000	1.03312600
C	1.98303000	3.79240500	-0.68022000
H	0.86302900	2.75525300	-2.19045900
C	2.79038100	2.45800700	1.14413000

H	2.28816500	0.36946100	1.09300100
C	3.27946400	-3.04433600	-0.47564200
H	3.14210800	-1.43998700	-1.89530000
C	1.43658300	-3.27536200	1.04443400
H	-0.14675700	-1.83503000	0.84866900
C	-3.77652300	0.07990400	0.05579200
H	-4.14170400	-0.99522400	-1.79866600
H	-2.97869400	1.13610400	1.78055700
C	2.69619600	3.70975400	0.52447800
H	1.89401600	4.75252300	-1.18475900
H	3.33627100	2.36619300	2.08115100
C	2.67687500	-3.73465900	0.58634100
H	4.24345300	-3.37930800	-0.85362700
H	0.94764100	-3.79201200	1.86813000
C	3.36580300	4.92855600	1.11572900
H	4.33491200	5.12306300	0.63650000
H	2.75429400	5.82800100	0.98110400
H	3.55213200	4.80315600	2.18759100
C	3.33467800	-4.95226200	1.19312000
H	3.16188200	-5.84663000	0.57924100
H	4.42005200	-4.82380000	1.27512700
H	2.94240300	-5.16293900	2.19361000
N	-5.10243000	0.11819900	0.46439600
C	-5.42619000	0.58303900	1.80196500
C	-6.09714300	-0.65051500	-0.26353100
H	-4.96826100	-0.03407700	2.59171800
H	-5.09749200	1.61898800	1.95030300
H	-6.50951600	0.55962100	1.93612700
H	-6.16074100	-0.32463200	-1.30903300
H	-5.88875400	-1.73247100	-0.25802400
H	-7.07665400	-0.48941500	0.19111500

P(*para*–Me–phenyl)(*para*–NMe$_2$–phenyl)$_2$

0 1

P	0.01850300	0.63650900	-1.54378900
C	-1.42399100	-0.26603700	-0.82813900
C	-0.03059900	2.23885400	-0.61016300

C	1.47048600	-0.23079200	-0.80413100
C	-2.00277600	-1.29061300	-1.59424400
C	-2.01298200	0.00653300	0.41634300
C	-0.90808800	3.23358800	-1.07719600
C	0.77607600	2.54443000	0.49438700
C	2.70668000	-0.11217300	-1.45992200
C	1.43568300	-1.03654900	0.34414200
C	-3.09263300	-2.02608900	-1.14109500
H	-1.59574800	-1.51643100	-2.57758700
C	-3.10971500	-0.71245400	0.88266300
H	-1.61713300	0.80752800	1.03460600
C	-0.98916900	4.47427900	-0.45043100
H	-1.53620000	3.03142600	-1.94229000
C	0.69925700	3.79484600	1.11332300
H	1.47010200	1.80206400	0.87696000
C	3.85660300	-0.73574600	-0.98767000
H	2.77288800	0.47863700	-2.37118900
C	2.57347600	-1.67682200	0.82611200
H	0.49668600	-1.18115200	0.87101200
C	-3.67251200	-1.76302200	0.12153100
H	-3.49838000	-2.80024500	-1.78164200
H	-3.52928100	-0.44784900	1.84628000
C	-0.18181800	4.78059000	0.65542400
H	-1.68358600	5.22170300	-0.82962700
H	1.33608500	4.00507900	1.97056200
C	3.82360400	-1.53105200	0.18109000
H	4.77963800	-0.61012000	-1.54123500
H	2.48201800	-2.29676300	1.71036800
N	4.97083000	-2.14126800	0.67600000
N	-4.74775300	-2.50679700	0.59518500
C	-5.45481600	-2.05719500	1.78205200
H	-4.78375800	-2.02009000	2.64844500
H	-5.90761300	-1.05954300	1.66091200
H	-6.25068600	-2.76806100	2.01418000
C	-5.43459000	-3.41580800	-0.30627300
H	-5.88384100	-2.90429200	-1.17321500
H	-4.75022600	-4.18413200	-0.68517200

H	-6.23066000	-3.92644100	0.23975500
C	4.85028700	-3.12838300	1.73514700
H	4.40183900	-2.68773300	2.63350500
H	4.24052300	-3.99925200	1.44398900
H	5.84649900	-3.48387400	2.00681100
C	6.17583000	-2.15297300	-0.13551600
H	6.04312300	-2.67851400	-1.09533200
H	6.51202100	-1.13230100	-0.35330700
H	6.97481100	-2.64992500	0.41882500
C	-0.24538900	6.14168500	1.30903100
H	0.19522600	6.12549800	2.31146300
H	0.30183500	6.89253400	0.72302100
H	-1.27870200	6.49647700	1.39964600

PhI-FigureS1

0 1

C	0.00000000	1.21222400	-1.25424500
C	0.00000000	0.00000000	-0.57271000
C	0.00000000	-1.21222400	-1.25424500
C	0.00000000	-1.20402400	-2.64743900
C	0.00000000	0.00000000	-3.34513700
C	0.00000000	1.20402400	-2.64743900
H	0.00000000	2.15195900	-0.71334900
H	0.00000000	-2.15195900	-0.71334900
H	0.00000000	-2.14758800	-3.18474300
H	0.00000000	0.00000000	-4.43073700
H	0.00000000	2.14758800	-3.18474300
I	0.00000000	0.00000000	1.55762700

PPh_3-FigureS1

0 1

P	0.00416700	0.00229000	1.26399800
C	-0.64156300	-1.51836900	0.44692400
C	1.64019300	0.20698500	0.44098600
C	-0.99466100	1.31252300	0.43859300
C	-1.79189700	-2.09469500	1.00032600
C	-0.06300500	-2.11836200	-0.67586500

C	2.74109000	-0.40421300	1.05308100
C	1.84082500	0.91765500	-0.74712500
C	-1.01239800	2.57518400	1.04266500
C	-1.71306400	1.12361400	-0.74686000
C	-2.36213600	-3.23039500	0.43469500
H	-2.24491700	-1.64794200	1.88224100
C	-0.62740300	-3.26248200	-1.23581400
H	0.83202000	-1.69096000	-1.11771300
C	4.00817800	-0.32307900	0.48353400
H	2.60379500	-0.94534600	1.98618700
C	3.11009600	1.00684900	-1.31274700
H	1.00121600	1.40500200	-1.23390400
C	-1.71436900	3.62988600	0.46709400
H	-0.47303400	2.73190600	1.97374000
C	-2.42254100	2.17656700	-1.31897700
H	-1.71723800	0.14938900	-1.22678100
C	-1.77872300	-3.81845500	-0.68538600
H	-3.25711100	-3.66173200	0.87354000
H	-0.16596700	-3.71807700	-2.10730500
C	4.19516200	0.38399300	-0.70150700
H	4.85144500	-0.80545100	0.96924700
H	3.25016400	1.56168100	-2.23604800
C	-2.42148100	3.43171200	-0.71616500
H	-1.71519700	4.60423900	0.94683300
H	-2.97417400	2.01563500	-2.24079600
H	-2.21784300	-4.70950800	-1.12445500
H	5.18412400	0.45480000	-1.14485300
H	-2.97362100	4.25250100	-1.16462200

5-FigureS1

0 1

Pd	-1.19679900	-0.46821400	-0.02853100
P	1.11363100	-0.27263100	-0.00273900
I	-3.76438500	-1.04371300	0.01461800
C	1.92315800	0.85970700	-1.18346300
C	1.80914400	-1.92328100	-0.36378100
C	1.78403900	0.18831700	1.62953600

C	2.62235000	0.37804300	-2.29315500
C	1.79110600	2.24225200	-0.99958300
C	1.11715900	-2.74199700	-1.26452200
C	2.99409000	-2.38723700	0.21584000
C	1.04384500	-0.15123800	2.76723100
C	3.02068300	0.82421400	1.77780500
C	3.18051900	1.26749500	-3.20794000
H	2.73651300	-0.69032400	-2.44767400
C	2.35320700	3.12442100	-1.91409100
H	1.24784600	2.63323200	-0.14444600
C	1.60737400	-4.00381800	-1.58685500
H	0.19286500	-2.39152500	-1.71992800
C	3.47918100	-3.65046200	-0.10640100
H	3.53454000	-1.76612400	0.92373600
C	1.53751000	0.13403300	4.03589100
H	0.07444400	-0.63243800	2.65613600
C	3.51054700	1.11067600	3.04871600
H	3.59768900	1.10208700	0.90065100
C	3.04645000	2.63969800	-3.02105400
H	3.72107500	0.88320800	-4.06751600
H	2.23749900	4.19309100	-1.76305400
C	2.78795500	-4.45872600	-1.00663200
H	1.06050900	-4.63206700	-2.28273500
H	4.39739400	-4.00679000	0.35036000
C	2.77108300	0.76505300	4.17718000
H	0.95531000	-0.13130500	4.91288400
H	4.47051200	1.60610600	3.15702200
H	3.47958000	3.33147300	-3.73738000
H	3.16830500	-5.44599500	-1.25066200
H	3.15491300	0.99127800	5.16738700
C	-1.28474900	1.49981000	-0.05432900
C	-1.46865900	2.13541200	-1.27838400
C	-1.15429300	2.22794800	1.12350400
C	-1.50358000	3.52826000	-1.32061900
H	-1.58014700	1.56046200	-2.19139800
C	-1.18873600	3.62263000	1.06581100
H	-1.01617200	1.72797200	2.07626200

C	-1.35614500	4.27378300	-0.15343400
H	-1.64547500	4.02789600	-2.27457400
H	-1.08406200	4.19514800	1.98309400
H	-1.38189000	5.35871600	-0.19301500

6-FigureS1

0 1

P	-2.37069900	-0.00140400	-0.02870600
C	-3.10139000	-0.40073300	-1.65767400
C	-3.13251600	1.61619600	0.37850100
C	-2.36164600	-1.14309200	-2.58230300
C	-4.39845300	0.01078900	-1.99163600
C	-3.14258500	-1.13522200	1.17968700
Pd	0.00004400	-0.09805200	-0.00017100
C	-3.66454600	1.87726600	1.64207000
C	-3.08374400	2.64739400	-0.56690200
C	-2.91346200	-1.47475400	-3.81677900
H	-1.36192700	-1.48042500	-2.32688900
C	-4.94666700	-0.32396400	-3.22489200
H	-4.97785500	0.60435100	-1.29045800
C	-2.49572100	-1.31928900	2.40583600
C	-4.35869000	-1.77716500	0.94407000
C	0.00006300	1.92198500	-0.00012000
C	-4.13081500	3.15189400	1.95804900
H	-3.71798100	1.08995600	2.38709300
C	-3.54761900	3.91628300	-0.24949500
H	-2.66105300	2.46414600	-1.54934300
C	-4.20426600	-1.06809000	-4.13944000
H	-2.33036200	-2.05745000	-4.52329300
H	-5.95362200	-0.00092500	-3.47173900
C	-3.06722100	-2.11714500	3.38976100
H	-1.53106500	-0.84943800	2.57959900
C	-4.92269800	-2.58762500	1.92555000
H	-4.86287400	-1.66169900	-0.01001200
C	-0.20458500	2.63479500	1.18367000
C	0.20471100	2.63482200	-1.18389300
C	-4.07012600	4.17287200	1.01675100

H	-4.54494800	3.34122000	2.94400600
H	-3.48850200	4.70872900	-0.98892800
H	-4.63310000	-1.32735900	-5.10298500
C	-4.28219600	-2.75463500	3.14952100
H	-2.55503700	-2.25651600	4.33681500
H	-5.86398900	-3.09231200	1.72978900
C	-0.20329100	4.02871200	1.18506400
H	-0.38450000	2.10518900	2.11636800
C	0.20340800	4.02873800	-1.18525800
H	0.38463900	2.10523700	-2.11659900
H	-4.42918500	5.16711700	1.26616800
H	-4.72263900	-3.39033900	3.91190200
C	0.00005100	4.73052400	-0.00009000
H	-0.37122500	4.56478800	2.11550400
H	0.37133800	4.56483400	-2.11568700
H	0.00004000	5.81699800	-0.00008000
P	2.37079200	-0.00138300	0.02869500
C	3.14300000	-1.13523800	-1.17944300
C	3.10104500	-0.40069500	1.65786800
C	3.13261700	1.61622300	-0.37845300
C	2.49630000	-1.31956200	-2.40563700
C	4.35918300	-1.77696100	-0.94360800
C	4.39788200	0.01109400	1.99236700
C	2.36115400	-1.14340200	2.58210800
C	3.08372300	2.64748600	0.56687000
C	3.66469300	1.87724700	-1.64201600
C	3.06803200	-2.11744800	-3.38940500
H	1.53158800	-0.84989000	-2.57955800
C	4.92341900	-2.58745600	-1.92492700
H	4.86324500	-1.66128800	0.01051600
C	4.94571500	-0.32368100	3.22579000
H	4.97740900	0.60488000	1.29148300
C	2.91259800	-1.47510800	3.81673500
H	1.36162500	-1.48098000	2.32626500
C	3.54752900	3.91638600	0.24939800
H	2.66098800	2.46428300	1.54929900
C	4.13089000	3.15188300	-1.95806000

H	3.71822000	1.08989400	-2.38698800
C	4.28307500	-2.75472100	-3.14894900
H	2.55596700	-2.25701700	-4.33649400
H	5.86476500	-3.09198000	-1.72900300
C	4.20316600	-1.06812900	4.13995100
H	5.95248900	-0.00040000	3.47306400
H	2.32939100	-2.05807600	4.52293500
C	4.07008600	4.17292300	-1.01683400
H	3.48831700	4.70887400	0.98877700
H	4.54505700	3.34116900	-2.94401000
H	4.72370300	-3.39045800	-3.91119600
H	4.63170400	-1.32741500	5.10362500
H	4.42908600	5.16717600	-1.26630400
I	-0.00007100	-2.87719000	-0.00034800

TS7-FigureS1

0 1

P	2.18649000	0.13493100	0.18588000
C	3.56319800	-0.88801100	-0.44585700
C	3.05478800	1.67259900	0.73039900
C	3.27529100	-2.04678100	-1.17424800
C	4.89662100	-0.56425300	-0.16482400
C	1.62361200	-0.59936100	1.78213800
Pd	0.03942500	-0.45994000	-0.42585900
C	3.32101900	1.92541400	2.07889400
C	3.58283000	2.54491500	-0.23305700
C	4.30732000	-2.86849500	-1.61636900
H	2.24232900	-2.32487100	-1.36883200
C	5.92288100	-1.38994300	-0.61098300
H	5.14038200	0.32734300	0.40225000
C	0.72833300	0.12900200	2.58158000
C	1.93991200	-1.91549900	2.12684500
C	1.17405900	1.05047600	-1.39061500
C	4.06004000	3.04431600	2.45895700
H	2.96059100	1.24803800	2.84406400
C	4.32787900	3.65351100	0.14743300
H	3.42468700	2.35394700	-1.28917500

C	5.63089200	-2.54138700	-1.33828100
H	4.06642500	-3.76888700	-2.17268100
H	6.95379700	-1.13260500	-0.38752200
C	0.15690600	-0.45388600	3.70525100
H	0.48074800	1.15370100	2.31909600
C	1.37161400	-2.48951200	3.25891600
H	2.59513000	-2.50462700	1.49446600
C	0.71899400	2.36955000	-1.22940100
C	1.54047900	0.60121000	-2.66761300
C	4.55988300	3.91341200	1.49679800
H	4.24621600	3.22809800	3.51270600
H	4.72680600	4.31726500	-0.61346500
H	6.43517500	-3.18443300	-1.68355800
C	0.47697100	-1.76629500	4.04296300
H	-0.55832100	0.10647000	4.29953800
H	1.61162800	-3.51733300	3.51162700
C	0.58288200	3.20076200	-2.33144200
H	0.46635000	2.74176100	-0.24218700
C	1.41335800	1.44763000	-3.76862500
H	1.92319400	-0.40474200	-2.80202800
H	5.13566800	4.78506200	1.79354000
H	0.01755600	-2.22853000	4.91127600
C	0.93115300	2.74154500	-3.60284700
H	0.19554800	4.20548300	-2.19468200
H	1.69199100	1.08833600	-4.75470100
H	0.83387400	3.39879100	-4.46204200
P	-2.22432100	0.39385500	0.02584700
C	-3.50660900	0.02220500	-1.22685500
C	-2.95540000	-0.19370000	1.60525300
C	-2.30134300	2.22104700	0.17862200
C	-3.10266400	-0.57737400	-2.42186900
C	-4.85962100	0.32122000	-1.02976200
C	-3.82584500	0.57408700	2.38851000
C	-2.61679300	-1.48291800	2.02952600
C	-1.78511700	2.84000400	1.32565500
C	-2.68497100	3.02452400	-0.89789200
C	-4.03961300	-0.86552900	-3.41245100

H	-2.05758000	-0.83887900	-2.56445100
C	-5.79243300	0.03204900	-2.01792900
H	-5.18525800	0.77575900	-0.09818900
C	-4.34140800	0.06443000	3.57655300
H	-4.09161500	1.58121700	2.07936000
C	-3.14470700	-1.99472100	3.21149200
H	-1.93659000	-2.08799800	1.43516000
C	-1.65413100	4.22232400	1.39368000
H	-1.49467500	2.23260100	2.17897900
C	-2.55531600	4.41047500	-0.82977100
H	-3.08177400	2.56746300	-1.79919900
C	-5.38151500	-0.56114300	-3.21180900
H	-3.71741600	-1.34077800	-4.33385600
H	-6.84160800	0.26146200	-1.85602200
C	-4.00216700	-1.22240500	3.98946600
H	-5.01068900	0.67274700	4.17830000
H	-2.87451000	-2.99902000	3.52394900
C	-2.03533200	5.01382900	0.31084200
H	-1.25448300	4.68267500	2.29263100
H	-2.86166900	5.01877900	-1.67612500
H	-6.11279400	-0.79295400	-3.98085400
H	-4.40838800	-1.62118900	4.91482400
H	-1.93185000	6.09366600	0.36150900
I	-0.34774600	-3.21857200	-0.83290100

8-FigureS1

0 1

P	2.81168500	0.19206500	0.09879900
C	3.78920400	-1.32700200	0.08203700
C	3.96180000	1.59597100	0.03726100
C	3.15425600	-2.53396500	-0.23030900
C	5.15638700	-1.30963700	0.38287100
C	1.71401400	0.25085600	-1.30044500
Pd	-0.31874400	-0.43519200	-0.64567800
C	4.13766400	2.27608100	-1.17097800
C	4.68560000	1.98751400	1.17096600
C	3.88359900	-3.71813900	-0.22219800

H	2.09364500	-2.56251700	-0.47261200
C	5.87643500	-2.49871500	0.38433400
H	5.66394400	-0.37618500	0.60211700
C	0.70750200	1.29582900	-1.28401400
C	2.18372000	-0.25286300	-2.56910200
C	1.87702600	0.34860200	1.63801200
C	5.04009500	3.33371000	-1.24423300
H	3.56972100	1.98353600	-2.04960800
C	5.58543300	3.04388600	1.09014700
H	4.53717300	1.47423800	2.11726300
C	5.24089800	-3.70238600	0.08555400
H	3.37676100	-4.64843200	-0.45751400
H	6.93744300	-2.48295300	0.61351000
C	0.24519800	1.79562100	-2.55269600
H	0.64037400	1.98473600	-0.44307400
C	1.66962900	0.22660700	-3.73773100
H	2.94235700	-1.02963200	-2.58287500
C	1.56158700	1.61296900	2.14771300
C	1.31851000	-0.79766200	2.21331500
C	5.76352100	3.71547700	-0.11844100
H	5.17395200	3.85976700	-2.18402300
H	6.14356500	3.34580200	1.97087700
H	5.80761300	-4.62879600	0.08877300
C	0.68959600	1.26579100	-3.72854300
H	-0.47282600	2.61078100	-2.54458500
H	2.01173600	-0.18213700	-4.68334200
C	0.67408100	1.72600600	3.21351500
H	1.98811800	2.50823800	1.70513100
C	0.43335100	-0.67329400	3.27615500
H	1.52943500	-1.78202200	1.80926100
H	6.46638700	4.54087100	-0.17912300
H	0.31305500	1.64942900	-4.67232400
C	0.09959200	0.58535300	3.76772700
H	0.41943300	2.70837400	3.59989500
H	-0.02597900	-1.56234100	3.69335900
H	-0.62931200	0.67533000	4.56705700
P	-2.40733000	0.44531500	-0.03537100

C	-2.88191400	0.26992500	1.73388000
C	-3.89895900	-0.17552700	-0.89737500
C	-2.46312100	2.25728800	-0.32374000
C	-2.73467900	-1.00247800	2.29917100
C	-3.37856900	1.31002700	2.52426800
C	-5.18876200	0.24250300	-0.54777100
C	-3.73220300	-1.10251300	-1.92804900
C	-3.17745700	2.83282700	-1.37737600
C	-1.61229600	3.07409300	0.43484200
C	-3.07991600	-1.22676200	3.62769300
H	-2.33374300	-1.81511700	1.69699800
C	-3.70554700	1.08717900	3.86047300
H	-3.50945900	2.30163700	2.10171600
C	-6.29412200	-0.25013200	-1.23030100
H	-5.32567500	0.95449100	0.26232600
C	-4.84292300	-1.59906200	-2.60835100
H	-2.73339900	-1.45178400	-2.17602000
C	-3.04599200	4.19128800	-1.66329500
H	-3.83431600	2.21806400	-1.98497800
C	-1.48978700	4.42978500	0.15680600
H	-1.03984900	2.63544300	1.24897600
C	-3.55774300	-0.18096500	4.41565600
H	-2.96566300	-2.22122300	4.04989100
H	-4.08598600	1.90630100	4.46454500
C	-6.12067200	-1.17255500	-2.26268800
H	-7.29225600	0.07803500	-0.95453000
H	-4.70504800	-2.32898100	-3.40025600
C	-2.20467800	4.99371700	-0.89929000
H	-3.60597000	4.62141000	-2.48870100
H	-0.83128500	5.04778500	0.76099400
H	-3.81839400	-0.35509800	5.45590600
H	-6.98621600	-1.56383800	-2.78982100
H	-2.10381600	6.05154900	-1.12330400
I	-0.58405200	-3.22751100	-0.31594300

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Pd	0.34093300	-0.05403100	-0.45047500
P	-2.10405000	-0.04646000	-0.21204500
C	-2.89488300	-1.14831100	1.03699700
C	-2.90840100	-0.51842500	-1.80572600
C	-2.78640800	1.62621300	0.15621500
C	-2.30063500	-1.24509700	2.30711700
C	-4.05526900	-1.89046400	0.76760200
C	-2.31818500	-1.55189600	-2.55308000
C	-4.05767400	0.11091600	-2.30814900
C	-2.11868800	2.73788000	-0.38448600
C	-3.92678100	1.83621800	0.94546200
C	-2.86745700	-2.05855500	3.28850900
H	-1.39259400	-0.69232400	2.52532400
C	-4.61418200	-2.70873300	1.75166900
H	-4.52222400	-1.83397700	-0.21060000
C	-2.87178300	-1.95576500	-3.76781700
H	-1.41871800	-2.03863100	-2.18233700
C	-4.60563600	-0.28981800	-3.52875600
H	-4.52292500	0.91746000	-1.74973000
C	-2.59104800	4.03004800	-0.15507700
H	-1.22229400	2.58550300	-0.98157600
C	-4.39316400	3.13178500	1.18077100
H	-4.44868900	0.98999200	1.38171400
C	-4.02348600	-2.79276100	3.01353900
H	-2.39689500	-2.12452400	4.26566000
H	-5.51115300	-3.28076700	1.52909900
C	-4.01631600	-1.32337100	-4.25913500
H	-5.49336000	0.20886800	-3.90880900
C	-3.72944300	4.22929100	0.62994200
H	-2.06539200	4.88027300	-0.58130600
H	-5.27561700	3.28151400	1.79722200
H	-4.45872700	-3.43160200	3.77747800
H	-4.44300000	-1.63065300	-5.21009800
H	-4.09328600	5.23612100	0.81649700
C	0.94956900	0.17715800	1.47101900
C	0.72537300	1.39148700	2.13492100
C	1.47304700	-0.90529800	2.18875100

C	1.00390900	1.51193500	3.50176100
H	0.32070100	2.24806500	1.60253800
C	1.74537000	-0.78105500	3.55677800
H	1.67962500	-1.84746300	1.69012000
C	1.51221400	0.42619400	4.21796700
H	0.82093400	2.45984600	4.00336900
H	2.14951300	-1.63263200	4.10017200
H	1.72939000	0.52245100	5.27879200
P	2.45069100	-0.10982800	-1.33967700
C	3.41718400	-1.55759000	-0.74578700
C	4.34214600	-1.51892600	0.31467100
C	3.17416900	-2.79575000	-1.36988300
C	5.00488400	-2.67601100	0.72550000
H	4.53905900	-0.57976800	0.82152800
C	3.82936700	-3.95419600	-0.95169000
H	2.47093300	-2.84472100	-2.19819700
C	4.75139200	-3.89736400	0.09595200
H	5.71569800	-2.62443200	1.54668600
H	3.62803300	-4.89877300	-1.45092400
H	5.26885200	-4.79702200	0.41884600
C	3.53775700	1.33763300	-1.02475900
C	4.92165400	1.29022200	-1.27899200
C	2.97293100	2.57675600	-0.67334600
C	5.71081100	2.43509000	-1.16508000
H	5.38538200	0.35164900	-1.56878100
C	3.76154300	3.72146900	-0.56475900
H	1.90679200	2.63470100	-0.47342100
C	5.13583800	3.65602000	-0.80634300
H	6.77840600	2.37214600	-1.36146200
H	3.30275900	4.66595900	-0.28218500
H	5.75160900	4.54714900	-0.71743200
H	-2.40368100	-2.75623400	-4.33418900

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P	0.19378000	-2.17034600	-0.21940500
C	1.83842100	-2.76042200	0.40822200

C	0.12935600	-2.68879300	-1.99161600
C	-0.96587200	-3.39024000	0.57071800
C	2.20811500	-2.37627100	1.70884400
C	2.72132200	-3.57005500	-0.32064200
C	-0.01046200	-1.69841500	-2.97505400
C	0.17499500	-4.03509300	-2.39324000
C	-2.16942400	-3.71884600	-0.07872100
C	-0.71463900	-3.94979900	1.83373900
C	3.40049100	-2.82143300	2.28047000
H	1.56300600	-1.71862100	2.28281000
C	3.92131900	-4.00472800	0.24623200
H	2.48192700	-3.86119600	-1.33698400
C	-0.07281300	-2.03842600	-4.32885800
H	-0.09760100	-0.65881200	-2.66910800
C	0.11728100	-4.37512500	-3.74509500
H	0.23996500	-4.82057000	-1.64626700
C	-3.08818400	-4.58247400	0.52024500
H	-2.39214200	-3.30108300	-1.05229900
C	-1.63545300	-4.81324100	2.42855800
H	0.21035200	-3.73254000	2.35600600
C	4.26051100	-3.64288300	1.55027000
H	3.65875500	-2.51542100	3.29078100
H	4.59178400	-4.63024600	-0.33738800
C	-0.00210400	-3.37708100	-4.71596300
H	-0.18692800	-1.25789000	-5.07639900
H	0.15608300	-5.42052500	-4.03979500
C	-2.82695500	-5.13147400	1.77526600
H	-4.01225300	-4.82079100	0.00048300
H	-1.41491100	-5.24059500	3.40335400
H	5.19220100	-3.98890200	1.98999200
H	-0.05326800	-3.64463800	-5.76809600
H	-3.54396100	-5.80305400	2.23994100
Pd	-0.40052500	0.32611300	-0.04704400
P	1.94486400	1.28870900	0.09159200
C	2.26962600	2.98075000	-0.60536300
C	3.31671900	0.30567100	-0.67267900
C	2.44027000	1.54115400	1.85548400

C	1.70405800	4.09423100	0.03942800
C	3.04129400	3.19340000	-1.75792000
C	3.12421000	-0.14490100	-1.98995900
C	4.53090500	0.01124300	-0.03679100
C	1.63467400	1.00370800	2.86949000
C	3.57262000	2.28995000	2.22036000
C	1.91883500	5.38221500	-0.44870200
H	1.08631700	3.96024200	0.92082700
C	3.24731600	4.48513000	-2.24859400
H	3.49939500	2.35733400	-2.27436100
C	4.12836700	-0.83917100	-2.66508700
H	2.18211900	0.04837600	-2.49398000
C	5.53102600	-0.69521300	-0.70833100
H	4.70092100	0.32733600	0.98635400
C	1.96344700	1.18322000	4.21533800
H	0.73323500	0.46155000	2.59677600
C	3.90448500	2.46571300	3.56384900
H	4.18756200	2.74862100	1.45173800
C	2.69046900	5.58385800	-1.59468900
H	1.46791400	6.22678400	0.06470800
H	3.85275700	4.62745500	-3.14013200
C	5.33833500	-1.11409300	-2.02515400
H	3.95896500	-1.17178900	-3.68569400
H	6.46417200	-0.91681000	-0.19708700
C	3.10239500	1.90966900	4.56413700
H	1.32337600	0.76543000	4.98788400
H	4.78430400	3.04556600	3.83003600
H	2.85405700	6.58866000	-1.97539700
H	6.12131200	-1.65866400	-2.54621600
H	3.35821000	2.05432700	5.61043300
C	-1.14186400	2.23808500	0.13805000
C	-1.46014700	2.76535800	1.39985800
C	-1.25975400	3.08498600	-0.97465500
C	-1.87030600	4.09696300	1.54578700
H	-1.41147400	2.13693200	2.28526000
C	-1.67311400	4.41293900	-0.83397200
H	-1.04034600	2.71008800	-1.97139400

C	-1.97845000	4.92710800	0.42789700
H	-2.11530400	4.47814600	2.53543500
H	-1.75758100	5.04495500	-1.71545100
H	-2.30482400	5.95864300	0.53818000
P	-2.70911600	-0.32922400	-0.33355900
C	-3.67665800	0.86878200	-1.35489300
C	-4.41151100	1.96418700	-0.86791300
C	-3.69309700	0.62935700	-2.74164700
C	-5.14218100	2.77807300	-1.73338500
H	-4.40010500	2.18840300	0.19355900
C	-4.40704200	1.45497600	-3.61156300
H	-3.14758600	-0.22409500	-3.13977300
C	-5.14155600	2.53063100	-3.10861600
H	-5.70264100	3.61945900	-1.33268900
H	-4.40258000	1.24815000	-4.67936400
H	-5.70927000	3.16923300	-3.78085900
C	-3.52031800	-0.25968600	1.32056400
C	-4.92443900	-0.25961500	1.44458300
C	-2.76707000	-0.38963700	2.50240800
C	-5.54052100	-0.36259700	2.69126700
H	-5.54181800	-0.17819900	0.55459400
C	-3.38246700	-0.50729300	3.74957900
H	-1.68198600	-0.39837400	2.43534900
C	-4.77407400	-0.48714800	3.85287400
H	-6.62627500	-0.35090100	2.75431800
H	-2.77120900	-0.60505600	4.64412900
H	-5.25572100	-0.56843500	4.82389600

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C	1.51773000	2.99450900	-1.73881000
C	1.22301400	2.38884900	-2.97960500
C	2.50465500	4.00453000	-1.74348300
C	1.88428900	2.75596100	-4.15299600
H	0.46727000	1.60817800	-3.01793900
C	3.17198600	4.36671900	-2.91272800
H	2.74857400	4.51754500	-0.81800100

C	2.87093400	3.74465500	-4.12847100
H	1.63097000	2.26228700	-5.08929800
H	3.92947100	5.14692500	-2.87538100
H	3.38977200	4.03165400	-5.03961100
Pd	-0.12027200	0.22371900	-0.42229200
P	-2.67467100	0.14638400	-0.02174800
C	-4.41231400	0.24401500	-0.74234300
C	-2.71839200	1.72595300	0.97541100
C	-2.79152300	-1.18603800	1.25084200
C	-4.81974500	-0.62024100	-1.77562400
C	-5.37835000	1.10256400	-0.18612700
C	-2.74741300	2.95826900	0.29966200
C	-2.75040700	1.71939900	2.37962400
C	-1.67571700	-1.46104500	2.05843100
C	-3.96675800	-1.92742400	1.44164200
C	-6.13344100	-0.60993200	-2.24719400
H	-4.11726100	-1.31439200	-2.21922500
C	-6.69058300	1.11422100	-0.66171000
H	-5.11222400	1.77115100	0.62243800
C	-2.87578000	4.15061000	1.01115800
H	-2.69827100	2.98892900	-0.78397600
C	-2.85719300	2.91917900	3.08597800
H	-2.72267600	0.78578700	2.92905500
C	-1.73327900	-2.45478900	3.03676400
H	-0.76077700	-0.89204300	1.92056800
C	-4.01966300	-2.92626500	2.41725900
H	-4.84272200	-1.73013600	0.83398600
C	-7.07340900	0.26202800	-1.69748700
H	-6.41735100	-1.28602000	-3.04923100
H	-7.41214700	1.79484600	-0.21784600
C	-2.93369000	4.13746100	2.40577100
H	-2.90977100	5.09224700	0.47073000
H	-2.89950600	2.89506000	4.17193400
C	-2.90661100	-3.19197300	3.21591100
H	-0.85965100	-2.64539500	3.65395200
H	-4.93652200	-3.49377400	2.55192600
H	-8.09444300	0.27395900	-2.06941300

H	-3.02662700	5.06836800	2.95830500
H	-2.95322300	-3.96762500	3.97571400
C	-1.85203900	-0.74813600	-1.52845200
C	-1.57465200	-2.12795300	-1.52354300
C	-1.79798200	-0.04648400	-2.75737900
C	-1.21882600	-2.78306100	-2.71005500
H	-1.64221300	-2.69388300	-0.60207800
C	-1.46098400	-0.70809100	-3.93345400
H	-2.03304300	1.01341000	-2.78337200
C	-1.16451700	-2.07912900	-3.91035600
H	-0.96783000	-3.83929400	-2.67846300
H	-1.43311800	-0.15885100	-4.87076900
H	-0.89426500	-2.59092800	-4.83010600
P	1.79166400	-1.44238000	0.08467300
C	1.68689700	-3.20350000	-0.49188000
C	2.41577100	-3.66730000	-1.59799000
C	0.76391900	-4.07960100	0.11022800
C	2.23587700	-4.96642600	-2.08068700
H	3.13354600	-3.01437700	-2.08407400
C	0.59319400	-5.37987600	-0.36478900
H	0.18112300	-3.74737500	0.96541100
C	1.32904000	-5.82991100	-1.46530700
H	2.81577400	-5.30407900	-2.93601900
H	-0.11477300	-6.04293500	0.12645200
H	1.19655600	-6.84286800	-1.83613900
C	2.12114300	-1.63388900	1.89994400
C	1.89040400	-0.51751200	2.72179600
C	2.60431500	-2.81476900	2.48946500
C	2.13808700	-0.58021200	4.09469400
H	1.52460000	0.40743800	2.28660400
C	2.84202300	-2.87804500	3.86422600
H	2.79052300	-3.69150000	1.87743200
C	2.60962900	-1.76133500	4.67071300
H	1.96507200	0.30169800	4.70461700
H	3.21419100	-3.80065200	4.30289300
H	2.79867800	-1.81173100	5.74001800
C	3.43617900	-0.91505100	-0.58047500

C	4.65644200	-1.29027200	0.00451800
C	3.45446000	-0.10869500	-1.72741800
C	5.86469600	-0.86815000	-0.55047400
H	4.66455600	-1.90359800	0.90033600
C	4.66476500	0.31206700	-2.28457900
H	2.52094300	0.21608700	-2.17460200
C	5.87171500	-0.06696500	-1.69591100
H	6.80217900	-1.16107200	-0.08442500
H	4.65305200	0.95324600	-3.16137200
H	6.81499400	0.26684000	-2.12068600
P	0.46255300	2.62065700	-0.26948800
C	1.61823800	2.86375500	1.15605900
C	1.05085800	3.27656900	2.37992400
C	3.01134400	2.64270200	1.13299800
C	1.83260400	3.45562900	3.52283900
H	-0.01756000	3.46998700	2.42854200
C	3.79579700	2.83962700	2.27001700
H	3.48623500	2.31011600	0.21517900
C	3.21319100	3.24504300	3.47425200
H	1.36322300	3.78113600	4.44916300
H	4.86799900	2.66353000	2.21687500
H	3.82638400	3.39764600	4.35897600

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P	-3.24885400	0.07172200	0.17833000
C	-3.87883800	1.78099900	0.23695500
C	-4.69903800	-1.02544200	-0.08013700
C	-2.97812200	2.85975700	0.20326100
C	-5.26130700	2.03002200	0.30547100
C	-2.07411800	-0.14209000	-1.16324700
Pd	0.09008600	-0.03853700	-0.42234400
C	-4.95967400	-1.52331100	-1.36610500
C	-5.57012100	-1.34787200	0.97540200
C	-3.46414200	4.16746300	0.24420600
H	-1.89915600	2.70180400	0.16901900
C	-5.73285600	3.34153400	0.34446400

H	-5.97051600	1.21020900	0.32006200
C	-1.38206600	-1.42568900	-1.26372600
C	-2.36011600	0.57590700	-2.39016400
C	-2.56194100	-0.41178300	1.79749000
C	-6.07668500	-2.33057500	-1.59027000
H	-4.29211000	-1.28375300	-2.18762000
C	-6.68506200	-2.15307300	0.74379000
H	-5.37519400	-0.97707400	1.97732000
C	-4.83626100	4.41226600	0.31271200
H	-2.75516700	4.99029400	0.22124800
H	-6.80266400	3.52429700	0.39432400
C	-1.05786300	-1.91840000	-2.57336900
H	-1.47745500	-2.16281400	-0.46935800
C	-1.97047900	0.08030500	-3.60716000
H	-2.87833800	1.52854800	-2.33397600
C	-2.54201700	-1.76480600	2.17768300
C	-2.01252400	0.55561800	2.65216400
C	-6.93869900	-2.64575700	-0.53905700
H	-6.26830400	-2.71508100	-2.58791100
H	-7.35222200	-2.39854700	1.56536800
H	-5.20806200	5.43309800	0.33898400
C	-1.31618800	-1.18657200	-3.70491000
H	-0.59524600	-2.89813500	-2.64818100
H	-2.17222200	0.65409600	-4.50789500
C	-1.97163700	-2.14107100	3.39309000
H	-2.97377100	-2.52361200	1.53274600
C	-1.44948500	0.17124100	3.86878600
H	-2.00801500	1.60109600	2.36600500
H	-7.80565700	-3.27626600	-0.71640800
H	-1.04475100	-1.57643300	-4.68213800
C	-1.42549600	-1.17421600	4.23958300
H	-1.95533700	-3.18931400	3.67774400
H	-1.01788200	0.92594800	4.51906400
H	-0.97981800	-1.47025800	5.18489900
P	2.03986600	-1.40785900	-0.20225600
C	2.55637100	-1.87938400	1.51189600
C	3.57492600	-0.69934900	-0.95596600

C	1.91444500	-3.05992100	-1.03475700
C	2.24307000	-0.99593800	2.55572700
C	3.26260900	-3.05728300	1.81269600
C	4.87104500	-1.10795400	-0.60414600
C	3.41862300	0.29367700	-1.93441400
C	2.50204000	-3.31330600	-2.28324600
C	1.08771400	-4.05127400	-0.47363600
C	2.63992800	-1.27422100	3.86534300
H	1.69622800	-0.08515400	2.33768400
C	3.64916500	-3.33868100	3.12406500
H	3.50357900	-3.76327800	1.02362700
C	5.98366900	-0.53688100	-1.22293200
H	5.01571100	-1.86255500	0.16287600
C	4.53293000	0.86225100	-2.55657500
H	2.42317200	0.64455000	-2.18680500
C	2.27332900	-4.52073400	-2.94918300
H	3.14308300	-2.56572700	-2.73935600
C	0.86730600	-5.25936800	-1.13381300
H	0.62178600	-3.87869900	0.49338800
C	3.34176000	-2.44553600	4.15343400
H	2.40449000	-0.56525800	4.65421300
H	4.19358000	-4.25475100	3.33993400
C	5.81725100	0.44769400	-2.20104600
H	6.98232500	-0.85755000	-0.93671600
H	4.38866900	1.64238100	-3.29880200
C	1.45747800	-5.49838100	-2.37912200
H	2.74075300	-4.69636800	-3.91492000
H	0.23398400	-6.01586000	-0.67667200
H	3.64913700	-2.66319300	5.17335200
H	6.68672900	0.89539000	-2.67578800
H	1.28341300	-6.43818500	-2.89645300
P	0.58536800	2.31872600	0.27976700
C	1.89143400	2.49263700	1.57868100
C	1.47802000	2.73874400	2.90379400
C	3.27787000	2.35230400	1.35695300
C	2.39193800	2.81815900	3.95761100
H	0.41930700	2.89284000	3.10163800

C	4.19488800	2.45226000	2.40317700
H	3.64043400	2.16196900	0.35139200
C	3.75944200	2.67873300	3.71262400
H	2.03646700	3.01568900	4.96729400
H	5.25699800	2.34060800	2.19600800
H	4.47633000	2.75291500	4.52658900
C	1.30831200	3.18027900	-1.18131300
C	2.21506400	4.25758700	-1.08499700
C	0.85052900	2.84763100	-2.47599800
C	2.65463400	4.94444300	-2.21673500
H	2.58252200	4.56136300	-0.10917400
C	1.28018600	3.54304500	-3.60661800
H	0.15406700	2.02025200	-2.59489200
C	2.19336300	4.59479200	-3.48900200
H	3.36045000	5.76489400	-2.10166900
H	0.90595700	3.25350800	-4.58687300
H	2.53542500	5.13312900	-4.36940900

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1 1

P	-2.15215100	0.25498900	-0.01276200
C	-2.36000000	0.40058100	1.80135600
C	-3.86216500	0.18018800	-0.72192700
C	-1.56126400	1.90369700	-0.61683200
C	-1.22325400	0.35828700	2.62761500
C	-3.62415800	0.60445300	2.37823300
C	-4.68696900	-0.93352300	-0.47073200
C	-4.38685500	1.25881600	-1.45258100
C	-1.14245900	2.04735800	-1.95083300
C	-1.61439400	3.03042300	0.21679900
C	-1.35104700	0.51473300	4.00705600
H	-0.23934300	0.20524200	2.19256800
C	-3.74396000	0.75838200	3.76071500
H	-4.51206200	0.64570800	1.75771500
C	-5.99853600	-0.96155100	-0.93860800
H	-4.31295900	-1.77939800	0.09557400
C	-5.69892900	1.21778800	-1.93096500

H	-3.78309400	2.13432900	-1.65544400
C	-0.80343800	3.30431200	-2.44790600
H	-1.08563200	1.18107400	-2.60435000
C	-1.26539700	4.28683000	-0.28756500
H	-1.93777800	2.93855200	1.24790300
C	-2.61187000	0.71242100	4.57590500
H	-0.46398600	0.47806800	4.63253900
H	-4.72565400	0.91484000	4.19796000
C	-6.50694100	0.11121800	-1.67645300
H	-6.62218300	-1.82608400	-0.73082400
H	-6.08433500	2.05761400	-2.50150300
C	-0.86848800	4.42777100	-1.61794200
H	-0.48572700	3.40557300	-3.48130800
H	-1.31631100	5.15536500	0.36283900
H	-2.71141500	0.83003600	5.65106900
H	-7.52696000	0.08225500	-2.04831600
H	-0.60910300	5.40751100	-2.00831800
Pd	0.02459800	-0.73713000	-0.38227600
P	2.35823500	-0.09580100	-0.11477100
C	3.34412700	-1.45841000	-0.86645000
C	2.87945200	-0.06779800	1.65384900
C	3.05534000	1.44804600	-0.83074300
C	2.89470500	-2.01019100	-2.07831700
C	4.51544500	-1.96275000	-0.28029400
C	2.35019300	-1.04434500	2.51606300
C	3.77501400	0.88012500	2.16952000
C	2.35859800	2.65239800	-0.64100600
C	4.26945400	1.46316700	-1.53471700
C	3.60694000	-3.03766500	-2.69683600
H	1.98553000	-1.63134500	-2.54078200
C	5.22239800	-2.99607200	-0.89862800
H	4.87524300	-1.55365400	0.65872300
C	2.71638700	-1.07720600	3.86141900
H	1.65596800	-1.78740100	2.12896400
C	4.13139900	0.85159700	3.52050800
H	4.19638500	1.64132200	1.52108800
C	2.87840000	3.85087700	-1.12940500

H	1.41014600	2.65645000	-0.11128700
C	4.77911400	2.66386000	-2.03301200
H	4.81861900	0.54106300	-1.69464700
C	4.77123000	-3.53378700	-2.10581100
H	3.25028000	-3.45411500	-3.63464500
H	6.12659900	-3.38039600	-0.43516800
C	3.60590900	-0.12482000	4.36753900
H	2.30919500	-1.84519300	4.51339700
H	4.82491500	1.59284000	3.90749300
C	4.08816900	3.85915500	-1.82788800
H	2.33304800	4.77667300	-0.97072600
H	5.71841400	2.66288500	-2.57869400
H	5.32305700	-4.33875700	-2.58264700
H	3.88844800	-0.14623200	5.41619700
H	4.48859300	4.79257900	-2.21324400
C	-1.72532300	-1.83313900	-0.42650300
C	-1.83544900	-2.69187400	0.68259200
C	-2.01384300	-2.30786000	-1.72145100
C	-2.19424300	-4.02911000	0.48587600
H	-1.65168300	-2.32022500	1.68538800
C	-2.35295800	-3.64781900	-1.90437300
H	-1.98238200	-1.63733100	-2.57483600
C	-2.44654200	-4.50531900	-0.80255400
H	-2.27480000	-4.69498000	1.34032400
H	-2.55712100	-4.02001300	-2.90416200
H	-2.72743100	-5.54413800	-0.94941600

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1 1

P	2.30343700	1.09051500	0.19592700
C	2.51520600	2.91718400	0.13241400
C	3.99415300	0.39896100	-0.08378200
C	1.97727800	0.77630500	2.00856500
C	1.37848400	3.73994500	0.17847800
C	3.78723100	3.50942300	0.11345700
C	4.64339900	0.63868500	-1.31140700
C	4.68593800	-0.30051400	0.91777600

C	1.83680200	-0.54276000	2.47995500
C	1.89601200	1.83740800	2.92711100
C	1.50990300	5.12841200	0.19126900
H	0.38748700	3.29864800	0.20620100
C	3.91364700	4.90020500	0.12584300
H	4.68036500	2.89601100	0.09496100
C	5.94097300	0.18015100	-1.52841800
H	4.14576900	1.19976500	-2.09406500
C	5.98194300	-0.76910000	0.68954400
H	4.22883000	-0.47978000	1.88233400
C	1.62836800	-0.79211500	3.83676100
H	1.91964100	-1.37945200	1.79716000
C	1.68594000	1.57919700	4.28366100
H	2.00850800	2.86277800	2.59737200
C	2.77895000	5.71141800	0.16152900
H	0.61795200	5.74655800	0.21852900
H	4.90393300	5.34610500	0.11033400
C	6.61182000	-0.53293900	-0.53130700
H	6.42766800	0.38192900	-2.47820400
H	6.49749900	-1.31282400	1.47573900
C	1.54870500	0.26767800	4.74263300
H	1.53598500	-1.81862800	4.17903500
H	1.64061500	2.41019900	4.98196200
H	2.88256300	6.79266400	0.16885900
H	7.62165800	-0.89364900	-0.70449200
H	1.39208000	0.07248400	5.79967000
Pd	0.13081900	0.13491400	-0.21793800
P	-2.16663500	1.34338400	-0.07395600
C	-3.57493000	0.63209000	-1.04722200
C	-2.19333400	3.12378500	-0.58522500
C	-2.83963300	1.39482700	1.64772900
C	-3.77153700	-0.75798100	-1.00470600
C	-4.47473900	1.41570700	-1.78798400
C	-1.89045100	3.44627100	-1.92149100
C	-2.47640700	4.16693400	0.30902600
C	-1.93695900	1.43489000	2.72203400
C	-4.21730400	1.40828700	1.91847800

C	-4.83596500	-1.34972000	-1.68465900
H	-3.10374000	-1.38322700	-0.42295500
C	-5.53379500	0.81947400	-2.47677600
H	-4.35839900	2.49277900	-1.82985600
C	-1.88359400	4.77267200	-2.35187800
H	-1.67751900	2.65337900	-2.63353000
C	-2.45891600	5.49748400	-0.12242600
H	-2.72372200	3.94622500	1.34203500
C	-2.39981700	1.49602700	4.03810300
H	-0.86723900	1.41565000	2.53227500
C	-4.67820700	1.46132900	3.23491300
H	-4.93226100	1.37245000	1.10260000
C	-5.71760200	-0.56295500	-2.42842800
H	-4.97043100	-2.42644600	-1.63359300
H	-6.21885200	1.44171700	-3.04610300
C	-2.16569900	5.80458600	-1.45156100
H	-1.66324000	5.00144000	-3.39109400
H	-2.69116100	6.29137800	0.58238300
C	-3.77206300	1.50626800	4.29725900
H	-1.68682200	1.52882600	4.85708300
H	-5.74705400	1.46845700	3.42976000
H	-6.54331800	-1.02319600	-2.96379000
H	-2.16387300	6.83772100	-1.78731300
H	-4.13405900	1.54890200	5.32079400
C	1.49869300	0.68911400	-1.76367600
C	1.14299800	1.80792600	-2.53725700
C	1.98789600	-0.46419800	-2.40725800
C	1.23389000	1.75117100	-3.93043900
H	0.80150900	2.71936400	-2.06475100
C	2.05915400	-0.51717500	-3.79911200
H	2.32496600	-1.30881700	-1.81939400
C	1.68279500	0.59007300	-4.56362500
H	0.95491300	2.62139000	-4.51840800
H	2.41766800	-1.42120500	-4.28290400
H	1.75400600	0.55329600	-5.64689400
P	-0.19635700	-2.51495400	-0.05667100
C	-1.64387400	-3.04369500	0.96921600

C	-2.42442400	-4.17369200	0.67660400
C	-1.96560900	-2.27167300	2.09734000
C	-3.50009800	-4.51986500	1.49612000
H	-2.20086300	-4.78051000	-0.19486600
C	-3.03619300	-2.62456700	2.92118300
H	-1.38555400	-1.38256300	2.32718700
C	-3.80707400	-3.74860000	2.61980800
H	-4.09886900	-5.39410600	1.25565800
H	-3.27443000	-2.00936000	3.78410800
H	-4.64699900	-4.01993300	3.25317200
C	1.16721800	-3.57974000	0.61715800
C	2.34749900	-3.75752200	-0.12757600
C	1.09611700	-4.14981200	1.89890600
C	3.41959300	-4.48354500	0.39121300
H	2.42030000	-3.35746200	-1.13474600
C	2.17349200	-4.87226500	2.41930600
H	0.19260900	-4.04444800	2.49053400
C	3.33803700	-5.04069800	1.66987100
H	4.31592400	-4.61949000	-0.20762700
H	2.09306100	-5.31485300	3.40853500
H	4.17157700	-5.60848500	2.07323200
C	-0.51810200	-3.25469100	-1.71719000
C	-0.27134500	-4.60612300	-2.01722800
C	-1.05820100	-2.42873200	-2.71607200
C	-0.56831300	-5.11664300	-3.28171500
H	0.15881000	-5.26117500	-1.26576000
C	-1.36192800	-2.94337100	-3.97777000
H	-1.24177200	-1.37889800	-2.50613000
C	-1.11693900	-4.28751400	-4.26321300
H	-0.37212600	-6.16302500	-3.49881600
H	-1.78431500	-2.29137100	-4.73722300
H	-1.34809200	-4.68752300	-5.24653000

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0 1

P	1.96408800	-1.03059200	0.11323900
C	2.40875300	0.00699300	1.54779300

C	3.58870300	-1.72571800	-0.46536200
C	1.14339700	-2.56654100	0.77041200
C	1.60536200	1.09699200	1.90932500
C	3.54767000	-0.30160500	2.31895000
C	4.61367800	-0.83402100	-0.83260600
C	3.83856300	-3.10369200	-0.51756000
C	0.45181700	-3.42447600	-0.10007700
C	1.27624400	-2.92140800	2.12049700
C	1.93452300	1.87699700	3.01990900
H	0.74246600	1.37707700	1.31368400
C	3.85451500	0.46471600	3.44056400
H	4.19176900	-1.13007300	2.04279700
C	5.85768100	-1.31380000	-1.23248300
H	4.43996000	0.23715900	-0.80591300
C	5.08543400	-3.58097000	-0.93466200
H	3.07073500	-3.81336600	-0.23381000
C	-0.07737800	-4.62656300	0.36700300
H	0.31909900	-3.14890900	-1.14269900
C	0.73586600	-4.12355100	2.58436500
H	1.80153300	-2.26878400	2.80939400
C	3.05032200	1.55505600	3.79051700
H	1.33305000	2.75411500	3.23445600
H	4.73249200	0.22024200	4.03236100
C	6.09625700	-2.69063000	-1.28981500
H	6.64010400	-0.61107500	-1.50464200
H	5.26040300	-4.65255600	-0.97497200
C	0.06513700	-4.97987100	1.71117100
H	-0.61063400	-5.28074100	-0.31675800
H	0.84458200	-4.38742100	3.63292000
H	3.30855800	2.16411900	4.65239100
H	7.06550400	-3.06309800	-1.60976300
H	-0.35307300	-5.91379300	2.07551300
Pd	-0.10175800	-0.17945700	-0.81427700
P	-2.43310300	-0.33051600	-0.17719600
C	-3.43388600	-0.21419600	-1.72589800
C	-3.04500600	1.03476400	0.88871400
C	-3.06537000	-1.85184000	0.65653600

C	-2.90516900	-0.75871400	-2.90769300
C	-4.69028800	0.40930100	-1.76977400
C	-2.35971000	2.25851400	0.85994700
C	-4.18575400	0.90404000	1.70136700
C	-2.60264100	-2.14072000	1.95131300
C	-3.97425900	-2.72979100	0.04967400
C	-3.62218200	-0.69691900	-4.10342500
H	-1.92204200	-1.22455700	-2.89049700
C	-5.40309000	0.47658100	-2.96788900
H	-5.10582000	0.85407500	-0.87108100
C	-2.80687800	3.33882300	1.62337700
H	-1.46383000	2.39740200	0.25798400
C	-4.62947700	1.98558200	2.46241300
H	-4.72071300	-0.03998200	1.74688700
C	-3.05621100	-3.27037800	2.62953300
H	-1.89287900	-1.47458500	2.43452300
C	-4.41721800	-3.86911900	0.72743100
H	-4.34686000	-2.52227300	-0.94833900
C	-4.87307600	-0.07768100	-4.13502800
H	-3.19829900	-1.11997500	-5.01021200
H	-6.37145800	0.96905700	-2.98971500
C	-3.94216500	3.20290800	2.42305200
H	-2.23764600	4.26384000	1.58651200
H	-5.51060500	1.87511200	3.08958200
C	-3.96496000	-4.13934200	2.01891500
H	-2.69747000	-3.47369800	3.63478700
H	-5.12558900	-4.53804800	0.24558100
H	-5.42829700	-0.01840400	-5.06722300
H	-4.28908200	4.04054400	3.02265200
H	-4.31823400	-5.02027000	2.54836300
C	1.76470300	0.21548900	-1.63136200
C	2.02727900	1.58807800	-1.49481700
C	1.97838500	-0.43900200	-2.86390500
C	2.47145700	2.31061900	-2.60927100
H	1.85638600	2.13781500	-0.57043900
C	2.42280700	0.29535200	-3.95949300
H	1.81638300	-1.50885400	-2.95822300

C	2.67224200	1.66896600	-3.83004900
H	2.62901100	3.37929500	-2.49400000
H	2.58052000	-0.20187300	-4.91293600
H	3.02356600	2.23500700	-4.68868300
I	0.81200100	4.62875100	0.43086700

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0 1

P	0.63481500	2.21966500	0.61990400
C	-0.18732500	3.83564300	0.27019800
C	2.39557800	2.65227500	0.98404600
C	0.03810600	1.81396500	2.35449100
C	-1.58084400	3.89057100	0.09906400
C	0.55861900	5.01607400	0.14484100
C	3.47155500	2.40852300	0.12059500
C	2.64454700	3.31755100	2.20611900
C	0.70580100	0.78973600	3.05070900
C	-0.97677600	2.52807400	3.01221300
C	-2.21621500	5.10234400	-0.17244700
H	-2.17246200	2.98168400	0.15723400
C	-0.08051600	6.22721700	-0.13071500
H	1.63634900	4.99545100	0.25936300
C	4.76873400	2.79247700	0.47632800
H	3.35170400	1.90116800	-0.82546000
C	3.93243000	3.72312100	2.54038500
H	1.83335000	3.52346900	2.89572800
C	0.35974200	0.48260700	4.36598900
H	1.51745600	0.24796900	2.57924800
C	-1.31429400	2.22023800	4.33352700
H	-1.48985300	3.34198800	2.51445100
C	-1.46597000	6.27524600	-0.28592000
H	-3.29338900	5.12051900	-0.30969500
H	0.51175000	7.13304500	-0.22606300
C	5.00116500	3.45440700	1.67815200
H	5.57833300	2.52622000	-0.19673600
H	4.10209200	4.23817700	3.48229600
C	-0.65368900	1.19476200	5.01201500

H	0.89493700	-0.30999900	4.88039500
H	-2.08845000	2.79716500	4.83295600
H	-1.95870200	7.21937000	-0.50159700
H	6.00961100	3.75373400	1.95097200
H	-0.91581900	0.96216400	6.04060200
Pd	-0.46154000	0.21091300	-0.05011500
P	-2.97045300	-0.11302700	-0.64555100
C	-3.43590000	-1.54964600	-1.72540500
C	-3.80802300	1.30877000	-1.49141800
C	-4.04989900	-0.38530300	0.83421100
C	-2.93768900	-2.81506100	-1.37228800
C	-4.27077800	-1.44690500	-2.84913500
C	-3.33198300	1.71620000	-2.75123700
C	-4.87017500	2.02216200	-0.91503200
C	-3.65399500	0.16514500	2.06193800
C	-5.25481300	-1.10397400	0.77273100
C	-3.26653800	-3.94582600	-2.11906400
H	-2.29789300	-2.92386200	-0.50335000
C	-4.58950000	-2.57977700	-3.60249900
H	-4.67966400	-0.48637600	-3.14226100
C	-3.91230500	2.79399500	-3.41977500
H	-2.50421400	1.18637100	-3.21327800
C	-5.44148700	3.11103100	-1.58089200
H	-5.26324600	1.72626100	0.05178400
C	-4.44419300	0.00812800	3.20270000
H	-2.71965900	0.71445300	2.13070800
C	-6.04083300	-1.26670200	1.91439500
H	-5.57778400	-1.54188700	-0.16647900
C	-4.09017200	-3.83130800	-3.24080100
H	-2.86936600	-4.91312600	-1.82461200
H	-5.23496800	-2.47949000	-4.47120000
C	-4.96811900	3.49837600	-2.83491700
H	-3.53699400	3.08539300	-4.39720100
H	-6.26776400	3.64643200	-1.12010600
C	-5.63869400	-0.71110100	3.13172500
H	-4.11740500	0.44110300	4.14417500
H	-6.96857500	-1.82935600	1.85222800

H	-4.33982300	-4.71049600	-3.82860900
H	-5.41837700	4.33959000	-3.35483100
H	-6.25246400	-0.84054000	4.01924300
C	0.65436000	1.43497900	-1.43228300
C	-0.03603300	2.24083100	-2.35573500
C	1.73382700	0.65022700	-1.87033700
C	0.34241400	2.23564900	-3.69884400
H	-0.85967400	2.86683100	-2.04167100
C	2.10440600	0.65201200	-3.21838800
H	2.32559300	0.05150200	-1.18890800
C	1.40829900	1.44165900	-4.13280500
H	-0.19791000	2.86310400	-4.40386800
H	2.97212800	0.06300100	-3.50413900
H	1.70798300	1.45576300	-5.17725700
P	0.62316600	-2.11224700	0.61023500
C	-0.53302000	-3.31814400	1.41975500
C	-0.49833800	-4.69889100	1.16593300
C	-1.48396900	-2.82496100	2.32782200
C	-1.39411700	-5.55985300	1.80301400
H	0.22628100	-5.10209500	0.46566000
C	-2.37351800	-3.68749400	2.97156100
H	-1.53577300	-1.75905000	2.52948100
C	-2.33262900	-5.05761100	2.70745500
H	-1.35605100	-6.62563800	1.59274000
H	-3.10659100	-3.28290700	3.66408700
H	-3.03057000	-5.72998100	3.19932700
C	2.10056800	-2.17775900	1.72591600
C	3.32643200	-1.66904300	1.26207900
C	2.02017300	-2.65113700	3.04641500
C	4.44455000	-1.63963200	2.09630500
H	3.46033600	-1.32119500	0.23950400
C	3.14037800	-2.61097000	3.88112500
H	1.08979500	-3.06294100	3.42444300
C	4.35376200	-2.10441300	3.41008800
H	5.37642600	-1.25709600	1.68899200
H	3.06387800	-2.99054700	4.89737700
H	5.22424800	-2.08075900	4.06057700

C	1.19145700	-3.00690300	-0.90179400
C	2.24166500	-3.93971500	-0.88666200
C	0.53714300	-2.74520500	-2.11604500
C	2.62041000	-4.59765700	-2.05715100
H	2.78107100	-4.13697100	0.03379600
C	0.91011100	-3.41282900	-3.28310100
H	-0.26137500	-2.01002900	-2.15204500
C	1.95374200	-4.33895000	-3.25597300
H	3.44851300	-5.30017400	-2.03327600
H	0.39538100	-3.19514100	-4.21501500
H	2.25841200	-4.84473700	-4.16812100
I	5.55662900	-0.34016500	-1.75819200

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P	1.25509200	1.00029300	-0.08544600
C	1.61621000	0.52890200	1.64423600
C	2.78834000	1.82855100	-0.70139900
C	1.15825800	-0.49993500	-1.14952400
C	0.59802900	0.48756900	2.61551300
C	2.92522800	0.16076900	1.99555500
C	3.09104200	3.17391300	-0.41957700
C	3.74845000	1.03211300	-1.34953500
C	0.71232100	-0.35944600	-2.47872800
C	1.57854700	-1.75086100	-0.68332300
C	0.88919000	0.09334900	3.92019800
H	-0.41966300	0.76092900	2.34493400
C	3.20131600	-0.25722200	3.29952800
H	3.72765300	0.12838700	1.26462900
C	4.31424200	3.71304500	-0.80863300
H	2.38538400	3.80397200	0.10709700
C	4.97899000	1.57940600	-1.72157500
H	3.58758100	-0.02556000	-1.52294200
C	0.67049600	-1.46656400	-3.31979400
H	0.40731300	0.61307000	-2.85684900
C	1.53984700	-2.85606400	-1.54125800
H	1.99361700	-1.87301700	0.31008300

C	2.19360700	-0.27947300	4.26254000
H	0.09864400	0.07296200	4.66546600
H	4.20928200	-0.58425800	3.53476900
C	5.25916600	2.91917000	-1.46660200
H	4.53220400	4.75477200	-0.58921100
H	5.71677300	0.93230600	-2.18507800
C	1.07817600	-2.72142300	-2.84688400
H	0.33502300	-1.35123600	-4.34715800
H	1.91263500	-3.80856700	-1.17956000
H	2.41799000	-0.59517700	5.27792300
H	6.21549300	3.34281800	-1.76119800
H	1.05581700	-3.58314600	-3.50808900
Pd	-1.15678000	1.20807700	-0.13719500
P	-2.90255800	-0.47435700	-0.00328400
C	-3.95080000	-0.49458600	-1.52293400
C	-4.08163800	-0.07101700	1.35855900
C	-2.47417100	-2.24233100	0.27998800
C	-3.30064700	-0.55014700	-2.76816100
C	-5.35183400	-0.44286000	-1.48849300
C	-4.26456000	1.27886500	1.70124200
C	-4.80042200	-1.05234100	2.05815600
C	-1.43702500	-2.54070800	1.17804900
C	-3.15300000	-3.29399100	-0.35445200
C	-4.03924900	-0.56575300	-3.95073700
H	-2.21525800	-0.59064500	-2.80993600
C	-6.08774500	-0.44815200	-2.67626300
H	-5.87182500	-0.39694200	-0.53692100
C	-5.15602400	1.64163300	2.71112600
H	-3.70190500	2.04869300	1.17659500
C	-5.68674200	-0.68796300	3.07396900
H	-4.66422200	-2.10144700	1.81425900
C	-1.09514200	-3.86570400	1.44767600
H	-0.88954400	-1.73757900	1.66250000
C	-2.80250400	-4.61918900	-0.08794500
H	-3.95038600	-3.08085200	-1.05950700
C	-5.43488600	-0.51059100	-3.90775100
H	-3.52458600	-0.61498300	-4.90656900

H	-7.17278900	-0.40413500	-2.63546600
C	-5.86780700	0.65730000	3.40077600
H	-5.28748100	2.69010800	2.96435600
H	-6.23381800	-1.45780700	3.61142400
C	-1.77599600	-4.90717300	0.81324700
H	-0.28675100	-4.08222000	2.14022000
H	-3.33163600	-5.42568800	-0.58844500
H	-6.00931000	-0.51433100	-4.83007100
H	-6.55602100	0.93737600	4.19359100
H	-1.50143300	-5.93886900	1.01496300
C	0.00445100	2.90109700	-0.12517500
C	-0.01158400	3.61928600	1.08357600
C	-0.03378500	3.59313600	-1.35096800
C	-0.11895400	5.01378200	1.06105500
H	0.07152600	3.09932100	2.03206600
C	-0.15464200	4.98316600	-1.36061000
H	0.03698900	3.05408100	-2.29080300
C	-0.19529300	5.69336000	-0.15660500
H	-0.13668700	5.56552000	1.99712600
H	-0.20236300	5.51238700	-2.30841300
H	-0.27159600	6.77705200	-0.16920100
I	5.18902700	-2.26183700	0.18126300

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P	1.90240600	-0.17061500	-0.74199300
C	2.73009900	1.41701700	-1.12435400
C	3.04023400	-1.46492300	-1.39789000
C	2.01809600	-0.38518600	1.08902500
C	2.00536100	2.61948700	-1.13551800
C	4.12244900	1.44474200	-1.30748800
C	3.18637200	-1.66058700	-2.78619800
C	3.89487500	-2.15041000	-0.51942200
C	1.43314000	-1.51457100	1.69722600
C	2.76571200	0.51063500	1.86966000
C	2.65567300	3.83109800	-1.35890800
H	0.93445500	2.60556800	-0.96942300

C	4.76935300	2.66590100	-1.51170500
H	4.72082500	0.54426600	-1.23315800
C	4.13086600	-2.55839800	-3.27329600
H	2.57940500	-1.10296800	-3.48936300
C	4.84230300	-3.04890000	-1.01904200
H	3.87633200	-1.96030300	0.54564700
C	1.56431600	-1.71780300	3.06857300
H	0.90603300	-2.24771700	1.09607800
C	2.89137400	0.29480300	3.24603100
H	3.29235600	1.34068100	1.41635600
C	4.04085500	3.85349400	-1.55173400
H	2.07970700	4.75183000	-1.37702700
H	5.85053900	2.67252900	-1.60645300
C	4.95358900	-3.26517700	-2.38901500
H	4.23244300	-2.69834500	-4.34615700
H	5.51261300	-3.54285100	-0.32307700
C	2.28186600	-0.80316000	3.84854500
H	1.12016100	-2.59841300	3.52432800
H	3.51806700	0.96545000	3.82507500
H	4.55102100	4.79908800	-1.71566600
H	5.69508000	-3.96038600	-2.77353200
H	2.39683900	-0.97153800	4.91580500
Pd	-0.51982800	-0.00629400	-0.44843100
P	-1.83408900	2.17578900	0.11000600
C	-3.69277300	2.09027000	0.10802700
C	-1.51364000	3.59254800	-1.04344100
C	-1.49000500	2.88258000	1.78119500
C	-4.32470800	1.36205500	1.13169200
C	-4.49232800	2.67369400	-0.88659700
C	-1.61790700	3.36081000	-2.42704300
C	-1.14993000	4.87459000	-0.60490500
C	-0.30686600	2.50766400	2.43359300
C	-2.35808100	3.78815800	2.41632400
C	-5.71165400	1.22286400	1.15820500
H	-3.73544700	0.90769300	1.92089500
C	-5.88223800	2.52668900	-0.86128000
H	-4.04094200	3.25861400	-1.68011400

C	-1.39046700	4.38796900	-3.34338700
H	-1.87268600	2.36910100	-2.79089400
C	-0.90771600	5.89852000	-1.52504200
H	-1.05196400	5.07914500	0.45563800
C	0.00954900	3.02853000	3.69050000
H	0.37210100	1.80362500	1.96231900
C	-2.04175900	4.30603900	3.67223200
H	-3.28392300	4.08404400	1.93233000
C	-6.49712700	1.80120700	0.15868400
H	-6.17381400	0.65574100	1.96127900
H	-6.48223600	2.99264300	-1.63879000
C	-1.03210800	5.66141300	-2.89445300
H	-1.48475500	4.19088300	-4.40803700
H	-0.62574200	6.88471100	-1.16572800
C	-0.85741900	3.92789100	4.31168700
H	0.93081200	2.72237700	4.17769000
H	-2.72152600	5.00480900	4.15272700
H	-7.57788000	1.69004900	0.17764800
H	-0.84603800	6.45990700	-3.60733900
H	-0.61484300	4.33207400	5.29084100
C	0.31991600	-0.45765100	-2.32126200
C	0.31295900	0.56122400	-3.28768300
C	0.08370800	-1.78582200	-2.72135200
C	-0.00193100	0.26162300	-4.61827000
H	0.56130500	1.57953400	-3.01589800
C	-0.25157600	-2.07148600	-4.04465200
H	0.17649000	-2.59316200	-2.00454900
C	-0.29829600	-1.04847500	-4.99674600
H	-0.00575400	1.05891800	-5.35726800
H	-0.45542400	-3.09860500	-4.33654200
H	-0.53961600	-1.27683800	-6.03126600
P	-2.16215700	-2.02546600	0.28541700
C	-2.92363200	-1.80273500	1.96224100
C	-4.19742600	-2.28026400	2.30796700
C	-2.17644200	-1.11330300	2.93159200
C	-4.70760400	-2.07528200	3.59122300
H	-4.80149900	-2.80244000	1.57333400

C	-2.68355300	-0.91751600	4.21860000
H	-1.19383500	-0.72479900	2.68124500
C	-3.95241700	-1.39546300	4.55025400
H	-5.69715300	-2.44892400	3.84170300
H	-2.08929800	-0.38154500	4.95345600
H	-4.35249400	-1.23661700	5.54802300
C	-1.46139100	-3.74017100	0.41142300
C	-1.23579500	-4.49760900	-0.75310500
C	-1.04672900	-4.27467600	1.64232800
C	-0.61372200	-5.74470400	-0.68645700
H	-1.56939700	-4.12265200	-1.71608700
C	-0.42000900	-5.52149800	1.70598500
H	-1.22300600	-3.72244600	2.55987200
C	-0.19804800	-6.25968100	0.54328800
H	-0.45611500	-6.31508700	-1.59800700
H	-0.11029400	-5.91628300	2.66994000
H	0.28978400	-7.22894300	0.59422700
C	-3.60605300	-2.26586800	-0.84372300
C	-4.33504000	-3.46534100	-0.92832500
C	-3.99700700	-1.18363800	-1.64654600
C	-5.43045100	-3.57132000	-1.78627800
H	-4.03928200	-4.32360900	-0.33267500
C	-5.09734800	-1.28802200	-2.49946500
H	-3.43870500	-0.25404000	-1.60020700
C	-5.81543900	-2.48210900	-2.57189600
H	-5.98220900	-4.50609500	-1.84154000
H	-5.38856600	-0.43569000	-3.10682700
H	-6.66849600	-2.56703200	-3.23983800
I	6.41943600	0.06844100	1.39769100

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0 1

P	1.64484100	-0.24314000	1.23378400
C	2.68151900	1.25384600	1.47455000
C	2.73163900	-1.72441200	1.36154300
C	0.63678900	-0.31413800	2.81731400
C	2.04068900	2.49618400	1.64526300

C	4.08062600	1.20616400	1.41471500
C	3.77177200	-1.90683000	0.43195700
C	2.58384700	-2.65367900	2.40947600
C	-0.38114200	-1.27421100	2.96733900
C	0.91027400	0.54291500	3.89730500
C	2.79039900	3.66076100	1.78762800
H	0.95712800	2.55485200	1.66194200
C	4.82623100	2.38224100	1.53827600
H	4.61608000	0.28429400	1.22752600
C	4.64416000	-2.98906900	0.55159700
H	3.97305900	-1.19602100	-0.36460400
C	3.44246500	-3.74896900	2.50376400
H	1.81163900	-2.52700300	3.15774500
C	-1.11246500	-1.36465700	4.15272800
H	-0.58309100	-1.97868400	2.17160200
C	0.17423000	0.45021800	5.08139600
H	1.70345100	1.27621400	3.82712400
C	4.18801600	3.60409500	1.73564900
H	2.28065700	4.61107200	1.91602000
H	5.90516900	2.32031100	1.43949500
C	4.47291700	-3.92074800	1.57497600
H	5.46721500	-3.05689400	-0.15390500
H	3.31433200	-4.45690600	3.31863800
C	-0.84261700	-0.49679000	5.21273300
H	-1.88654300	-2.12162100	4.24470300
H	0.41002700	1.11733200	5.90613100
H	4.77244000	4.51554000	1.82919300
H	5.14914900	-4.76713800	1.66257300
H	-1.40808700	-0.56905900	6.13790300
Pd	-0.44371700	0.01454300	-0.00145100
P	-1.74073600	2.23752400	-0.25967900
C	-2.87834500	2.38487600	-1.72214100
C	-0.76834900	3.81212900	-0.35563600
C	-2.88561500	2.55229000	1.16091400
C	-3.84235600	1.37890100	-1.90663400
C	-2.82541900	3.43796700	-2.64767800
C	0.18787100	3.94787700	-1.37826400

C	-0.93028700	4.86673000	0.55532500
C	-2.52567500	2.06911500	2.42879400
C	-4.08680700	3.26714900	1.02646400
C	-4.72896800	1.42636900	-2.98166200
H	-3.91456000	0.56031400	-1.19914800
C	-3.70638000	3.47672300	-3.73207100
H	-2.10150200	4.23569400	-2.52737900
C	0.95055000	5.10978400	-1.49355300
H	0.33548000	3.14202300	-2.09117900
C	-0.15691600	6.02607500	0.44470500
H	-1.66290800	4.79193200	1.35173500
C	-3.34311700	2.29893100	3.53763900
H	-1.60454500	1.50647500	2.55161300
C	-4.90764000	3.48847600	2.13352100
H	-4.38474900	3.64855800	0.05482300
C	-4.66028400	2.47374000	-3.90332600
H	-5.46849000	0.63882100	-3.09771700
H	-3.64671900	4.30022300	-4.43884900
C	0.78202300	6.15297900	-0.57938900
H	1.68211000	5.19609200	-2.29216200
H	-0.29826100	6.83346800	1.15860600
C	-4.53813000	3.00614400	3.39154800
H	-3.04458200	1.91796100	4.51024700
H	-5.83560200	4.04115800	2.01245900
H	-5.34517300	2.50768500	-4.74631500
H	1.38032600	7.05579000	-0.66537300
H	-5.17803600	3.18133400	4.25238100
C	1.46130400	-0.16642300	-0.94563800
C	2.03316400	0.99324000	-1.49393600
C	1.53104000	-1.37729000	-1.65892800
C	2.63958800	0.94411500	-2.74993800
H	2.04908900	1.91684700	-0.93027700
C	2.11559700	-1.40785600	-2.92489400
H	1.14687500	-2.29397600	-1.23058600
C	2.67595400	-0.25094400	-3.46899000
H	3.12260100	1.83268800	-3.14350400
H	2.16152800	-2.34764400	-3.46767000

H	3.17880600	-0.28970200	-4.43019800
P	-2.03576300	-2.05119400	-0.41400800
C	-3.83336700	-1.77501600	-0.05787300
C	-4.86589900	-2.18196100	-0.91775300
C	-4.16933000	-1.10844800	1.13255800
C	-6.20088200	-1.92929200	-0.59084200
H	-4.62902000	-2.69307800	-1.84578500
C	-5.50296300	-0.86346100	1.46096900
H	-3.38439100	-0.76290400	1.79967200
C	-6.52266200	-1.27177100	0.59813300
H	-6.98914700	-2.24896600	-1.26756200
H	-5.74058000	-0.33647000	2.38081900
H	-7.56139100	-1.07276800	0.84754800
C	-1.73728700	-3.67955600	0.43061400
C	-0.41107000	-4.09738300	0.63319400
C	-2.77541900	-4.51504800	0.87516100
C	-0.12702300	-5.31892300	1.24449100
H	0.41278800	-3.45945100	0.32916400
C	-2.49116600	-5.73599800	1.49158100
H	-3.80946700	-4.21603600	0.73866400
C	-1.16850100	-6.14305200	1.67503600
H	0.90813600	-5.61288000	1.39244600
H	-3.30806400	-6.36917800	1.82795500
H	-0.95092900	-7.09278200	2.15604900
C	-2.01337000	-2.51454000	-2.20351600
C	-2.18783100	-3.83163100	-2.65826200
C	-1.80158300	-1.49456200	-3.14592700
C	-2.16189800	-4.11763000	-4.02475200
H	-2.33876900	-4.63715900	-1.94635300
C	-1.78573600	-1.78155700	-4.51129000
H	-1.64103300	-0.47397800	-2.81022000
C	-1.96433200	-3.09388200	-4.95350500
H	-2.29365900	-5.14237500	-4.36190400
H	-1.62045800	-0.98069800	-5.22657400
H	-1.94109200	-3.31926400	-6.01628900
I	6.47448300	0.04259000	-1.40718300

IRC of tetraphenylphosphonium C−P oxidative -Point1

0 1

P	-2.39021400	0.39581500	0.14886500
C	-3.69642100	-0.66814400	-0.58638100
C	-3.30737500	1.91767100	0.70762500
C	-3.35465500	-1.88980700	-1.19192100
C	-5.04610700	-0.28068000	-0.53247000
C	-1.86189200	-0.35646700	1.75214300
Pd	-0.01787300	-0.34100200	-0.26882400
C	-3.67111400	2.11475200	2.04802200
C	-3.71869700	2.86503600	-0.24802200
C	-4.35038500	-2.70029700	-1.73906300
H	-2.31835800	-2.22044800	-1.21661200
C	-6.03365000	-1.09881900	-1.08199300
H	-5.33393700	0.65310000	-0.06441100
C	-1.01173400	0.34953300	2.62719200
C	-2.33166700	-1.62710900	2.12807100
C	-1.33923500	1.16780700	-1.24144500
C	-4.40107900	3.24407500	2.42776100
H	-3.38544900	1.39187500	2.80306400
C	-4.45686200	3.98472100	0.13158800
H	-3.46661200	2.72907000	-1.29417600
C	-5.68892100	-2.30765500	-1.68868200
H	-4.06914500	-3.64323200	-2.19923400
H	-7.07363800	-0.78773400	-1.03318000
C	-0.63976700	-0.21348900	3.84860900
H	-0.66198700	1.34299100	2.36484100
C	-1.96278400	-2.17405100	3.35474100
H	-2.96811700	-2.19457500	1.46041700
C	-0.73816700	2.43740500	-1.06515600
C	-1.47917000	0.65601500	-2.55315300
C	-4.79216600	4.18239800	1.47328800
H	-4.66423700	3.38441300	3.47263600
H	-4.76600000	4.70500200	-0.62088000
H	-6.46095800	-2.94225200	-2.11579600
C	-1.11483900	-1.47372900	4.21597000
H	0.02381200	0.33565900	4.51072300

H	-2.33222700	-3.15738300	3.63085400
C	-0.25992400	3.14848200	-2.16171800
H	-0.64602800	2.86277200	-0.07191400
C	-1.00740500	1.38717000	-3.64476500
H	-1.96267000	-0.29920800	-2.71429500
H	-5.35933900	5.06028100	1.77084500
H	-0.82316800	-1.90844500	5.16782600
C	-0.39838000	2.62876700	-3.45361300
H	0.23215200	4.10310200	-2.00279600
H	-1.11701800	0.97862700	-4.64554000
H	-0.03125800	3.19194800	-4.30812600
P	2.32464500	0.48344300	0.10554700
C	3.45366600	0.08544600	-1.30492100
C	3.22294000	-0.18912100	1.57955500
C	2.54719900	2.31267600	0.31350000
C	2.87384000	-0.26399400	-2.53332500
C	4.85356300	0.11569200	-1.19804800
C	4.21160900	0.52310900	2.27955600
C	2.90041400	-1.49086100	1.99759600
C	2.02055700	2.92987600	1.46409400
C	3.11099600	3.13121000	-0.67635500
C	3.67655500	-0.55825700	-3.63792000
H	1.79214100	-0.32614600	-2.61218600
C	5.65381300	-0.18302500	-2.30074900
H	5.32104500	0.36204600	-0.24921900
C	4.86391800	-0.05434800	3.37074300
H	4.46989800	1.53423400	1.97946400
C	3.56124000	-2.06714100	3.08408200
H	2.13622900	-2.05375000	1.46723800
C	2.06519300	4.31404900	1.62363600
H	1.58774600	2.31684000	2.25105600
C	3.14988000	4.52054400	-0.52009100
H	3.52793200	2.68421200	-1.57296800
C	5.06639300	-0.51761500	-3.52397500
H	3.21305400	-0.83535700	-4.58102600
H	6.73631100	-0.16085100	-2.20338700
C	4.54156100	-1.35172900	3.77445300

H	5.62580700	0.51018900	3.90282100
H	3.30334500	-3.07759900	3.39019200
C	2.62871800	5.11799200	0.62754400
H	1.66288300	4.76642700	2.52677300
H	3.59803200	5.13394400	-1.29801300
H	5.69165500	-0.75619200	-4.38060900
H	5.05158000	-1.80107700	4.62294600
H	2.66366700	6.19734600	0.74938700
I	0.25130700	-3.14745600	-0.64316700

IRC of tetraphenylphosphonium C–P oxidative -Point2

0 1

P	-2.37457300	0.39019100	0.14827200
C	-3.68710600	-0.66898000	-0.58668600
C	-3.29201700	1.91437500	0.70608100
C	-3.34957900	-1.88914300	-1.19741000
C	-5.03631100	-0.28063700	-0.52667300
C	-1.86372800	-0.36549800	1.76136900
Pd	-0.02362900	-0.33962600	-0.26933900
C	-3.65395900	2.11809300	2.04592900
C	-3.70832500	2.85572700	-0.25341000
C	-4.34801600	-2.69640500	-1.74456000
H	-2.31398600	-2.22112900	-1.22631000
C	-6.02678200	-1.09531900	-1.07620800
H	-5.32153800	0.65131100	-0.05353300
C	-1.01459800	0.33450600	2.64185500
C	-2.34093000	-1.63447800	2.13327300
C	-1.33623400	1.17072100	-1.24658000
C	-4.38565000	3.24799900	2.42105100
H	-3.36517600	1.40041000	2.80458500
C	-4.44823400	3.97568300	0.12128600
H	-3.45956800	2.71394500	-1.29950700
C	-5.68581100	-2.30215800	-1.68890600
H	-4.06942200	-3.63776000	-2.20953600
H	-7.06610300	-0.78290000	-1.02247500
C	-0.65145900	-0.23165200	3.86457000
H	-0.65782300	1.32629200	2.38283500

C	-1.98122300	-2.18475100	3.36142600
H	-2.97708000	-2.19835100	1.46217800
C	-0.73527600	2.44160000	-1.07268200
C	-1.48232900	0.66390300	-2.56039100
C	-4.78098700	4.18029100	1.46254200
H	-4.64616200	3.39378800	3.46578000
H	-4.76080900	4.69025700	-0.63515100
H	-6.46003300	-2.93367600	-2.11656000
C	-1.13419300	-1.49007300	4.22794500
H	0.01104100	0.31327200	4.53119300
H	-2.35797300	-3.16615000	3.63477600
C	-0.27168900	3.16054500	-2.17114400
H	-0.63385900	2.86301400	-0.07865100
C	-1.02642000	1.40273700	-3.65421800
H	-1.96166200	-0.29359200	-2.72128400
H	-5.34930300	5.05869100	1.75614500
H	-0.85022700	-1.92769700	5.18083700
C	-0.42343100	2.64735200	-3.46398900
H	0.21590700	4.11774300	-2.01338000
H	-1.14685700	0.99955900	-4.65589800
H	-0.07450800	3.21895400	-4.31968400
P	2.32467900	0.48274700	0.10433700
C	3.45347700	0.08481000	-1.30614300
C	3.22239400	-0.18924000	1.57873800
C	2.54575900	2.31194900	0.31214000
C	2.87369900	-0.26395800	-2.53478100
C	4.85336000	0.11456600	-1.19899300
C	4.21120300	0.52346000	2.27803100
C	2.89949400	-1.49048000	1.99798900
C	2.01861400	2.92846300	1.46283900
C	3.10924700	3.13084200	-0.67753500
C	3.67653400	-0.55820300	-3.63930400
H	1.79198300	-0.32538900	-2.61414800
C	5.65369800	-0.18400300	-2.30165500
H	5.32071900	0.36036500	-0.24997200
C	4.86339100	-0.05312400	3.36970600
H	4.46958600	1.53427600	1.97699300

C	3.56014700	-2.06585400	3.08506100
H	2.13519300	-2.05376800	1.46829100
C	2.06294800	4.31258400	1.62289200
H	1.58562700	2.31499700	2.24938500
C	3.14781200	4.52010600	-0.52071700
H	3.52610500	2.68425600	-1.57439200
C	5.06637100	-0.51805600	-3.52506600
H	3.21316400	-0.83477400	-4.58262600
H	6.73618200	-0.16218000	-2.20411500
C	4.54068000	-1.35003500	3.77467000
H	5.62536300	0.51179700	3.90123200
H	3.30179200	-3.07583700	3.39231300
C	2.62654600	5.11693700	0.62719300
H	1.66012800	4.76451200	2.52600700
H	3.59567500	5.13393100	-1.29845100
H	5.69170500	-0.75654200	-4.38167100
H	5.05050000	-1.79859900	4.62368200
H	2.66121900	6.19624000	0.74946500
I	0.25440500	-3.14506000	-0.63911400

IRC of tetraphenylphosphonium C−P oxidative -Point3

0 1

P	-2.36076200	0.38254600	0.15107800
C	-3.67881000	-0.67011300	-0.58596400
C	-3.27690300	1.91088200	0.70446600
C	-3.34485900	-1.88856000	-1.20183200
C	-5.02747900	-0.28054600	-0.52139100
C	-1.86801900	-0.37494500	1.77225900
Pd	-0.02996900	-0.33775200	-0.26995500
C	-3.63790200	2.12113600	2.04358900
C	-3.69738600	2.84662600	-0.25889000
C	-4.34554100	-2.69281100	-1.74942800
H	-2.30990300	-2.22172700	-1.23402100
C	-6.02038700	-1.09192100	-1.07148500
H	-5.31057400	0.64991000	-0.04411000
C	-1.01873100	0.31969100	2.65650000
C	-2.35127500	-1.64243800	2.14026400

C	-1.32455300	1.17369300	-1.25467500
C	-4.37136100	3.25153900	2.41407800
H	-3.34769000	1.40784500	2.80571200
C	-4.43911600	3.96693000	0.11101800
H	-3.45157500	2.69954700	-1.30486300
C	-5.68265300	-2.29706400	-1.68931700
H	-4.06930300	-3.63293000	-2.21832100
H	-7.05915600	-0.77827000	-1.01408600
C	-0.66271700	-0.24914300	3.88002700
H	-0.65554800	1.30976100	2.39946500
C	-1.99872300	-2.19583600	3.36930300
H	-2.98692100	-2.20297000	1.46579100
C	-0.73016500	2.44723200	-1.08154800
C	-1.48269000	0.67212300	-2.56856700
C	-4.77020200	4.17814800	1.45164600
H	-4.63072800	3.40180200	3.45847300
H	-4.75479000	4.67643900	-0.64890900
H	-6.45875000	-2.92599400	-2.11740000
C	-1.15219700	-1.50596600	4.24002700
H	-0.00028800	0.29214200	4.54970200
H	-2.38071000	-3.17597900	3.63998600
C	-0.28419500	3.17468500	-2.18176600
H	-0.61964100	2.86408500	-0.08657700
C	-1.04533500	1.41921400	-3.66443600
H	-1.95654800	-0.28844900	-2.72804800
H	-5.34011700	5.05675600	1.74152700
H	-0.87365700	-1.94610000	5.19337600
C	-0.44806400	2.66679100	-3.47522300
H	0.19865200	4.13453500	-2.02518800
H	-1.17531000	1.02032600	-4.66667000
H	-0.11332000	3.24490100	-4.33221600
P	2.32474900	0.48192200	0.10286000
C	3.45347000	0.08408100	-1.30744000
C	3.22168100	-0.18949800	1.57787300
C	2.54428300	2.31111000	0.31071700
C	2.87382100	-0.26427300	-2.53626100
C	4.85333100	0.11363700	-1.19996800

C	4.21058900	0.52369700	2.27656600
C	2.89856000	-1.49029600	1.99823100
C	2.01673900	2.92692200	1.46157400
C	3.10762200	3.13034400	-0.67869700
C	3.67682900	-0.55843700	-3.64067500
H	1.79212300	-0.32526800	-2.61615000
C	5.65381400	-0.18477100	-2.30255100
H	5.32051100	0.35912000	-0.25078500
C	4.86266600	-0.05207100	3.36870800
H	4.46906300	1.53425100	1.97474700
C	3.55902700	-2.06479600	3.08588400
H	2.13432600	-2.05408000	1.46905500
C	2.06088200	4.31099300	1.62217600
H	1.58361600	2.31308200	2.24775900
C	3.14597900	4.51952900	-0.52128300
H	3.52451200	2.68418200	-1.57574700
C	5.06664900	-0.51851100	-3.52612400
H	3.21360700	-0.83465800	-4.58416000
H	6.73627600	-0.16308600	-2.20482000
C	4.53967800	-1.34856300	3.77483500
H	5.62470700	0.51318900	3.89975600
H	3.30037800	-3.07441000	3.39406300
C	2.62459100	5.11574500	0.62688800
H	1.65772100	4.76251800	2.52532300
H	3.59372300	5.13375700	-1.29875000
H	5.69210200	-0.75687900	-4.38266700
H	5.04937700	-1.79644200	4.62427200
H	2.65912800	6.19499700	0.74961700
I	0.25776300	-3.14255600	-0.63481300

IRC of tetraphenylphosphonium C–P oxidative -Point4

0 1

P	-2.34783400	0.37451100	0.15498600
C	-3.67106300	-0.67130200	-0.58485300
C	-3.26218200	1.90735300	0.70271300
C	-3.34042200	-1.88806500	-1.20557500
C	-5.01919500	-0.28041200	-0.51643700

C	-1.87350600	-0.38445100	1.78384800
Pd	-0.03620000	-0.33574700	-0.27045000
C	-3.62301900	2.12397600	2.04091100
C	-3.68601500	2.83763100	-0.26464400
C	-4.34312400	-2.68938500	-1.75387700
H	-2.30607900	-2.22235900	-1.24065800
C	-6.01430100	-1.08854000	-1.06737700
H	-5.30031800	0.64865100	-0.03532900
C	-1.02347000	0.30506700	2.67108300
C	-2.36226600	-1.65045100	2.14846500
C	-1.31003200	1.17669100	-1.26302500
C	-4.35838500	3.25483700	2.40647300
H	-3.33196000	1.41488800	2.80651100
C	-4.42962200	3.95832000	0.10024100
H	-3.44250700	2.68530300	-1.31031300
C	-5.67955700	-2.29211200	-1.68992800
H	-4.06906500	-3.62833100	-2.22642200
H	-7.05253100	-0.77363400	-1.00686200
C	-0.67341200	-0.26618800	3.89513300
H	-0.65424600	1.29338700	2.41556800
C	-2.01549400	-2.20686400	3.37802000
H	-2.99790700	-2.20777600	1.47119900
C	-0.72412100	2.45362700	-1.09079300
C	-1.48130000	0.68035700	-2.57660100
C	-4.75995500	4.17594100	1.44001700
H	-4.61732500	3.40940100	3.45036400
H	-4.74777800	4.66294700	-0.66320800
H	-6.45735900	-2.91851800	-2.11863300
C	-1.16891400	-1.52154100	4.25216000
H	-0.01065400	0.27167800	4.56726300
H	-2.40211300	-3.18586000	3.64638400
C	-0.29710600	3.18981900	-2.19277600
H	-0.60426500	2.86614500	-0.09509600
C	-1.06380900	1.43593200	-3.67452400
H	-1.94892500	-0.28367100	-2.73447300
H	-5.33157800	5.05474500	1.72594200
H	-0.89480000	-1.96409300	5.20568500

C	-0.47301900	2.68683900	-3.48660600
H	0.18005200	4.15280600	-2.03759900
H	-1.20352400	1.04111100	-4.67711500
H	-0.15290700	3.27144000	-4.34491400
P	2.32480900	0.48098200	0.10122200
C	3.45357700	0.08326200	-1.30879100
C	3.22081100	-0.18992500	1.57692700
C	2.54283000	2.31013300	0.30925400
C	2.87417900	-0.26490700	-2.53778600
C	4.85340400	0.11289400	-1.20092300
C	4.20972800	0.52379800	2.27512100
C	2.89754800	-1.49032500	1.99830400
C	2.01492300	2.92520800	1.46030100
C	3.10609700	3.12972400	-0.67984000
C	3.67747000	-0.55892600	-3.64202600
H	1.79252300	-0.32568800	-2.61826100
C	5.65414000	-0.18529900	-2.30336100
H	5.32031100	0.35823400	-0.25157700
C	4.86167500	-0.05116800	3.36773300
H	4.46824900	1.53411900	1.97259300
C	3.55780500	-2.06396000	3.08654700
H	2.13346700	-2.05464200	1.46957200
C	2.05899500	4.30921400	1.62154300
H	1.58158600	2.31097700	2.24606400
C	3.14435000	4.51881400	-0.52174600
H	3.52298100	2.68401300	-1.57711300
C	5.06725900	-0.51893800	-3.52709700
H	3.21449200	-0.83495900	-4.58567300
H	6.73657000	-0.16354400	-2.20538900
C	4.53848500	-1.34728400	3.77493400
H	5.62372100	0.51445500	3.89837000
H	3.29891800	-3.07324200	3.39557600
C	2.62288800	5.11438200	0.62672100
H	1.65552300	4.76031400	2.52474600
H	3.59201000	5.13345800	-1.29891500
H	5.69291600	-0.75713100	-4.38352800
H	5.04805200	-1.79449100	4.62479700

H	2.65737300	6.19357300	0.74997400
I	0.26104300	-3.14008700	-0.63066800

IRC of tetraphenylphosphonium C−P oxidative -Point5

0 1

P	-2.33551100	0.36611300	0.15966600
C	-3.66381300	-0.67256400	-0.58349800
C	-3.24778200	1.90374000	0.70073600
C	-3.33630000	-1.88773400	-1.20872800
C	-5.01142900	-0.28026600	-0.51187600
C	-1.88008200	-0.39388500	1.79610300
Pd	-0.04243500	-0.33361800	-0.27069800
C	-3.60946900	2.12637700	2.03779400
C	-3.67408400	2.82880700	-0.27067200
C	-4.34083400	-2.68621700	-1.75793200
H	-2.30255600	-2.22312300	-1.24635500
C	-6.00853800	-1.08522300	-1.06388400
H	-5.29071700	0.64751500	-0.02726400
C	-1.02875600	0.29091200	2.68548800
C	-2.37358200	-1.65846100	2.15793000
C	-1.29277900	1.17970900	-1.27147800
C	-4.34695800	3.25758500	2.39819200
H	-3.31822800	1.42123300	2.80684500
C	-4.41971300	3.94984500	0.08899700
H	-3.43211600	2.67143000	-1.31585200
C	-5.67658900	-2.28736700	-1.69074600
H	-4.06879900	-3.62406200	-2.23385200
H	-7.04623300	-0.76901500	-1.00075500
C	-0.68320200	-0.28244900	3.90973600
H	-0.65405200	1.27750300	2.43097900
C	-2.03098100	-2.21770200	3.38762600
H	-3.00971900	-2.21282300	1.47854400
C	-0.71674600	2.46063300	-1.10038700
C	-1.47790700	0.68851900	-2.58444900
C	-4.75037400	4.17349000	1.42768400
H	-4.60632700	3.41613100	3.44139300
H	-4.73966000	4.64983600	-0.67797900

H	-6.45595000	-2.91129600	-2.12025100
C	-1.18373100	-1.53655300	4.26426400
H	-0.01970000	0.25231900	4.58362800
H	-2.42146800	-3.19570400	3.65411400
C	-0.31028400	3.20584200	-2.20416000
H	-0.58698500	2.86897800	-0.10420700
C	-1.08197900	1.45287700	-3.68442400
H	-1.93839200	-0.27939200	-2.74051900
H	-5.32386600	5.05243100	1.70944500
H	-0.91280600	-1.98141600	5.21763700
C	-0.49870300	2.70756700	-3.49807700
H	0.16029700	4.17238200	-2.05059300
H	-1.23197600	1.06197500	-4.68710300
H	-0.19469000	3.29894000	-4.35761100
P	2.32480900	0.47993600	0.09945600
C	3.45375600	0.08237900	-1.31015100
C	3.21972600	-0.19050400	1.57592600
C	2.54135100	2.30903600	0.30777600
C	2.87474700	-0.26583200	-2.53931900
C	4.85353400	0.11237300	-1.20179500
C	4.20855200	0.52378800	2.27372300
C	2.89642400	-1.49056400	1.99821200
C	2.01317500	2.92334300	1.45907000
C	3.10459000	3.12899300	-0.68096000
C	3.67844900	-0.55963200	-3.64331000
H	1.79315400	-0.32662200	-2.62045100
C	5.65464900	-0.18553600	-2.30401000
H	5.32005900	0.35774500	-0.25227800
C	4.86037900	-0.05039400	3.36678600
H	4.46705200	1.53391500	1.97057000
C	3.55647900	-2.06335000	3.08703300
H	2.13258600	-2.05546100	1.46984600
C	2.05732600	4.30727000	1.62105000
H	1.57957200	2.30870800	2.24437100
C	3.14288600	4.51797200	-0.52209300
H	3.52137800	2.68375800	-1.57851000
C	5.06819100	-0.51928300	-3.52791900

H	3.21583100	-0.83563900	-4.58712700
H	6.73703800	-0.16348800	-2.20573300
C	4.53709400	-1.34619600	3.77495000
H	5.62235600	0.51562400	3.89708100
H	3.29743800	-3.07235000	3.39682000
C	2.62145700	5.11286400	0.62673200
H	1.65361600	4.75792200	2.52435200
H	3.59047900	5.13303900	-1.29894600
H	5.69415300	-0.75723400	-4.38418500
H	5.04654100	-1.79275100	4.62522000
H	2.65600500	6.19198100	0.75058500
I	0.26416100	-3.13769200	-0.62678400

IRC of tetraphenylphosphonium C–P oxidative -Point6

0 1

P	-2.32429800	0.35710700	0.16550500
C	-3.65735500	-0.67403900	-0.58177900
C	-3.23392900	1.89993800	0.69855900
C	-3.33263600	-1.88760300	-1.21129700
C	-5.00448300	-0.28026000	-0.50769500
C	-1.88794600	-0.40326500	1.80905800
Pd	-0.04866800	-0.33127900	-0.27070200
C	-3.59754900	2.12816900	2.03426400
C	-3.66159400	2.82015500	-0.27694600
C	-4.33873900	-2.68335200	-1.76171900
H	-2.29943500	-2.22396600	-1.25110500
C	-6.00331200	-1.08212500	-1.06113100
H	-5.28212900	0.64631600	-0.01985500
C	-1.03465100	0.27738100	2.69952900
C	-2.38516500	-1.66654500	2.16883700
C	-1.27167000	1.18275700	-1.28041000
C	-4.33733300	3.25962100	2.38928100
H	-3.30689000	1.42663200	2.80671600
C	-4.40934400	3.94153500	0.07735300
H	-3.42024700	2.65800800	-1.32143700
C	-5.67384300	-2.28294000	-1.69193200
H	-4.06849800	-3.62011300	-2.24081200

H	-7.04050200	-0.76461900	-0.99596400
C	-0.69180500	-0.29769300	3.92359500
H	-0.65521200	1.26231200	2.44535400
C	-2.04473700	-2.22836800	3.39823100
H	-3.02240400	-2.21827300	1.48815600
C	-0.70762600	2.46842200	-1.11058600
C	-1.47188100	0.69659100	-2.59230000
C	-4.74156200	4.17072600	1.41470000
H	-4.59807500	3.42176300	3.43160000
H	-4.73022600	4.63724800	-0.69313100
H	-6.45455600	-2.90444700	-2.12250600
C	-1.19612200	-1.55085000	4.27624400
H	-0.02708100	0.23440500	4.59842000
H	-2.43811500	-3.20559600	3.66340500
C	-0.32347200	3.22288300	-2.21617900
H	-0.56746700	2.87279800	-0.11418100
C	-1.09924700	1.46994200	-3.69432300
H	-1.92417100	-0.27569300	-2.74630200
H	-5.31705800	5.04975700	1.69208400
H	-0.92689700	-1.99785000	5.22911100
C	-0.52453400	2.72887000	-3.50986400
H	0.13943000	4.19349900	-2.06448300
H	-1.25995800	1.08271800	-4.69681400
H	-0.23772000	3.32710100	-4.37058100
P	2.32466500	0.47880800	0.09756800
C	3.45397200	0.08146200	-1.31147300
C	3.21833100	-0.19120600	1.57490200
C	2.53975700	2.30785100	0.30631200
C	2.87553600	-0.26702000	-2.54083100
C	4.85368300	0.11212400	-1.20249000
C	4.20695600	0.52372300	2.27240100
C	2.89515500	-1.49100500	1.99797400
C	2.01144100	2.92135800	1.45792700
C	3.10303600	3.12818500	-0.68201700
C	3.67981600	-0.56048900	-3.64447900
H	1.79403900	-0.32809000	-2.62273300
C	5.65534100	-0.18541600	-2.30438200

H	5.31968600	0.35769800	-0.25277700
C	4.85871500	-0.04968600	3.36587600
H	4.46532800	1.53370800	1.96871500
C	3.55505600	-2.06294300	3.08734500
H	2.13167200	-2.05655700	1.46989500
C	2.05586400	4.30519000	1.62075800
H	1.57751100	2.30631400	2.24272200
C	3.14158000	4.51703300	-0.52225600
H	3.51961200	2.68345300	-1.57991100
C	5.06948700	-0.51946500	-3.52849900
H	3.21770400	-0.83662400	-4.58849100
H	6.73767400	-0.16284700	-2.20570100
C	4.53549900	-1.34525000	3.77487900
H	5.62054300	0.51678200	3.89588600
H	3.29599000	-3.07172500	3.39778600
C	2.62031300	5.11121700	0.62699900
H	1.65200600	4.75536900	2.52421100
H	3.58914100	5.13252600	-1.29876900
H	5.69588700	-0.75708100	-4.38452700
H	5.04486900	-1.79116800	4.62552000
H	2.65507600	6.19024300	0.75154400
I	0.26700400	-3.13543100	-0.62328400

IRC of tetraphenylphosphonium C–P oxidative -Point7

0 1

P	-2.31476500	0.34721600	0.17276800
C	-3.65210400	-0.67593000	-0.57972200
C	-3.22104100	1.89580300	0.69626000
C	-3.32956000	-1.88778000	-1.21335300
C	-4.99883600	-0.28072800	-0.50418200
C	-1.89749700	-0.41261000	1.82269600
Pd	-0.05500800	-0.32856200	-0.27055400
C	-3.58767700	2.12909000	2.03045300
C	-3.64886500	2.81170400	-0.28326500
C	-4.33676100	-2.68101000	-1.76551900
H	-2.29678100	-2.22482800	-1.25485400
C	-5.99888900	-1.07968000	-1.05965200

H	-5.27521900	0.64469000	-0.01341200
C	-1.04154900	0.26475100	2.71297800
C	-2.39691500	-1.67489800	2.18118900
C	-1.24534800	1.18588100	-1.29028100
C	-4.32984900	3.26067800	2.38003400
H	-3.29842800	1.43072100	2.80618100
C	-4.39881900	3.93340100	0.06568600
H	-3.40709300	2.64524900	-1.32688300
C	-5.67130600	-2.27921400	-1.69399800
H	-4.06786900	-3.61664200	-2.24759500
H	-7.03565700	-0.76100300	-0.99323600
C	-0.69920800	-0.31154400	3.93640600
H	-0.65846200	1.24820800	2.45834400
C	-2.05620500	-2.23898800	3.40974300
H	-3.03581600	-2.22448800	1.50012300
C	-0.69590400	2.47708400	-1.12170400
C	-1.46218400	0.70449100	-2.60042400
C	-4.73383300	4.16751400	1.40146800
H	-4.59288100	3.42588800	3.42130500
H	-4.71972100	4.62532800	-0.70820400
H	-6.45300900	-2.89843000	-2.12609400
C	-1.20561500	-1.56424900	4.28785800
H	-0.03283500	0.21850500	4.61123700
H	-2.45107500	-3.21582500	3.67423400
C	-0.33596600	3.24095400	-2.22914400
H	-0.54484200	2.87768600	-0.12534200
C	-1.11458700	1.48690700	-3.70446600
H	-1.90507200	-0.27271600	-2.75200000
H	-5.31143000	5.04657900	1.67435300
H	-0.93627800	-2.01314000	5.23981800
C	-0.54952000	2.75051800	-3.52222100
H	0.11799400	4.21621900	-2.07962200
H	-1.28638300	1.10302200	-4.70645200
H	-0.28092100	3.35555400	-4.38406300
P	2.32436100	0.47770200	0.09568600
C	3.45429900	0.08065800	-1.31256400
C	3.21655500	-0.19194100	1.57403000

C	2.53801400	2.30669500	0.30505900
C	2.87670200	-0.26826400	-2.54218100
C	4.85391700	0.11226600	-1.20271200
C	4.20479600	0.52373400	2.27139800
C	2.89375100	-1.49159600	1.99770700
C	2.00957300	2.91935000	1.45702700
C	3.10149900	3.12744200	-0.68274000
C	3.68179600	-0.56123700	-3.64535300
H	1.79534400	-0.32990100	-2.62505700
C	5.65635200	-0.18478300	-2.30413800
H	5.31919600	0.35816100	-0.25273600
C	4.85653100	-0.04889800	3.36526100
H	4.46288800	1.53365100	1.96730900
C	3.55353100	-2.06267200	3.08762200
H	2.13080700	-2.05793000	1.46977900
C	2.05439500	4.30307500	1.62083000
H	1.57519900	2.30388200	2.24123400
C	3.14044100	4.51613700	-0.52195400
H	3.51784000	2.68326000	-1.58101200
C	5.07136500	-0.51924900	-3.52855900
H	3.22039700	-0.83760100	-4.58963100
H	6.73860700	-0.16149300	-2.20487500
C	4.53360800	-1.34433300	3.77493400
H	5.61806500	0.51811300	3.89509100
H	3.29462600	-3.07132700	3.39857100
C	2.61930600	5.10956500	0.62773900
H	1.65036600	4.75274000	2.52444400
H	3.58806800	5.13207500	-1.29805100
H	5.69838900	-0.75640500	-4.38424600
H	5.04292800	-1.78961700	4.62592800
H	2.65436700	6.18848800	0.75306700
I	0.26951100	-3.13340600	-0.62024500

IRC of tetraphenylphosphonium C–P oxidative -Point8

0 1

P	-2.30075700	0.21954000	0.15506800
C	-3.64172500	-0.79493200	-0.60375100

C	-3.20230800	1.77484900	0.66717700
C	-3.32063000	-2.00492200	-1.24136900
C	-4.98809400	-0.39818700	-0.52798200
C	-1.90124400	-0.53821200	1.80976900
Pd	-0.05468800	-0.44189600	-0.29784100
C	-3.57256500	2.01258900	1.99986700
C	-3.62909700	2.68727600	-0.31602600
C	-4.32846600	-2.79591600	-1.79566500
H	-2.28810000	-2.34225600	-1.28419700
C	-5.98885700	-1.19444700	-1.08602100
H	-5.26353800	0.52623900	-0.03477000
C	-1.04166200	0.13712600	2.69801800
C	-2.40078500	-1.79992400	2.16786800
C	-1.20479500	1.07251000	-1.32960700
C	-4.31683500	3.14430100	2.34440400
H	-3.28554900	1.31672300	2.77854700
C	-4.38105400	3.80936800	0.02807300
H	-3.38604100	2.51719900	-1.35868900
C	-5.66255000	-2.39290400	-1.72324000
H	-4.06048900	-3.73040100	-2.28050000
H	-7.02528700	-0.87468400	-1.01935200
C	-0.69712900	-0.43967000	3.92027800
H	-0.65634800	1.11935900	2.44178000
C	-2.05680000	-2.36572800	3.39494000
H	-3.04189800	-2.34806400	1.48747800
C	-0.67345500	2.36991700	-1.16174000
C	-1.44106500	0.59543000	-2.63677200
C	-4.71967700	4.04763000	1.36220700
H	-4.58278100	3.31185700	3.38456900
H	-4.70117400	4.49822400	-0.74888900
H	-6.44486200	-3.01004400	-2.15721800
C	-1.20364600	-1.69247200	4.27154200
H	-0.02858600	0.08916800	4.59392500
H	-2.45132900	-3.34268500	3.65956400
C	-0.33951400	3.14304500	-2.27105700
H	-0.51109500	2.76682600	-0.16564900
C	-1.11979300	1.38658600	-3.74277700

H	-1.87352500	-0.38717300	-2.78528300
H	-5.29929200	4.92670200	1.63078000
H	-0.93208400	-2.14275300	5.22221800
C	-0.56472000	2.65498700	-3.56307300
H	0.10431400	4.12346000	-2.12409300
H	-1.30283300	1.00557000	-4.74392700
H	-0.31426100	3.26620800	-4.42603600
P	2.33104000	0.35994600	0.06610200
C	3.46149100	-0.03694100	-1.34135400
C	3.22183800	-0.30944000	1.54544600
C	2.54353700	2.18890900	0.27615200
C	2.88465400	-0.38631900	-2.57118000
C	4.86102200	-0.00440600	-1.23069700
C	4.20987500	0.40693100	2.24253200
C	2.89957600	-1.60900300	1.96968300
C	2.01536900	2.80084200	1.42858500
C	3.10728000	3.00994100	-0.71120400
C	3.69048500	-0.67878100	-3.67392500
H	1.80346400	-0.44858000	-2.65501600
C	5.66415300	-0.30101800	-2.33169700
H	5.32563900	0.24184200	-0.28049500
C	4.86188600	-0.16503100	3.33655500
H	4.46758500	1.41682900	1.93813400
C	3.55950700	-2.17929700	3.05994400
H	2.13712100	-2.17614300	1.44200200
C	2.06087500	4.18446600	1.59329800
H	1.58054900	2.18508100	2.21230700
C	3.14694100	4.39847900	-0.54943300
H	3.52312300	2.56621600	-1.60992200
C	5.07995300	-0.63586700	-3.55639100
H	3.22973800	-0.95531600	-4.61844800
H	6.74633500	-0.27702400	-2.23188500
C	4.53937700	-1.46037600	3.74687000
H	5.62320500	0.40250800	3.86610900
H	3.30083600	-3.18785300	3.37137300
C	2.62620400	4.99128600	0.60074700
H	1.65688700	4.63371600	2.49712100

H	3.59461400	5.01476200	-1.32519800
H	5.70757400	-0.87253400	-4.41176200
H	5.04881700	-1.90508400	4.59808500
H	2.66172400	6.07010500	0.72681500
I	0.27874800	-3.24828500	-0.64528900

IRC of tetraphenylphosphonium C–P oxidative -Point9

0 1

P	-2.30461400	0.32687500	0.19200700
C	-3.64789000	-0.68036100	-0.57248800
C	-3.20149000	1.88811600	0.69406100
C	-3.32753500	-1.88871300	-1.21335700
C	-4.99396700	-0.28236600	-0.49694200
C	-1.91787000	-0.42833200	1.84913800
Pd	-0.06722300	-0.32238300	-0.27019900
C	-3.57421400	2.12946500	2.02569400
C	-3.62707200	2.79809200	-0.29190100
C	-4.33568800	-2.67805600	-1.76946500
H	-2.29511600	-2.22609100	-1.25703300
C	-5.99506300	-1.07658100	-1.05722400
H	-5.26877400	0.64124900	-0.00179100
C	-1.05470400	0.24593200	2.73472900
C	-2.41668300	-1.68968600	2.20738800
C	-1.18124600	1.19162800	-1.31255100
C	-4.31967400	3.26145400	2.36651900
H	-3.28897400	1.43548900	2.80661700
C	-4.38022800	3.92070700	0.04871100
H	-3.38285500	2.62530900	-1.33380800
C	-5.66946800	-2.27421500	-1.69650800
H	-4.06831200	-3.61164000	-2.25636800
H	-7.03127900	-0.75609400	-0.99050100
C	-0.70721200	-0.33092400	3.95580800
H	-0.66814600	1.22722600	2.47659000
C	-2.06871200	-2.25658200	3.43295600
H	-3.06004700	-2.23686600	1.52817000
C	-0.66638700	2.49421800	-1.14475500
C	-1.43534800	0.71778400	-2.61643200

C	-4.72151100	4.16219600	1.38159600
H	-4.58754700	3.43089400	3.40589400
H	-4.69944700	4.60745300	-0.73049000
H	-6.45216400	-2.88986100	-2.13192200
C	-1.21313700	-1.58393400	4.30750800
H	-0.03653900	0.19722400	4.62789300
H	-2.46224800	-3.23377200	3.69822000
C	-0.35460000	3.27466000	-2.25553800
H	-0.49443100	2.88813200	-0.14906900
C	-1.13613100	1.51573900	-3.72387800
H	-1.85911800	-0.26925400	-2.76210000
H	-5.30229800	5.04148000	1.64693900
H	-0.93885100	-2.03502900	5.25702400
C	-0.58905400	2.78792500	-3.54638600
H	0.08035300	4.25948900	-2.11089400
H	-1.32888200	1.13695400	-4.72410800
H	-0.35353300	3.40385000	-4.41022100
P	2.32334700	0.47567400	0.09181800
C	3.45404300	0.07882100	-1.31510100
C	3.21307100	-0.19360500	1.57192800
C	2.53514400	2.30460600	0.30243200
C	2.87757600	-0.27091200	-2.54497900
C	4.85353200	0.11193500	-1.20403200
C	4.20119500	0.52325400	2.26853400
C	2.89126700	-1.49306500	1.99670500
C	2.00755400	2.91611400	1.45531800
C	3.09893000	3.12572500	-0.68478000
C	3.68376000	-0.56310300	-3.64750600
H	1.79651500	-0.33361300	-2.62943400
C	5.65698700	-0.18449300	-2.30482100
H	5.31782700	0.35841000	-0.25374600
C	4.85367800	-0.04821400	3.36251500
H	4.45868800	1.53306200	1.96372100
C	3.55155700	-2.06276400	3.08709000
H	2.12907800	-2.06083800	1.46938000
C	2.05372100	4.29968200	1.62057700
H	1.57255900	2.30023600	2.23883700

C	3.13930600	4.51414600	-0.52238900
H	3.51404300	2.68224600	-1.58395300
C	5.07316600	-0.51963000	-3.52962100
H	3.22329800	-0.83980300	-4.59210800
H	6.73913200	-0.16015000	-2.20480000
C	4.53150000	-1.34345600	3.77344500
H	5.61513300	0.51964100	3.89151400
H	3.29314500	-3.07125400	3.39891000
C	2.61917700	5.10662200	0.62822200
H	1.65006000	4.74873600	2.52462400
H	3.58683600	5.13055600	-1.29811500
H	5.70103700	-0.75610300	-4.38485500
H	5.04132900	-1.78779100	4.62461100
H	2.65516700	6.18537300	0.75470800
I	0.27288900	-3.13048500	-0.61608100

IRC of tetraphenylphosphonium C−P oxidative -Point10

0 1

P	-2.30293300	0.31719400	0.20249900
C	-3.64787900	-0.68269500	-0.56812500
C	-3.19445000	1.88474300	0.69381900
C	-3.32785700	-1.88929200	-1.21226300
C	-4.99364200	-0.28338600	-0.49335100
C	-1.92743000	-0.43474100	1.86092100
Pd	-0.07245300	-0.31931500	-0.27014300
C	-3.56953100	2.12956800	2.02445600
C	-3.61838300	2.79263200	-0.29474200
C	-4.33611900	-2.67710500	-1.77033700
H	-2.29546400	-2.22652500	-1.25665400
C	-5.99483100	-1.07565800	-1.05608400
H	-5.26794200	0.63947400	0.00355700
C	-1.06040900	0.23898500	2.74320500
C	-2.42482900	-1.69585500	2.21960300
C	-1.14747100	1.19414100	-1.32413100
C	-4.31591700	3.26190000	2.36181600
H	-3.28625800	1.43723900	2.80746800
C	-4.37252500	3.91586200	0.04268000

H	-3.37273600	2.61741900	-1.33589300
C	-5.66965000	-2.27255000	-1.69712700
H	-4.06914700	-3.60974300	-2.25928500
H	-7.03087400	-0.75450400	-0.98975200
C	-0.70917300	-0.33765900	3.96295600
H	-0.67315800	1.21944600	2.48278700
C	-2.07199400	-2.26358800	3.44346600
H	-3.07060800	-2.24231700	1.54192600
C	-0.65068500	2.50190900	-1.15572600
C	-1.42086700	0.72315700	-2.62388800
C	-4.71655000	4.16031900	1.37433700
H	-4.58576800	3.43300400	3.40041200
H	-4.69057700	4.60077700	-0.73861200
H	-6.45254700	-2.88681300	-2.13414200
C	-1.21391500	-1.59103400	4.31545200
H	-0.03628900	0.19008400	4.63315000
H	-2.46394200	-3.24117100	3.70965900
C	-0.36173700	3.28946500	-2.26780200
H	-0.46898000	2.89284700	-0.16059900
C	-1.14397800	1.52760200	-3.73253600
H	-1.83556100	-0.26840100	-2.76655100
H	-5.29840600	5.03983200	1.63656400
H	-0.93634700	-2.04271000	5.26374400
C	-0.60488100	2.80350500	-3.55726600
H	0.06363000	4.27893300	-2.12556900
H	-1.34652200	1.15090400	-4.73167600
H	-0.38418000	3.42382600	-4.42187400
P	2.32282900	0.47479600	0.09000100
C	3.45366800	0.07789400	-1.31641300
C	3.21154400	-0.19441500	1.57086100
C	2.53404500	2.30371300	0.30116600
C	2.87749300	-0.27214200	-2.54631500
C	4.85312200	0.11151700	-1.20498300
C	4.19985500	0.52289700	2.26690700
C	2.89023900	-1.49377900	1.99617800
C	2.00718400	2.91487500	1.45453000
C	3.09788800	3.12484100	-0.68596200

C	3.68396600	-0.56410300	-3.64865700
H	1.79656200	-0.33520000	-2.63136200
C	5.65683300	-0.18478300	-2.30559500
H	5.31715100	0.35822100	-0.25463500
C	4.85291800	-0.04812200	3.36076200
H	4.45709100	1.53263800	1.96172200
C	3.55098400	-2.06291500	3.08661500
H	2.12827300	-2.06217700	1.46926000
C	2.05408000	4.29839800	1.62025000
H	1.57200800	2.29895200	2.23790100
C	3.13906300	4.51315400	-0.52302700
H	3.51217400	2.68154600	-1.58559800
C	5.07331600	-0.52017000	-3.53047600
H	3.22374400	-0.84090100	-4.59333100
H	6.73894500	-0.16012500	-2.20538800
C	4.53108200	-1.34326000	3.77232100
H	5.61452500	0.52004700	3.88918500
H	3.29281400	-3.07132800	3.39884900
C	2.61961300	5.10538400	0.62800400
H	1.65079900	4.74731500	2.52451700
H	3.58641700	5.12963900	-1.29876800
H	5.70141400	-0.75645600	-4.38558500
H	5.04132400	-1.78722900	4.62342100
H	2.65608000	6.18407300	0.75484900
I	0.27402200	-3.12951500	-0.61463900

IRC of tetraphenylphosphonium C–P oxidative -Point11

0 1

P	-2.30306700	0.30716100	0.21378500
C	-3.64887600	-0.68542200	-0.56346300
C	-3.18875300	1.88125700	0.69384500
C	-3.32857400	-1.89005600	-1.21095100
C	-4.99434700	-0.28486600	-0.49016500
C	-1.93716200	-0.44090900	1.87233300
Pd	-0.07737400	-0.31605500	-0.27025400
C	-3.56605500	2.12947800	2.02354100
C	-3.61060300	2.78740600	-0.29718300

C	-4.33655700	-2.67648000	-1.77141500
H	-2.29610800	-2.22691200	-1.25571400
C	-5.99521800	-1.07531500	-1.05583400
H	-5.26843800	0.63721200	0.00839000
C	-1.06622800	0.23275900	2.75087000
C	-2.43249600	-1.70196200	2.23139800
C	-1.11053400	1.19654100	-1.33687200
C	-4.31312700	3.26221400	2.35764500
H	-3.28488300	1.43860900	2.80852200
C	-4.36554200	3.91134400	0.03730600
H	-3.36325900	2.61005800	-1.33758600
C	-5.66994100	-2.27143600	-1.69842800
H	-4.06964000	-3.60808700	-2.26236300
H	-7.03117400	-0.75366800	-0.99041400
C	-0.71084400	-0.34348900	3.96920500
H	-0.67876100	1.21250800	2.48793400
C	-2.07432000	-2.27034800	3.45341000
H	-3.08057500	-2.24789800	1.55533300
C	-0.63347900	2.50939300	-1.16691700
C	-1.40463600	0.72808800	-2.63163300
C	-4.71238600	4.15853600	1.36775400
H	-4.58495700	3.43482400	3.39548100
H	-4.68217800	4.59472600	-0.74590700
H	-6.45274900	-2.88446300	-2.13733900
C	-1.21397600	-1.59738000	4.32263700
H	-0.03583700	0.18408900	4.63739300
H	-2.46412400	-3.24850900	3.72062000
C	-0.36803700	3.30395000	-2.27998800
H	-0.44198200	2.89730000	-0.17246700
C	-1.15036200	1.53884200	-3.74111700
H	-1.80996200	-0.26799300	-2.77126500
H	-5.29518700	5.03830800	1.62700300
H	-0.93286900	-2.04941200	5.26972000
C	-0.61926300	2.81839500	-3.56793500
H	0.04704500	4.29820400	-2.14005700
H	-1.36273500	1.16413400	-4.73902100
H	-0.41317500	3.44286300	-4.43315300

P	2.32231000	0.47404200	0.08836700
C	3.45335200	0.07712900	-1.31747500
C	3.20995200	-0.19515800	1.57003100
C	2.53293900	2.30295100	0.30018700
C	2.87755400	-0.27314200	-2.54745300
C	4.85276300	0.11127400	-1.20556000
C	4.19836500	0.52265100	2.26562200
C	2.88926000	-1.49448500	1.99577500
C	2.00668700	2.91375800	1.45397500
C	3.09698200	3.12409200	-0.68677400
C	3.68441200	-0.56482100	-3.64955400
H	1.79675800	-0.33650800	-2.63318400
C	5.65681600	-0.18484400	-2.30594500
H	5.31645300	0.35817100	-0.25510600
C	4.85198300	-0.04793500	3.35936800
H	4.45529000	1.53236000	1.96015100
C	3.55042500	-2.06305700	3.08628700
H	2.12761600	-2.06355700	1.46916900
C	2.05423200	4.29724100	1.62013600
H	1.57122800	2.29779000	2.23714100
C	3.13890000	4.51230100	-0.52330300
H	3.51054200	2.68099400	-1.58683000
C	5.07369500	-0.52043300	-3.53096500
H	3.22450200	-0.84165500	-4.59435100
H	6.73888600	-0.15986800	-2.20546500
C	4.53055500	-1.34301100	3.77147300
H	5.61365300	0.52058600	3.88729900
H	3.29256100	-3.07143500	3.39885200
C	2.61992100	5.10428400	0.62805100
H	1.65118500	4.74602000	2.52455900
H	3.58614700	5.12886600	-1.29901300
H	5.70208700	-0.75648800	-4.38591100
H	5.04116700	-1.78661300	4.62253200
H	2.65676600	6.18291700	0.75522900
I	0.27499500	-3.12872900	-0.61341300

IRC of tetraphenylphosphonium C−P oxidative -Point12

0 1

P	-2.30455300	0.29701900	0.22552700
C	-3.65057300	-0.68843500	-0.55852500
C	-3.18407500	1.87770400	0.69416600
C	-3.32962600	-1.89096800	-1.20943900
C	-4.99572700	-0.28661100	-0.48713000
C	-1.94675000	-0.44687400	1.88341600
Pd	-0.08203100	-0.31265200	-0.27050700
C	-3.56335100	2.12933100	2.02295800
C	-3.60352000	2.78235900	-0.29925900
C	-4.33713200	-2.67605500	-1.77251600
H	-2.29704700	-2.22735500	-1.25437300
C	-5.99606100	-1.07527300	-1.05599200
H	-5.26974200	0.63468400	0.01299600
C	-1.07191600	0.22704200	2.75795400
C	-2.43972000	-1.70794000	2.24284100
C	-1.07163200	1.19886600	-1.35044200
C	-4.31086600	3.26256000	2.35395500
H	-3.28432600	1.43981000	2.80982600
C	-4.35903400	3.90711700	0.03247700
H	-3.35436800	2.60304600	-1.33893100
C	-5.67042000	-2.27063000	-1.69997500
H	-4.07010500	-3.60659300	-2.26543500
H	-7.03197000	-0.75321100	-0.99177800
C	-0.71224100	-0.34869300	3.97485600
H	-0.68449900	1.20613700	2.49235100
C	-2.07602900	-2.27683600	3.46294700
H	-3.08998900	-2.25346200	1.56839900
C	-0.61529400	2.51658900	-1.17820100
C	-1.38728700	0.73266000	-2.63952600
C	-4.70866500	4.15691300	1.36174400
H	-4.58459200	3.43663100	3.39105700
H	-4.67409600	4.58918000	-0.75252400
H	-6.45299500	-2.88251800	-2.14089200
C	-1.21358400	-1.60315500	4.32932000
H	-0.03518200	0.17885700	4.64098800
H	-2.46341500	-3.25565800	3.73121600

C	-0.37383000	3.31801200	-2.29194900
H	-0.41401400	2.90154500	-0.18458600
C	-1.15582200	1.54954300	-3.74948300
H	-1.78319400	-0.26781600	-2.77624500
H	-5.29227400	5.03699100	1.61813300
H	-0.92886700	-2.05537900	5.27523400
C	-0.63274500	2.83269600	-3.57829500
H	0.03046000	4.31708500	-2.15410100
H	-1.37809200	1.17671400	-4.74598600
H	-0.44113900	3.46112600	-4.44395800
P	2.32178500	0.47335000	0.08684000
C	3.45302200	0.07643100	-1.31842200
C	3.20833000	-0.19587400	1.56932200
C	2.53184200	2.30225100	0.29935600
C	2.87759500	-0.27401400	-2.54848500
C	4.85239400	0.11107400	-1.20599500
C	4.19684300	0.52243600	2.26447600
C	2.88830400	-1.49519000	1.99544300
C	2.00617900	2.91272200	1.45354500
C	3.09614300	3.12337900	-0.68742600
C	3.68485000	-0.56540700	-3.65033700
H	1.79692300	-0.33760800	-2.63489000
C	5.65679200	-0.18485400	-2.30615400
H	5.31574400	0.35813500	-0.25542700
C	4.85103100	-0.04773700	3.35809400
H	4.45344100	1.53212800	1.95875200
C	3.54990200	-2.06321100	3.08601500
H	2.12700300	-2.06494200	1.46912300
C	2.05434600	4.29617200	1.62010200
H	1.57038400	2.29673100	2.23649200
C	3.13880100	4.51148800	-0.52345000
H	3.50899100	2.68046300	-1.58788800
C	5.07406700	-0.52061200	-3.53132300
H	3.22525600	-0.84223300	-4.59527000
H	6.73882000	-0.15958600	-2.20539100
C	4.53003800	-1.34276800	3.77071200
H	5.61275500	0.52113500	3.88554800

H	3.29237600	-3.07157300	3.39887100
C	2.62021400	5.10325200	0.62817500
H	1.65148200	4.74483800	2.52464500
H	3.58595600	5.12811500	-1.29913500
H	5.70275400	-0.75643900	-4.38610400
H	5.04102400	-1.78601700	4.62172100
H	2.65739600	6.18183500	0.75564400
I	0.27586900	-3.12805200	-0.61232100

IRC of tetraphenylphosphonium C−P oxidative -Point13

0 1

P	-2.30662200	0.28689400	0.23739400
C	-3.65269400	-0.69158600	-0.55344400
C	-3.17995600	1.87411800	0.69465900
C	-3.33091700	-1.89197900	-1.20777100
C	-4.99755100	-0.28852800	-0.48413800
C	-1.95632400	-0.45271900	1.89431800
Pd	-0.08651000	-0.30915900	-0.27084900
C	-3.56111900	2.12913400	2.02259700
C	-3.59681700	2.77739300	-0.30110700
C	-4.33783300	-2.67575800	-1.77361500
H	-2.29818800	-2.22781700	-1.25276500
C	-5.99722300	-1.07543300	-1.05636500
H	-5.27157800	0.63196900	0.01754200
C	-1.07755500	0.22159000	2.76472500
C	-2.44670900	-1.71386500	2.25413700
C	-1.03194200	1.20093800	-1.36400300
C	-4.30892400	3.26293800	2.35055000
H	-3.28425200	1.44090600	2.81131200
C	-4.35277100	3.90305100	0.02795200
H	-3.34572200	2.59616200	-1.34003400
C	-5.67105300	-2.27000500	-1.70169500
H	-4.07059400	-3.60519200	-2.26851500
H	-7.03310700	-0.75300000	-0.99352200
C	-0.71345800	-0.35355600	3.98018600
H	-0.69035800	1.20008000	2.49640600
C	-2.07735600	-2.28318800	3.47231700

H	-3.09921400	-2.25904400	1.58142300
C	-0.59655500	2.52362600	-1.18944900
C	-1.36923600	0.73694100	-2.64740500
C	-4.70517600	4.15540700	1.35605200
H	-4.58449000	3.43848000	3.38692700
H	-4.66611000	4.58390100	-0.75880300
H	-6.45330300	-2.88076800	-2.14476300
C	-1.21287900	-1.60862400	4.33576500
H	-0.03437700	0.17404000	4.64423100
H	-2.46218800	-3.26270700	3.74173200
C	-0.37928300	3.33196000	-2.30388200
H	-0.38538800	2.90561100	-0.19667600
C	-1.16070600	1.55998800	-3.75782500
H	-1.75554500	-0.26802200	-2.78116700
H	-5.28947400	5.03585900	1.60960500
H	-0.92448200	-2.06095600	5.28053300
C	-0.64582100	2.84680500	-3.58860100
H	0.01390900	4.33601100	-2.16818800
H	-1.39296300	1.18910800	-4.75294300
H	-0.46903100	3.47933900	-4.45471700
P	2.32124100	0.47269000	0.08538000
C	3.45266700	0.07576500	-1.31930200
C	3.20668600	-0.19658600	1.56867700
C	2.53076100	2.30157700	0.29861500
C	2.87760800	-0.27482100	-2.54945700
C	4.85200000	0.11089000	-1.20635300
C	4.19529300	0.52223100	2.26340100
C	2.88735200	-1.49590400	1.99515200
C	2.00566800	2.91172500	1.45318900
C	3.09533700	3.12267900	-0.68798800
C	3.68526100	-0.56592200	-3.65105800
H	1.79706100	-0.33862800	-2.63654100
C	5.65674400	-0.18484100	-2.30628700
H	5.31500600	0.35809500	-0.25566700
C	4.85007000	-0.04753800	3.35687600
H	4.45154800	1.53191000	1.95743100
C	3.54939800	-2.06337900	3.08577400

H	2.12640200	-2.06634300	1.46910800
C	2.05444900	4.29514600	1.62012200
H	1.56951700	2.29571500	2.23590900
C	3.13873700	4.51068800	-0.52352400
H	3.50746900	2.67993500	-1.58885200
C	5.07441300	-0.52074200	-3.53161100
H	3.22598700	-0.84271900	-4.59613700
H	6.73872900	-0.15929500	-2.20523800
C	4.52953200	-1.34253600	3.76999000
H	5.61184400	0.52168900	3.88385200
H	3.29223000	-3.07173600	3.39890400
C	2.62051300	5.10224900	0.62835200
H	1.65174800	4.74370800	2.52477100
H	3.58581000	5.12736500	-1.29918700
H	5.70339500	-0.75633900	-4.38622800
H	5.04090500	-1.78543800	4.62093700
H	2.65802500	6.18078400	0.75609700
I	0.27667600	-3.12743800	-0.61130300

IRC of tetraphenylphosphonium C−P oxidative -Point14

0 1

P	-2.30982400	0.27694800	0.24929300
C	-3.65530800	-0.69506400	-0.54804500
C	-3.17665800	1.87038300	0.69558700
C	-3.33248700	-1.89318500	-1.20590800
C	-4.99980600	-0.29072300	-0.48107300
C	-1.96538400	-0.45855000	1.90491300
Pd	-0.09068200	-0.30552100	-0.27134500
C	-3.55942000	2.12899000	2.02260200
C	-3.59051100	2.77238700	-0.30263300
C	-4.33869300	-2.67556600	-1.77477000
H	-2.29963500	-2.22854000	-1.25079400
C	-5.99868900	-1.07577000	-1.05692900
H	-5.27390300	0.62892900	0.02220500
C	-1.08296200	0.21632400	2.77124300
C	-2.45336700	-1.71971300	2.26523900
C	-0.99161100	1.20355900	-1.37866600

C	-4.30727100	3.26351200	2.34741500
H	-3.28476900	1.44206300	2.81318700
C	-4.34664100	3.89911100	0.02364900
H	-3.33736800	2.58922100	-1.34079300
C	-5.67185800	-2.26950100	-1.70360800
H	-4.07115800	-3.60384100	-2.27169200
H	-7.03455700	-0.75297100	-0.99563500
C	-0.71454400	-0.35818600	3.98530400
H	-0.69609100	1.19423000	2.50017100
C	-2.07847700	-2.28935500	3.48151800
H	-3.10801800	-2.26462400	1.59426300
C	-0.57699000	2.53034700	-1.20099700
C	-1.35019100	0.74112800	-2.65557600
C	-4.70183700	4.15405500	1.35055400
H	-4.58465100	3.44069200	3.38303700
H	-4.65804900	4.57884100	-0.76484600
H	-6.45370300	-2.87912600	-2.14896400
C	-1.21198900	-1.61386700	4.34201400
H	-0.03353100	0.16953000	4.64727100
H	-2.46075500	-3.26955300	3.75207000
C	-0.38428500	3.34523700	-2.31543400
H	-0.35597700	2.90987600	-0.20951000
C	-1.16482600	1.56994400	-3.76575900
H	-1.72707400	-0.26787500	-2.78694500
H	-5.28670400	5.03495400	1.60123300
H	-0.91992300	-2.06625200	5.28563300
C	-0.65862300	2.86051100	-3.59841900
H	-0.00249600	4.35396400	-2.18127000
H	-1.40715500	1.20069000	-4.75913000
H	-0.49685300	3.49696000	-4.46461600
P	2.32068100	0.47201900	0.08397500
C	3.45225100	0.07508300	-1.32015500
C	3.20500000	-0.19731400	1.56807900
C	2.52967000	2.30090100	0.29792500
C	2.87755100	-0.27560800	-2.55039700
C	4.85155200	0.11070400	-1.20666000
C	4.19370800	0.52203200	2.26234800

C	2.88638800	-1.49664000	1.99489000
C	2.00516000	2.91073700	1.45287900
C	3.09454900	3.12195000	-0.68851000
C	3.68562700	-0.56639800	-3.65174400
H	1.79710700	-0.33956800	-2.63806500
C	5.65664900	-0.18481100	-2.30637000
H	5.31421400	0.35804400	-0.25585100
C	4.84909800	-0.04733300	3.35566700
H	4.44960300	1.53170300	1.95613600
C	3.54891100	-2.06356000	3.08554600
H	2.12577200	-2.06775200	1.46913100
C	2.05455600	4.29412900	1.62016300
H	1.56857000	2.29472200	2.23533500
C	3.13872100	4.50986100	-0.52356300
H	3.50592500	2.67937200	-1.58978800
C	5.07471500	-0.52084500	-3.53185500
H	3.22668300	-0.84314000	-4.59698000
H	6.73859000	-0.15898300	-2.20502500
C	4.52903500	-1.34230200	3.76927300
H	5.61092000	0.52225900	3.88215700
H	3.29212300	-3.07191800	3.39894700
C	2.62083200	5.10124000	0.62854100
H	1.65198900	4.74260600	2.52489500
H	3.58570100	5.12657600	-1.29921800
H	5.70399500	-0.75620400	-4.38630800
H	5.04080700	-1.78485100	4.62015300
H	2.65865800	6.17972900	0.75653900
I	0.27742400	-3.12686200	-0.61033600

IRC of tetraphenylphosphonium C–P oxidative -Point15

0 1

P	-2.31350400	0.26723800	0.26100400
C	-3.65826300	-0.69876900	-0.54242500
C	-3.17390200	1.86652400	0.69682900
C	-3.33430100	-1.89456700	-1.20385000
C	-5.00238800	-0.29313500	-0.47793200
C	-1.97412200	-0.46437000	1.91535100

Pd	-0.09465100	-0.30171600	-0.27198500
C	-3.55813500	2.12884500	2.02287000
C	-3.58443300	2.76732800	-0.30390800
C	-4.33970900	-2.67546800	-1.77595100
H	-2.30135000	-2.22950200	-1.24848900
C	-6.00040100	-1.07625100	-1.05762300
H	-5.27660600	0.62568100	0.02689000
C	-1.08822300	0.21115200	2.77765300
C	-2.45978800	-1.72554700	2.27624600
C	-0.95110400	1.20605900	-1.39340100
C	-4.30581800	3.26422300	2.34447100
H	-3.28579600	1.44318700	2.81532900
C	-4.34055300	3.89524600	0.01950000
H	-3.32918300	2.58221200	-1.34128100
C	-5.67282700	-2.26909100	-1.70568900
H	-4.07180900	-3.60256200	-2.27488400
H	-7.03625600	-0.75308200	-0.99800400
C	-0.71554900	-0.36269800	3.99035100
H	-0.70169400	1.18847700	2.50380000
C	-2.07946700	-2.29543600	3.49066900
H	-3.11639200	-2.27025600	1.60689900
C	-0.55681100	2.53679900	-1.21266800
C	-1.33029600	0.74510000	-2.66385700
C	-4.69855500	4.15282200	1.34518800
H	-4.58500700	3.44315800	3.37931800
H	-4.64994500	4.57393700	-0.77068900
H	-6.45420700	-2.87756800	-2.15343000
C	-1.21099200	-1.61898500	4.34821600
H	-0.03265100	0.16522100	4.65021100
H	-2.45919000	-3.27631000	3.76229300
C	-0.38909600	3.35817000	-2.32674300
H	-0.32613500	2.91421300	-0.22266300
C	-1.16860700	1.57966000	-3.77344300
H	-1.69794600	-0.26772900	-2.79309400
H	-5.28389600	5.03422500	1.59299900
H	-0.91528500	-2.07135400	5.29069800
C	-0.67152200	2.87408100	-3.60793600

H	-0.01876300	4.37136300	-2.19365100
H	-1.42106500	1.21178400	-4.76484400
H	-0.52517600	3.51444600	-4.47399600
P	2.32007400	0.47133100	0.08260800
C	3.45179100	0.07437700	-1.32097500
C	3.20326600	-0.19806000	1.56750600
C	2.52859000	2.30020600	0.29727400
C	2.87745700	-0.27640400	-2.55130200
C	4.85106100	0.11050800	-1.20692100
C	4.19207900	0.52182400	2.26131000
C	2.88539300	-1.49739900	1.99464800
C	2.00465600	2.90974100	1.45260000
C	3.09379000	3.12119200	-0.68899700
C	3.68595900	-0.56685700	-3.65240200
H	1.79711200	-0.34052100	-2.63945300
C	5.65651500	-0.18477200	-2.30641100
H	5.31338000	0.35797500	-0.25598900
C	4.84809900	-0.04713300	3.35446300
H	4.44761400	1.53148900	1.95486700
C	3.54841600	-2.06376200	3.08532300
H	2.12509600	-2.06916700	1.46917700
C	2.05467000	4.29310300	1.62022500
H	1.56757600	2.29372700	2.23476600
C	3.13873800	4.50900500	-0.52357100
H	3.50441500	2.67877400	-1.59068200
C	5.07498300	-0.52092500	-3.53206400
H	3.22734300	-0.84352700	-4.59779700
H	6.73841200	-0.15866000	-2.20476500
C	4.52852900	-1.34207800	3.76855800
H	5.60996600	0.52282400	3.88047200
H	3.29202900	-3.07212500	3.39899500
C	2.62116900	5.10021200	0.62874800
H	1.65221500	4.74151100	2.52502200
H	3.58563300	5.12575600	-1.29921600
H	5.70456300	-0.75603300	-4.38635400
H	5.04071000	-1.78427400	4.61936600
H	2.65929400	6.17865900	0.75698300

I	0.27814000	-3.12629000	-0.60937300

IRC of tetraphenylphosphonium C−P oxidative -Point16

0 1

P	-2.31740900	0.25783200	0.27231800
C	-3.66149000	-0.70271200	-0.53658000
C	-3.17153200	1.86248600	0.69840500
C	-3.33635800	-1.89615700	-1.20158000
C	-5.00524900	-0.29580300	-0.47460300
C	-1.98258700	-0.47028700	1.92570400
Pd	-0.09840700	-0.29776200	-0.27268400
C	-3.55719500	2.12868300	2.02339800
C	-3.57840600	2.76209500	-0.30495900
C	-4.34090700	-2.67545100	-1.77717800
H	-2.30333700	-2.23074700	-1.24586200
C	-6.00233900	-1.07687200	-1.05838100
H	-5.27963600	0.62212400	0.03184100
C	-1.09341900	0.20590500	2.78412500
C	-2.46610900	-1.73146400	2.28735500
C	-0.91148000	1.20893200	-1.40829900
C	-4.30451400	3.26509000	2.34160100
H	-3.28725600	1.44433500	2.81779900
C	-4.33433400	3.89134700	0.01534700
H	-3.32083000	2.57491300	-1.34146400
C	-5.67396900	-2.26872200	-1.70797800
H	-4.07258500	-3.60129500	-2.27821300
H	-7.03817200	-0.75329300	-1.00054200
C	-0.71651500	-0.36726700	3.99549700
H	-0.70728500	1.18267300	2.50755400
C	-2.08042700	-2.30153500	3.49997800
H	-3.12471600	-2.27605400	1.61975400
C	-0.53599500	2.54304000	-1.22467200
C	-1.30951200	0.74906100	-2.67242300
C	-4.69521500	4.15168200	1.33975900
H	-4.58552600	3.44600600	3.37562100
H	-4.64145800	4.56899900	-0.77663000
H	-6.45483200	-2.87593500	-2.15834400

C	-1.20989600	-1.62415600	4.35454500
H	-0.03175400	0.16088300	4.65323700
H	-2.45766200	-3.28304400	3.77272500
C	-0.39353400	3.37078100	-2.33795000
H	-0.29571700	2.91883900	-0.23641100
C	-1.17189600	1.58921400	-3.78099100
H	-1.66806800	-0.26736400	-2.79991800
H	-5.28089800	5.03370900	1.58455700
H	-0.91049800	-2.07652300	5.29586300
C	-0.68481700	2.88776900	-3.61728000
H	-0.03479000	4.38829100	-2.20555400
H	-1.43467400	1.22259000	-4.77021900
H	-0.55495700	3.53231000	-4.48296000
P	2.31940200	0.47061100	0.08125800
C	3.45127500	0.07363000	-1.32178400
C	3.20145900	-0.19884200	1.56693500
C	2.52751500	2.29947100	0.29664000
C	2.87733000	-0.27723500	-2.55220000
C	4.85051300	0.11030000	-1.20715500
C	4.19037000	0.52160200	2.26025000
C	2.88434300	-1.49819600	1.99441200
C	2.00414500	2.90870300	1.45233200
C	3.09304700	3.12038800	-0.68946900
C	3.68626700	-0.56731700	-3.65305600
H	1.79708700	-0.34151500	-2.64076000
C	5.65633800	-0.18471500	-2.30642400
H	5.31247700	0.35789400	-0.25609500
C	4.84705000	-0.04692800	3.35322400
H	4.44552000	1.53126100	1.95355800
C	3.54790000	-2.06398200	3.08509600
H	2.12434500	-2.07061300	1.46924800
C	2.05479100	4.29203100	1.62030800
H	1.56650500	2.29268000	2.23415900
C	3.13876800	4.50810100	-0.52356200
H	3.50288900	2.67812800	-1.59157200
C	5.07522700	-0.52098100	-3.53225800
H	3.22799700	-0.84391600	-4.59862100

H	6.73818800	-0.15829600	-2.20446600
C	4.52800600	-1.34185300	3.76781500
H	5.60896300	0.52341200	3.87873000
H	3.29194000	-3.07235500	3.39905000
C	2.62152600	5.09913600	0.62897800
H	1.65244200	4.74037000	2.52516900
H	3.58557200	5.12489000	-1.29919800
H	5.70512200	-0.75581300	-4.38638100
H	5.04062200	-1.78368500	4.61854000
H	2.65996600	6.17754000	0.75745500
I	0.27883400	-3.12569800	-0.60838900

IRC of tetraphenylphosphonium C–P oxidative -Point17

0 1

P	-2.32142300	0.24870400	0.28321800
C	-3.66494400	-0.70688700	-0.53054900
C	-3.16949600	1.85826900	0.70026500
C	-3.33865100	-1.89797800	-1.19910500
C	-5.00835000	-0.29872500	-0.47107700
C	-1.99074300	-0.47629500	1.93592300
Pd	-0.10194200	-0.29361800	-0.27346000
C	-3.55658600	2.12848300	2.02414000
C	-3.57236200	2.75667800	-0.30583100
C	-4.34229600	-2.67551200	-1.77845500
H	-2.30558800	-2.23231700	-1.24292000
C	-6.00448000	-1.07761700	-1.05917300
H	-5.28294300	0.61826800	0.03704400
C	-1.09853700	0.20055400	2.79067800
C	-2.47232900	-1.73744300	2.29854400
C	-0.87266600	1.21180800	-1.42295500
C	-4.30333100	3.26610600	2.33874600
H	-3.28916100	1.44547200	2.82053900
C	-4.32791500	3.88740200	0.01113800
H	-3.31226900	2.56734600	-1.34139400
C	-5.67528700	-2.26836500	-1.71048000
H	-4.07351200	-3.60004600	-2.28166500
H	-7.04027700	-0.75358100	-1.00318700

C	-0.71747200	-0.37194200	4.00077300
H	-0.71279500	1.17678600	2.51149800
C	-2.08142300	-2.30764300	3.50944300
H	-3.13294400	-2.28198300	1.63277300
C	-0.51470400	2.54920700	-1.23697200
C	-1.28797700	0.75297900	-2.68129300
C	-4.69176000	4.15063200	1.33420700
H	-4.58619100	3.44923000	3.37188300
H	-4.63253900	4.56401000	-0.78270300
H	-6.45558900	-2.87417800	-2.16370600
C	-1.20876200	-1.62941400	4.36102900
H	-0.03088100	0.15647900	4.65638300
H	-2.45629800	-3.28972900	3.78332800
C	-0.39771700	3.38318400	-2.34906100
H	-0.26482500	2.92377000	-0.25067600
C	-1.17487300	1.59867000	-3.78845400
H	-1.63742600	-0.26690600	-2.80740000
H	-5.27764600	5.03339900	1.57585100
H	-0.90568400	-2.08178400	5.30116600
C	-0.69856900	2.90152200	-3.62639100
H	-0.05054000	4.40479800	-2.21705100
H	-1.44797300	1.23313000	-4.77531600
H	-0.58594500	3.55027800	-4.49133800
P	2.31863000	0.46985000	0.07990600
C	3.45069800	0.07283100	-1.32258900
C	3.19956600	-0.19966500	1.56635000
C	2.52646300	2.29867800	0.29601700
C	2.87717500	-0.27811000	-2.55310600
C	4.84990300	0.11006600	-1.20736500
C	4.18857200	0.52135700	2.25915600
C	2.88322200	-1.49903400	1.99417900
C	2.00362800	2.90761100	1.45206200
C	3.09233600	3.11952700	-0.68992600
C	3.68656300	-0.56779600	-3.65371500
H	1.79703500	-0.34252500	-2.64203400
C	5.65611900	-0.18464900	-2.30641000
H	5.31149700	0.35778700	-0.25617000

C	4.84594000	-0.04672400	3.35194300
H	4.44332000	1.53100700	1.95219700
C	3.54734800	-2.06422600	3.08485800
H	2.12350400	-2.07209500	1.46933800
C	2.05492400	4.29089700	1.62040800
H	1.56535600	2.29156400	2.23349500
C	3.13880800	4.50714000	-0.52354000
H	3.50139200	2.67742000	-1.59244500
C	5.07545500	-0.52102600	-3.53243800
H	3.22865900	-0.84432100	-4.59946000
H	6.73792100	-0.15789500	-2.20412600
C	4.52745100	-1.34163100	3.76703800
H	5.60789900	0.52401600	3.87692700
H	3.29184200	-3.07261000	3.39910900
C	2.62190500	5.09800000	0.62922900
H	1.65267600	4.73916600	2.52533000
H	3.58552100	5.12397200	-1.29916600
H	5.70568500	-0.75555300	-4.38638800
H	5.04052900	-1.78308700	4.61767200
H	2.66067300	6.17635800	0.75795400
I	0.27951000	-3.12507200	-0.60736600

IRC of tetraphenylphosphonium C−P oxidative -Point18

0 1

P	-2.32545900	0.23985100	0.29364500
C	-3.66859300	-0.71131300	-0.52432700
C	-3.16775000	1.85384700	0.70241900
C	-3.34117600	-1.90005100	-1.19642800
C	-5.01166100	-0.30192100	-0.46731100
C	-1.99856400	-0.48243600	1.94602600
Pd	-0.10524500	-0.28929000	-0.27426600
C	-3.55630200	2.12823300	2.02508900
C	-3.56624800	2.75103700	-0.30653000
C	-4.34388800	-2.67565100	-1.77979100
H	-2.30809800	-2.23422100	-1.23969300
C	-6.00681100	-1.07848300	-1.05996400
H	-5.28649000	0.61407400	0.04258300

C	-1.10356300	0.19504100	2.79735900
C	-2.47845900	-1.74350900	2.30983900
C	-0.83519700	1.21512900	-1.43763600
C	-4.30225600	3.26727700	2.33586000
H	-3.29153100	1.44659500	2.82356200
C	-4.32122800	3.88338500	0.00682200
H	-3.30346300	2.55945100	-1.34107400
C	-5.67678600	-2.26799600	-1.71320800
H	-4.07461600	-3.59880500	-2.28528000
H	-7.04255200	-0.75392900	-1.00589000
C	-0.71843700	-0.37678400	4.00623800
H	-0.71822700	1.17077100	2.51570500
C	-2.08251400	-2.31378100	3.51911000
H	-3.14112100	-2.28806200	1.64600100
C	-0.49291100	2.55525200	-1.24963500
C	-1.26563900	0.75692200	-2.69054600
C	-4.68813400	4.14967600	1.32846700
H	-4.58701600	3.45285800	3.36804600
H	-4.62307400	4.55893100	-0.78899300
H	-6.45649000	-2.87223800	-2.16956800
C	-1.20763100	-1.63480900	4.36772000
H	-0.03005000	0.15193200	4.65972200
H	-2.45519900	-3.29637000	3.79417000
C	-0.40154200	3.39531800	-2.36008300
H	-0.23353200	2.92902000	-0.26554600
C	-1.17737800	1.60798300	-3.79584200
H	-1.60598800	-0.26624700	-2.81572500
H	-5.27406000	5.03332500	1.56678600
H	-0.90088300	-2.08720600	5.30665700
C	-0.71287300	2.91539500	-3.63526100
H	-0.06605100	4.42090800	-2.22816200
H	-1.46082900	1.24337900	-4.78016700
H	-0.61884400	3.56869700	-4.49917100
P	2.31775200	0.46903900	0.07854000
C	3.45004400	0.07196800	-1.32340600
C	3.19756700	-0.20054000	1.56574000
C	2.52542600	2.29781500	0.29539800

C	2.87698300	-0.27903600	-2.55404600
C	4.84921400	0.10979800	-1.20755800
C	4.18666300	0.52108200	2.25800800
C	2.88201300	-1.49992200	1.99394200
C	2.00309800	2.90644500	1.45178400
C	3.09165600	3.11859800	-0.69037100
C	3.68685300	-0.56830000	-3.65439200
H	1.79694500	-0.34353100	-2.64335300
C	5.65585200	-0.18457000	-2.30636900
H	5.31041300	0.35764400	-0.25621600
C	4.84475400	-0.04651800	3.35060000
H	4.44098500	1.53072300	1.95076100
C	3.54675100	-2.06449400	3.08460400
H	2.12255600	-2.07362400	1.46944900
C	2.05506500	4.28968300	1.62052400
H	1.56412000	2.29036100	2.23276800
C	3.13885200	4.50610900	-0.52350800
H	3.49993300	2.67664200	-1.59329800
C	5.07567300	-0.52106100	-3.53260800
H	3.22934400	-0.84474700	-4.60033500
H	6.73760400	-0.15744400	-2.20373700
C	4.52685600	-1.34141000	3.76621400
H	5.60675700	0.52464600	3.87503700
H	3.29172500	-3.07289200	3.39917100
C	2.62230200	5.09678600	0.62950000
H	1.65291600	4.73787500	2.52550900
H	3.58547300	5.12299000	-1.29911900
H	5.70626500	-0.75525000	-4.38637600
H	5.04042700	-1.78247400	4.61674400
H	2.66141100	6.17509600	0.75848500
I	0.28017000	-3.12439400	-0.60629000

IRC of triphenylphosphonin C−P oxidative -Point1

0 1

P	0.53178400	2.42447200	0.47713100
C	-0.60132300	3.90049200	0.49512500
C	2.16706500	3.13733600	0.99230100

Pd	0.01420100	0.13904400	-0.05514400
C	-1.95435500	3.68110400	0.18780600
C	-0.17272900	5.22018500	0.70630400
C	2.87113700	4.03193300	0.16663200
C	2.77986500	2.69547000	2.17293400
C	0.84388800	2.27726500	-1.36961600
C	-2.83346400	4.75100200	0.01051800
H	-2.31803000	2.66629400	0.05833300
C	-1.05724200	6.28921900	0.55168000
H	0.85803700	5.42297400	0.97585300
C	4.16248900	4.44122700	0.48839700
H	2.41759500	4.38643300	-0.75283800
C	4.07240200	3.11589000	2.50614000
H	2.25338800	1.99859000	2.82098400
C	2.11302200	1.88440500	-1.83963000
C	-0.14810400	2.58223000	-2.31579800
C	-2.38369500	6.06135500	0.18052700
H	-3.86774700	4.55292500	-0.25795300
H	-0.70227500	7.30476600	0.70959400
C	4.77059100	3.97645600	1.65728400
H	4.69601900	5.11779100	-0.17427900
H	4.53652700	2.75912900	3.42202900
C	2.40556500	1.89968000	-3.20056500
H	2.88963400	1.60358200	-1.13881100
C	0.14426400	2.58034400	-3.67997300
H	-1.14082200	2.87048700	-1.99313800
C	1.42831300	2.27064300	-4.12758700
H	3.40283600	1.62353000	-3.53497500
H	-0.63299500	2.84781200	-4.39281400
P	1.71930200	-1.59055500	-0.02934700
C	1.35642600	-2.96879900	-1.22147500
C	1.84988300	-2.44086500	1.61927900
C	3.52327100	-1.28058800	-0.37726900
C	0.82826700	-2.59938200	-2.46977100
C	1.57543000	-4.33012200	-0.96261400
C	2.93368700	-3.25844700	1.98387500
C	0.82354000	-2.23516300	2.55438000

C	4.18227800	-0.31083500	0.39858600
C	4.24965400	-1.93499200	-1.38305700
C	0.54590200	-3.56149800	-3.43991200
H	0.62778300	-1.54968200	-2.67089600
C	1.27599900	-5.29521200	-1.92784700
H	1.97289700	-4.64485000	-0.00283100
C	2.97321400	-3.87171100	3.23739000
H	3.75709500	-3.40609900	1.29091000
C	0.86109100	-2.85059100	3.80786900
H	0.00168400	-1.57185700	2.29887400
C	5.52689600	-0.01232800	0.18387400
H	3.63723400	0.22312800	1.17192900
C	5.59720200	-1.63091600	-1.60257900
H	3.76823800	-2.68724700	-1.99908200
C	0.76530800	-4.91413600	-3.16966700
H	0.14147200	-3.25525300	-4.40121700
C	1.93472900	-3.67324600	4.15099900
H	3.81946300	-4.50063300	3.50251800
H	0.05473500	-2.67608900	4.51544300
C	6.24093700	-0.67227400	-0.82072800
H	6.01075400	0.74526400	0.79474400
H	6.14179100	-2.15013700	-2.38747500
H	0.53340900	-5.66607400	-3.91948900
H	1.96938700	-4.14912500	5.12769600
H	7.28785300	-0.43677500	-0.99372900
H	1.44494300	-6.34642800	-1.70715900
H	-3.06403700	6.89739400	0.04047500
H	5.78168500	4.28743100	1.90723800
H	1.66173000	2.29389500	-5.19450500
C	-3.58379700	0.38825900	-0.79306500
C	-3.36677400	0.66391200	-2.15533700
C	-4.74005400	0.89991800	-0.18440900
C	-4.28966000	1.40600500	-2.89138200
H	-2.46343400	0.29975600	-2.63837300
C	-5.65447000	1.66262200	-0.91804500
H	-4.93284300	0.70451000	0.86537600
C	-5.43677900	1.91253500	-2.27332100

H	-4.10796900	1.59852900	-3.94571400
H	-6.54256100	2.05275400	-0.42697900
H	-6.15157600	2.49954400	-2.84403000
C	-2.74824100	-2.33464400	-0.43511700
C	-3.83777700	-2.63280500	-1.26768300
C	-1.95809300	-3.39717400	0.03451800
C	-4.12445700	-3.95419300	-1.62298500
H	-4.47126800	-1.83604500	-1.64246100
C	-2.25145100	-4.71553700	-0.30988600
H	-1.10546300	-3.19382800	0.67471200
C	-3.33479600	-4.99940300	-1.14503000
H	-4.97171500	-4.16203600	-2.27196700
H	-1.62301300	-5.51942900	0.06326300
H	-3.55853300	-6.02639100	-1.42199100
P	-2.29006900	-0.60821600	0.09586400
C	-2.93196900	-0.61843900	1.84581200
C	-2.37604000	0.27630500	2.77437900
C	-3.95576100	-1.48022400	2.27611000
C	-2.83699400	0.31572800	4.09301300
H	-1.57196000	0.93543900	2.45741600
C	-4.41212200	-1.44410100	3.59510100
H	-4.39703800	-2.18577200	1.57906900
C	-3.85479500	-0.54528000	4.50755600
H	-2.39431500	1.01657900	4.79626100
H	-5.20308100	-2.12062700	3.90909000
H	-4.20925900	-0.51907600	5.53482200

IRC of triphenylphosphonin C–P oxidative -Point2

0 1

P	0.52699600	2.42040400	0.49028700
C	-0.60241300	3.89859400	0.49562900
C	2.16392600	3.13268500	0.99700300
Pd	0.01874400	0.14899300	-0.06311700
C	-1.95464500	3.68068400	0.18324300
C	-0.17288600	5.21775600	0.70742700
C	2.86396900	4.02372400	0.16434000
C	2.78193100	2.69489600	2.17655100

C	0.83834300	2.25794400	-1.35845700
C	-2.83156800	4.75148400	0.00136200
H	-2.31940600	2.66608100	0.05492700
C	-1.05553400	6.28776500	0.54872000
H	0.85710000	5.41933700	0.98104200
C	4.15679200	4.43406200	0.47807700
H	2.40563900	4.37497700	-0.75404400
C	4.07615000	3.11673400	2.50188600
H	2.25816800	2.00084400	2.83001600
C	2.11075800	1.87435500	-1.83134000
C	-0.15333700	2.56227000	-2.30642400
C	-2.38080100	6.06139400	0.17244300
H	-3.86507600	4.55461100	-0.27114600
H	-0.69987700	7.30294000	0.70747900
C	4.77019200	3.97399200	1.64612700
H	4.68733200	5.10778700	-0.19006200
H	4.54481400	2.76389900	3.41707500
C	2.40743200	1.90737400	-3.19191700
H	2.88774600	1.59280600	-1.13110300
C	0.14361900	2.57919700	-3.67027200
H	-1.14883900	2.84167800	-1.98346600
C	1.43185200	2.28583900	-4.11793600
H	3.40780800	1.64258600	-3.52565000
H	-0.63332700	2.85063500	-4.38108200
P	1.72010200	-1.59121400	-0.02958900
C	1.35652700	-2.96955700	-1.22155500
C	1.84994000	-2.44176300	1.61914600
C	3.52422100	-1.28202300	-0.37680700
C	0.82887000	-2.59979000	-2.46995300
C	1.57483200	-4.33105000	-0.96275600
C	2.93353100	-3.25946600	1.98437000
C	0.82343100	-2.23554500	2.55389700
C	4.18295700	-0.31214700	0.39914800
C	4.25075100	-1.93616400	-1.38265500
C	0.54615300	-3.56171300	-3.44021900
H	0.62912600	-1.54991200	-2.67094000
C	1.27518900	-5.29589900	-1.92817300

H	1.97190800	-4.64605300	-0.00289500
C	2.97278800	-3.87201100	3.23825800
H	3.75707100	-3.40760300	1.29166800
C	0.86058700	-2.85047700	3.80767700
H	0.00189600	-1.57191500	2.29821100
C	5.52731300	-0.01278400	0.18403100
H	3.63784400	0.22141600	1.17273600
C	5.59811400	-1.63138700	-1.60240300
H	3.76955600	-2.68858400	-1.99866000
C	0.76485600	-4.91446300	-3.17005600
H	0.14209600	-3.25515800	-4.40158100
C	1.93412200	-3.67294800	4.15154900
H	3.81895200	-4.50081600	3.50393600
H	0.05408300	-2.67552000	4.51497000
C	6.24144000	-0.67224700	-0.82081900
H	6.01086700	0.74510500	0.79476500
H	6.14283800	-2.15032700	-2.38738900
H	0.53274600	-5.66622500	-3.91999000
H	1.96854700	-4.14820100	5.12855900
H	7.28813900	-0.43604600	-0.99418800
H	1.44362600	-6.34721400	-1.70757300
H	-3.05949100	6.89824100	0.02908200
H	5.78254200	4.28604300	1.88993600
H	1.67060400	2.33583500	-5.17798300
C	-3.58521900	0.38759300	-0.79177600
C	-3.36829800	0.66157500	-2.15441900
C	-4.74099000	0.90069200	-0.18344200
C	-4.29050000	1.40388900	-2.89103900
H	-2.46534400	0.29619100	-2.63724900
C	-5.65478200	1.66358800	-0.91773400
H	-4.93376600	0.70651700	0.86659000
C	-5.43697500	1.91219800	-2.27323300
H	-4.10877400	1.59516300	-3.94559000
H	-6.54241600	2.05507300	-0.42691000
H	-6.15122300	2.49950800	-2.84432000
C	-2.74897500	-2.33501900	-0.43376800
C	-3.83817800	-2.63325000	-1.26687100

C	-1.95877400	-3.39758500	0.03571600
C	-4.12423600	-3.95455200	-1.62299300
H	-4.47185200	-1.83657800	-1.64149200
C	-2.25139000	-4.71587800	-0.30974200
H	-1.10670500	-3.19450500	0.67675300
C	-3.33423500	-4.99973300	-1.14550800
H	-4.97124300	-4.16232700	-2.27231900
H	-1.62275700	-5.51970400	0.06321200
H	-3.55736200	-6.02664400	-1.42324400
P	-2.29101800	-0.60830400	0.09721200
C	-2.93326600	-0.61896700	1.84747400
C	-2.37764900	0.27577500	2.77617600
C	-3.95714700	-1.48089900	2.27769300
C	-2.83876900	0.31499100	4.09482400
H	-1.57345800	0.93496600	2.45951800
C	-4.41356200	-1.44500600	3.59671200
H	-4.39834400	-2.18645900	1.58061200
C	-3.85638600	-0.54622500	4.50933000
H	-2.39622000	1.01586300	4.79813200
H	-5.20443900	-2.12170300	3.91054500
H	-4.21086100	-0.52021000	5.53660100

IRC of triphenylphosphonin C−P oxidative -Point3

0 1

P	0.52205300	2.41618100	0.50357500
C	-0.60337200	3.89648600	0.49566400
C	2.16066600	3.12719600	1.00203200
Pd	0.02353000	0.15975500	-0.07055000
C	-1.95479600	3.68017500	0.17834600
C	-0.17304300	5.21518900	0.70836100
C	2.85640300	4.01463900	0.16239000
C	2.78401000	2.69387500	2.18053900
C	0.83351200	2.23724900	-1.34906300
C	-2.82968500	4.75184000	-0.00738600
H	-2.32068300	2.66585200	0.05090400
C	-1.05390500	6.28614100	0.54609300
H	0.85611000	5.41569100	0.98587600

C	4.15034400	4.42669600	0.46821200
H	2.39324400	4.36236200	-0.75484900
C	4.07965200	3.11756500	2.49795000
H	2.26323900	2.00276100	2.83949500
C	2.10868400	1.86313400	-1.82499600
C	-0.15776500	2.54189200	-2.29863600
C	-2.37805800	6.06130200	0.16511200
H	-3.86247700	4.55608100	-0.28338800
H	-0.69762500	7.30092800	0.70596100
C	4.76912900	3.97177200	1.63541300
H	4.67751000	5.09789400	-0.20512200
H	4.55283800	2.76894900	3.41244500
C	2.40901800	1.91473700	-3.18455800
H	2.88623600	1.57905400	-1.12644800
C	0.14340500	2.57895000	-3.66144000
H	-1.15584100	2.81241100	-1.97647900
C	1.43532800	2.30235700	-4.10896700
H	3.41187300	1.65960300	-3.51811600
H	-0.63342500	2.85479900	-4.37050500
P	1.72100700	-1.59206700	-0.02974900
C	1.35667000	-2.97037400	-1.22164900
C	1.85010000	-2.44282900	1.61904000
C	3.52518500	-1.28346400	-0.37636400
C	0.82950300	-2.60021900	-2.47013800
C	1.57428200	-4.33204100	-0.96294600
C	2.93351100	-3.26057300	1.98493600
C	0.82340200	-2.23606500	2.55341200
C	4.18357000	-0.31338400	0.39964700
C	4.25186900	-1.93731900	-1.38227800
C	0.54638000	-3.56194200	-3.44052600
H	0.63061400	-1.55015800	-2.67106100
C	1.27442900	-5.29662700	-1.92856300
H	1.97102300	-4.64732600	-0.00303300
C	2.97249200	-3.87233300	3.23922500
H	3.75721100	-3.40914700	1.29252000
C	0.86015900	-2.85043100	3.80750700
H	0.00213900	-1.57217200	2.29753300

C	5.52765400	-0.01312200	0.18413200
H	3.63828500	0.21991200	1.17331100
C	5.59903400	-1.63179400	-1.60224000
H	3.77090900	-2.68990400	-1.99827600
C	0.76440200	-4.91480900	-3.17047800
H	0.14266600	-3.25507000	-4.40192600
C	1.93361300	-3.67267300	4.15215900
H	3.81860400	-4.50095600	3.50549700
H	0.05350400	-2.67501400	4.51450800
C	6.24190600	-0.67213200	-0.82091500
H	6.01082500	0.74516900	0.79465700
H	6.14391500	-2.15043000	-2.38731300
H	0.53207900	-5.66638100	-3.92053700
H	1.96781800	-4.14726300	5.12949700
H	7.28838300	-0.43520400	-0.99463100
H	1.44243400	-6.34803900	-1.70809800
H	-3.05528200	6.89890900	0.01930600
H	5.78233400	4.28556500	1.87341300
H	1.67814300	2.37205100	-5.16635700
C	-3.58665900	0.38694100	-0.79051200
C	-3.36971600	0.65932300	-2.15347600
C	-4.74198500	0.90144000	-0.18256000
C	-4.29115200	1.40193400	-2.89069900
H	-2.46713700	0.29275400	-2.63606700
C	-5.65509600	1.66454700	-0.91754100
H	-4.93481500	0.70841100	0.86768200
C	-5.43704200	1.91194400	-2.27322500
H	-4.10923300	1.59213400	-3.94540600
H	-6.54233500	2.05730300	-0.42703000
H	-6.15068000	2.49959800	-2.84471700
C	-2.74986700	-2.33545700	-0.43246700
C	-3.83869200	-2.63376200	-1.26614300
C	-1.95951900	-3.39801500	0.03681000
C	-4.12409000	-3.95498300	-1.62307400
H	-4.47255500	-1.83718500	-1.64062000
C	-2.25135000	-4.71624100	-0.30969700
H	-1.10798600	-3.19515800	0.67863500

C	-3.33373000	-5.00010600	-1.14603400
H	-4.97084600	-4.16272700	-2.27273400
H	-1.62248500	-5.51998600	0.06302800
H	-3.55626100	-6.02694700	-1.42449100
P	-2.29231400	-0.60854600	0.09872700
C	-2.93487800	-0.61956200	1.84920100
C	-2.37943900	0.27522600	2.77792800
C	-3.95877100	-1.48164400	2.27945900
C	-2.84055800	0.31427100	4.09663500
H	-1.57520300	0.93450500	2.46146600
C	-4.41507000	-1.44593400	3.59856000
H	-4.39996200	-2.18724100	1.58240600
C	-3.85793600	-0.54715200	4.51123800
H	-2.39803700	1.01519600	4.79990600
H	-5.20581500	-2.12279000	3.91238200
H	-4.21228200	-0.52129100	5.53855700

IRC of triphenylphosphonin C–P oxidative -Point4

0 1

P	0.51681700	2.41188200	0.51763500
C	-0.60423800	3.89431800	0.49550600
C	2.15733500	3.12116600	1.00741600
Pd	0.02843500	0.17108800	-0.07731900
C	-1.95487700	3.67963600	0.17336800
C	-0.17321100	5.21263000	0.70916800
C	2.84861900	4.00505400	0.16084600
C	2.78612900	2.69247700	2.18489100
C	0.82903800	2.21500900	-1.34146800
C	-2.82792200	4.75210900	-0.01556200
H	-2.32195100	2.66565400	0.04664500
C	-1.05241700	6.28447400	0.54374600
H	0.85511300	5.41214400	0.99042600
C	4.14341400	4.41938000	0.45900200
H	2.38065500	4.34911000	-0.75527400
C	4.08301900	3.11831500	2.49445100
H	2.26848000	2.00429400	2.84934600
C	2.10680000	1.85085200	-1.82082500

C	-0.16147600	2.52129200	-2.29251500
C	-2.37558200	6.06113300	0.15857400
H	-3.86005600	4.55738300	-0.29473800
H	-0.69555400	7.29887600	0.70478600
C	4.76763400	3.96984300	1.62535200
H	4.66701800	5.08828600	-0.21937700
H	4.56073100	2.77400000	3.40823500
C	2.41054600	1.92165900	-3.17915900
H	2.88508100	1.56359100	-1.12440900
C	0.14364800	2.57938000	-3.65403000
H	-1.16204000	2.78305900	-1.97120200
C	1.43886000	2.31916100	-4.10168600
H	3.41569300	1.67542200	-3.51265100
H	-0.63336300	2.85985800	-4.36120600
P	1.72199100	-1.59308600	-0.02985700
C	1.35684300	-2.97123200	-1.22176900
C	1.85033200	-2.44399800	1.61894900
C	3.52613300	-1.28487200	-0.37596500
C	0.83013300	-2.60067300	-2.47033600
C	1.57378800	-4.33306700	-0.96317600
C	2.93360000	-3.26170500	1.98553300
C	0.82343100	-2.23667100	2.55292800
C	4.18410800	-0.31451800	0.40006000
C	4.25296600	-1.93842900	-1.38195100
C	0.54657200	-3.56220600	-3.44082900
H	0.63214700	-1.55043200	-2.67123800
C	1.27373400	-5.29738700	-1.92899100
H	1.97022800	-4.64862400	-0.00322100
C	2.97230700	-3.87265600	3.24022600
H	3.75746700	-3.41067900	1.29340300
C	0.85980200	-2.85043300	3.80734900
H	0.00240800	-1.57255700	2.29684300
C	5.52792300	-0.01336100	0.18417100
H	3.63860200	0.21858500	1.17370900
C	5.59993100	-1.63215000	-1.60210700
H	3.77224900	-2.69118600	-1.99793500
C	0.76395300	-4.91518400	-3.17091500

H	0.14316600	-3.25502000	-4.40225500
C	1.93319500	-3.67241900	4.15278100
H	3.81838200	-4.50106500	3.50711400
H	0.05299500	-2.67456400	4.51405800
C	6.24232800	-0.67196800	-0.82102100
H	6.01068300	0.74537200	0.79445500
H	6.14498400	-2.15048100	-2.38725500
H	0.53141900	-5.66656500	-3.92109800
H	1.96718400	-4.14633900	5.13044900
H	7.28859000	-0.43432800	-0.99504800
H	1.44135500	-6.34889000	-1.70867900
H	-3.05149100	6.89945300	0.01081400
H	5.78149200	4.28578500	1.85771800
H	1.68522900	2.40691600	-5.15720600
C	-3.58806600	0.38631000	-0.78931800
C	-3.37098300	0.65720600	-2.15255800
C	-4.74298100	0.90214100	-0.18177300
C	-4.29162800	1.40015200	-2.89037700
H	-2.46873100	0.28953600	-2.63486500
C	-5.65539300	1.66546000	-0.91744200
H	-4.93591200	0.71017200	0.86865100
C	-5.43700500	1.91174100	-2.27327800
H	-4.10944600	1.58939900	-3.94520400
H	-6.54228900	2.05940600	-0.42727900
H	-6.15002600	2.49973900	-2.84518300
C	-2.75084300	-2.33593700	-0.43125200
C	-3.83926900	-2.63431500	-1.26551400
C	-1.96027000	-3.39844800	0.03777600
C	-4.12400800	-3.95546000	-1.62320200
H	-4.47331600	-1.83783100	-1.63985100
C	-2.25132200	-4.71661400	-0.30972800
H	-1.10925500	-3.19578100	0.68035400
C	-3.33328900	-5.00050700	-1.14655900
H	-4.97051900	-4.16320500	-2.27317500
H	-1.62220800	-5.52026700	0.06275700
H	-3.55525600	-6.02728800	-1.42567000
P	-2.29388900	-0.60891000	0.10033100

C	-2.93669800	-0.62019000	1.85092700
C	-2.38130900	0.27467400	2.77957800
C	-3.96053500	-1.48242900	2.28131500
C	-2.84228800	0.31358700	4.09837900
H	-1.57705800	0.93403100	2.46322000
C	-4.41657900	-1.44685300	3.60053600
H	-4.40176600	-2.18808000	1.58433200
C	-3.85939600	-0.54803200	4.51318000
H	-2.39972400	1.01458000	4.80154900
H	-5.20715900	-2.12385400	3.91445400
H	-4.21352200	-0.52229300	5.54057600

IRC of triphenylphosphonin C–P oxidative -Point5

0 1

P	0.51121600	2.40748600	0.53278800
C	-0.60503300	3.89218300	0.49529900
C	2.15399500	3.11483800	1.01315000
Pd	0.03333400	0.18275100	-0.08336100
C	-1.95490100	3.67910600	0.16842100
C	-0.17340600	5.21018600	0.70988100
C	2.84074400	3.99520100	0.15972400
C	2.78834600	2.69082000	2.18956600
C	0.82482700	2.19145100	-1.33531700
C	-2.82631700	4.75231100	-0.02306400
H	-2.32321100	2.66554200	0.04214600
C	-1.05109900	6.28284800	0.54161900
H	0.85411200	5.40880700	0.99468400
C	4.13615100	4.41227700	0.45056200
H	2.36800000	4.33534700	-0.75533700
C	4.08634800	3.11895500	2.49139800
H	2.27391900	2.00554900	2.85950400
C	2.10505500	1.83746900	-1.81913500
C	-0.16441900	2.50044000	-2.28839200
C	-2.37343100	6.06092200	0.15286300
H	-3.85783800	4.55851200	-0.30513400
H	-0.69367400	7.29688200	0.70375300
C	4.76583600	3.96824500	1.61604000

H	4.65602900	5.07910300	-0.23271000
H	4.56859500	2.77889400	3.40440200
C	2.41207500	1.92799500	-3.17617200
H	2.88434700	1.54644100	-1.12535800
C	0.14444200	2.58036100	-3.64847800
H	-1.16745500	2.75350700	-1.96799600
C	1.44254300	2.33604100	-4.09655400
H	3.41945100	1.69069800	-3.50941000
H	-0.63277900	2.86658800	-4.35314500
P	1.72303900	-1.59423000	-0.02991900
C	1.35702900	-2.97209500	-1.22191800
C	1.85060600	-2.44521100	1.61887100
C	3.52704900	-1.28621600	-0.37560800
C	0.83074900	-2.60113200	-2.47055300
C	1.57334900	-4.33409000	-0.96343500
C	2.93376800	-3.26280800	1.98613500
C	0.82349500	-2.23731500	2.55245300
C	4.18456700	-0.31553000	0.40039200
C	4.25401500	-1.93946300	-1.38167700
C	0.54672200	-3.56249300	-3.44112700
H	0.63371800	-1.55072000	-2.67150000
C	1.27311400	-5.29814900	-1.92944100
H	1.96951900	-4.64990100	-0.00344700
C	2.97221100	-3.87295900	3.24121700
H	3.75780300	-3.41213700	1.29428600
C	0.85950400	-2.85045900	3.80720000
H	0.00268000	-1.57302200	2.29616300
C	5.52812200	-0.01351300	0.18416200
H	3.63881400	0.21744400	1.17395600
C	5.60078200	-1.63245000	-1.60200100
H	3.77354000	-2.69238800	-1.99765300
C	0.76351800	-4.91557500	-3.17135300
H	0.14359300	-3.25500700	-4.40256900
C	1.93285300	-3.67218200	4.15338400
H	3.81826200	-4.50113300	3.50872600
H	0.05255500	-2.67415400	4.51363200
C	6.24270100	-0.67177400	-0.82111800

H	6.01045800	0.74568700	0.79418200
H	6.14602000	-2.15047600	-2.38721600
H	0.53078100	-5.66677000	-3.92165800
H	1.96663500	-4.14545000	5.13137100
H	7.28876300	-0.43346100	-0.99541600
H	1.44041000	-6.34973700	-1.70929800
H	-3.04820200	6.89989100	0.00362200
H	5.78015800	4.28671300	1.84292200
H	1.69232900	2.44296600	-5.14944300
C	-3.58939800	0.38571700	-0.78822000
C	-3.37208400	0.65525000	-2.15169300
C	-4.74392200	0.90279500	-0.18107500
C	-4.29194500	1.39855600	-2.89007700
H	-2.47011700	0.28656400	-2.63369500
C	-5.65565400	1.66630300	-0.91740700
H	-4.93697100	0.71180200	0.86950800
C	-5.43688400	1.91157100	-2.27336500
H	-4.10945500	1.58697500	-3.94499200
H	-6.54225300	2.06134500	-0.42760500
H	-6.14930300	2.49990000	-2.84567400
C	-2.75183300	-2.33643000	-0.43015000
C	-3.83985800	-2.63487200	-1.26499000
C	-1.96098400	-3.39886500	0.03860400
C	-4.12397300	-3.95594900	-1.62336000
H	-4.47407500	-1.83847400	-1.63919800
C	-2.25129600	-4.71697600	-0.30981700
H	-1.11046900	-3.19636700	0.68190000
C	-3.33291600	-5.00090900	-1.14705500
H	-4.97025900	-4.16371600	-2.27361200
H	-1.62193400	-5.52053700	0.06243000
H	-3.55437400	-6.02764100	-1.42673200
P	-2.29567800	-0.60935600	0.10198100
C	-2.93863500	-0.62082200	1.85261400
C	-2.38318500	0.27414100	2.78110500
C	-3.96235700	-1.48322400	2.28318800
C	-2.84391900	0.31295000	4.10002100
H	-1.57894600	0.93356900	2.46478300

C	-4.41804600	-1.44774200	3.60255300
H	-4.40366600	-2.18894100	1.58631200
C	-3.86074400	-0.54884800	4.51508700
H	-2.40126300	1.01401700	4.80305400
H	-5.20843900	-2.12487100	3.91665900
H	-4.21459000	-0.52320200	5.54258100

IRC of triphenylphosphonin C–P oxidative -Point6

0 1

P	0.50507000	2.40310800	0.54989900
C	-0.60577800	3.89015100	0.49523800
C	2.15070800	3.10852000	1.01911700
Pd	0.03811100	0.19448200	-0.08861900
C	-1.95486200	3.67860400	0.16364300
C	-0.17363200	5.20795500	0.71051200
C	2.83297800	3.98540700	0.15899400
C	2.79067000	2.68904800	2.19438600
C	0.82085000	2.16638900	-1.33124800
C	-2.82488600	4.75244300	-0.02978800
H	-2.32438200	2.66551100	0.03746100
C	-1.04996400	6.28133400	0.53964700
H	0.85309800	5.40580000	0.99865500
C	4.12879600	4.40554800	0.44303500
H	2.35558900	4.32152200	-0.75508200
C	4.08965200	3.11943900	2.48877500
H	2.27944400	2.00666800	2.86969000
C	2.10352400	1.82325100	-1.82024900
C	-0.16650000	2.47973200	-2.28667300
C	-2.37163800	6.06068700	0.14800100
H	-3.85583700	4.55944100	-0.31448600
H	-0.69200300	7.29504000	0.70269300
C	4.76387700	3.96696800	1.60761700
H	4.64490800	5.07052300	-0.24487300
H	4.57632800	2.78342700	3.40093000
C	2.41374700	1.93384700	-3.17586500
H	2.88409800	1.52788600	-1.12966300
C	0.14586800	2.58196900	-3.64515300

H	-1.17196900	2.72419200	-1.96728200
C	1.44641200	2.35260000	-4.09390200
H	3.42332000	1.70533500	-3.50873300
H	-0.63161900	2.87474800	-4.34694800
P	1.72413900	-1.59547900	-0.02995600
C	1.35722000	-2.97293900	-1.22209800
C	1.85088600	-2.44640300	1.61880200
C	3.52791600	-1.28746700	-0.37529800
C	0.83133300	-2.60157900	-2.47079400
C	1.57296700	-4.33508100	-0.96371500
C	2.93398100	-3.26382400	1.98671200
C	0.82356400	-2.23795600	2.55200200
C	4.18494100	-0.31640400	0.40064600
C	4.25499000	-1.94040100	-1.38146400
C	0.54683000	-3.56279500	-3.44141700
H	0.63529500	-1.55101600	-2.67187000
C	1.27257300	-5.29889200	-1.92989800
H	1.96890200	-4.65112000	-0.00370000
C	2.97217900	-3.87322500	3.24214700
H	3.75818100	-3.41344600	1.29512700
C	0.85925700	-2.85049100	3.80706200
H	0.00289900	-1.57355000	2.29552600
C	5.52825300	-0.01359100	0.18411900
H	3.63892900	0.21651900	1.17405700
C	5.60156800	-1.63270100	-1.60192000
H	3.77474500	-2.69348100	-1.99743500
C	0.76310700	-4.91596800	-3.17178000
H	0.14394500	-3.25503400	-4.40286800
C	1.93257300	-3.67196200	4.15393500
H	3.81821500	-4.50115800	3.51025200
H	0.05218400	-2.67378200	4.51324200
C	6.24301900	-0.67157600	-0.82119700
H	6.01016600	0.74608700	0.79385800
H	6.14699500	-2.15042900	-2.38719200
H	0.53018200	-5.66698900	-3.92220000
H	1.96616400	-4.14462200	5.13221800
H	7.28890000	-0.43264400	-0.99571400

H	1.43960600	-6.35055600	-1.70993100
H	-3.04547100	6.90021700	-0.00229000
H	5.77848300	4.28823200	1.82925400
H	1.69931200	2.47833700	-5.14402500
C	-3.59060400	0.38517800	-0.78724300
C	-3.37300700	0.65347400	-2.15091600
C	-4.74475400	0.90339500	-0.18046500
C	-4.29212700	1.39715400	-2.88980400
H	-2.47131500	0.28383300	-2.63263300
C	-5.65586200	1.66704900	-0.91740900
H	-4.93791100	0.71328800	0.87026300
C	-5.43669600	1.91141600	-2.27346500
H	-4.10931600	1.58487100	-3.94478000
H	-6.54221100	2.06306800	-0.42795900
H	-6.14855700	2.50004600	-2.84615200
C	-2.75278400	-2.33691500	-0.42918300
C	-3.84042400	-2.63540800	-1.26457100
C	-1.96162600	-3.39925300	0.03928900
C	-4.12397300	-3.95642200	-1.62353000
H	-4.47479100	-1.83908400	-1.63866000
C	-2.25127000	-4.71731900	-0.30994800
H	-1.11157700	-3.19690500	0.68325100
C	-3.33261000	-5.00129200	-1.14750200
H	-4.97005800	-4.16422800	-2.27402200
H	-1.62167500	-5.52079400	0.06207600
H	-3.55362800	-6.02798700	-1.42765200
P	-2.29762500	-0.60985900	0.10364600
C	-2.94060200	-0.62143000	1.85422400
C	-2.38498900	0.27364500	2.78249200
C	-3.96415900	-1.48400600	2.28501000
C	-2.84541600	0.31237100	4.10153100
H	-1.58078600	0.93315000	2.46616900
C	-4.41942900	-1.44858100	3.60452600
H	-4.40556600	-2.18979200	1.58825600
C	-3.86196200	-0.54958800	4.51689200
H	-2.40263700	1.01351100	4.80440800
H	-5.20962800	-2.12581600	3.91888400

H	-4.21550000	-0.52400700	5.54449200

IRC of triphenylphosphonin C−P oxidative -Point7

0 1

P	0.49830900	2.39889700	0.56951300
C	-0.60646700	3.88828100	0.49540100
C	2.14755800	3.10252000	1.02506700
Pd	0.04263700	0.20595400	-0.09307100
C	-1.95476100	3.67813600	0.15915800
C	-0.17387200	5.20600400	0.71104400
C	2.82557000	3.97605100	0.15855600
C	2.79304500	2.68728900	2.19909200
C	0.81708800	2.13995200	-1.32974800
C	-2.82363500	4.75250200	-0.03564700
H	-2.32537000	2.66552700	0.03266500
C	-1.04900600	6.27998300	0.53780500
H	0.85209800	5.40319400	1.00229500
C	4.12164800	4.39936600	0.43651700
H	2.34378600	4.30813200	-0.75462700
C	4.09287100	3.11973900	2.48655500
H	2.28484900	2.00776300	2.87952000
C	2.10233200	1.80853300	-1.82422600
C	-0.16778900	2.45961100	-2.28758200
C	-2.37020400	6.06044300	0.14398100
H	-3.85406000	4.56016400	-0.32270500
H	-0.69053500	7.29340500	0.70152700
C	4.76189400	3.96598100	1.60020700
H	4.63410300	5.06272500	-0.25565600
H	4.58372000	2.78743600	3.39782900
C	2.41573900	1.93926900	-3.17827100
H	2.88436200	1.50850000	-1.13718500
C	0.14788300	2.58421100	-3.64426700
H	-1.17557100	2.69578900	-1.96917400
C	1.45044500	2.36837400	-4.09378700
H	3.42749700	1.71965200	-3.51066100
H	-0.62970600	2.88447000	-4.34288900
P	1.72525900	-1.59678700	-0.02998600

C	1.35740800	-2.97374100	-1.22230200
C	1.85114200	-2.44751500	1.61874200
C	3.52871300	-1.28859600	-0.37503500
C	0.83187200	-2.60199900	-2.47105000
C	1.57264400	-4.33601100	-0.96400100
C	2.93420800	-3.26471000	1.98723900
C	0.82361900	-2.23855600	2.55158800
C	4.18522800	-0.31713200	0.40083100
C	4.25586300	-1.94122400	-1.38130800
C	0.54689600	-3.56309900	-3.44169200
H	0.63685000	-1.55130300	-2.67234200
C	1.27211300	-5.29959300	-1.93034200
H	1.96838000	-4.65224900	-0.00396600
C	2.97218500	-3.87344200	3.24297500
H	3.75856300	-3.41455500	1.29589300
C	0.85905300	-2.85051500	3.80693800
H	0.00302700	-1.57411700	2.29496900
C	5.52832300	-0.01361300	0.18405700
H	3.63896600	0.21580600	1.17404100
C	5.60226900	-1.63290700	-1.60185700
H	3.77583100	-2.69444100	-1.99728100
C	0.76272700	-4.91634800	-3.17218200
H	0.14422600	-3.25509200	-4.40314900
C	1.93234600	-3.67176000	4.15441000
H	3.81821500	-4.50114400	3.51162700
H	0.05187700	-2.67344200	4.51290200
C	6.24327600	-0.67138800	-0.82124900
H	6.00982600	0.74653700	0.79351100
H	6.14788400	-2.15035400	-2.38717600
H	0.52963800	-5.66720900	-3.92270900
H	1.96576500	-4.14387800	5.13295600
H	7.28900200	-0.43191000	-0.99593600
H	1.43894000	-6.35132500	-1.71055400
H	-3.04330500	6.90043200	-0.00697800
H	5.77662000	4.29018400	1.81696200
H	1.70618300	2.51254700	-5.14081600
C	-3.59164800	0.38470700	-0.78640200

C	-3.37375000	0.65189800	-2.15024500
C	-4.74544400	0.90393500	-0.17993900
C	-4.29219800	1.39595000	-2.88955900
H	-2.47234500	0.28135000	-2.63173600
C	-5.65601000	1.66767800	-0.91742400
H	-4.93867900	0.71462400	0.87091900
C	-5.43646400	1.91126500	-2.27355800
H	-4.10907900	1.58308700	-3.94457400
H	-6.54215100	2.06454000	-0.42830000
H	-6.14782900	2.50015700	-2.84658500
C	-2.75365100	-2.33737700	-0.42836400
C	-3.84094200	-2.63590200	-1.26424600
C	-1.96217900	-3.39960700	0.03983700
C	-4.12399900	-3.95686100	-1.62369900
H	-4.47543500	-1.83963800	-1.63822700
C	-2.25124300	-4.71763600	-0.31009900
H	-1.11255600	-3.19738900	0.68440200
C	-3.33236600	-5.00164400	-1.14789100
H	-4.96991100	-4.16471600	-2.27439000
H	-1.62144100	-5.52103300	0.06172200
H	-3.55301600	-6.02831000	-1.42842300
P	-2.29964800	-0.61039000	0.10528900
C	-2.94250500	-0.62199200	1.85572700
C	-2.38665900	0.27320200	2.78372600
C	-3.96586300	-1.48475100	2.28671500
C	-2.84675100	0.31185600	4.10288600
H	-1.58251200	0.93280500	2.46741000
C	-4.42069400	-1.44935300	3.60637300
H	-4.40738000	-2.19060100	1.59008700
C	-3.86303700	-0.55024200	4.51853700
H	-2.40384100	1.01306500	4.80560200
H	-5.21070400	-2.12667100	3.92102100
H	-4.21627100	-0.52470600	5.54624200

IRC of triphenylphosphonin C−P oxidative -Point8

0 1

P	0.49098900	2.39506800	0.59174800

C	-0.60708100	3.88658500	0.49576800
C	2.14460900	3.09704100	1.03071300
Pd	0.04682600	0.21690000	-0.09675600
C	-1.95462000	3.67770000	0.15506900
C	-0.17410800	5.20434400	0.71145700
C	2.81873100	3.96744800	0.15829700
C	2.79537900	2.68562600	2.20343200
C	0.81358300	2.11234500	-1.33139100
C	-2.82256500	4.75249400	-0.04061400
H	-2.32612300	2.66554800	0.02790700
C	-1.04820800	6.27880600	0.53610100
H	0.85113600	5.40099900	1.00556200
C	4.11497500	4.39384800	0.43102500
H	2.33292000	4.29570600	-0.75408000
C	4.09589900	3.11984800	2.48469700
H	2.28989000	2.00888700	2.88861200
C	2.10165100	1.79374900	-1.83076700
C	-0.16846800	2.44057500	-2.29101400
C	-2.36908700	6.06020600	0.14072600
H	-3.85251700	4.56070000	-0.32974200
H	-0.68925400	7.29198900	0.70028300
C	4.76000200	3.96521800	1.59386500
H	4.62403400	5.05585000	-0.26492400
H	4.59050400	2.79084200	3.39513100
C	2.41819500	1.94434500	-3.18301900
H	2.88507000	1.48894100	-1.14730700
C	0.15031300	2.58707600	-3.64566400
H	-1.17834100	2.66899700	-1.97336800
C	1.45453600	2.38293400	-4.09583300
H	3.43207200	1.73367300	-3.51499900
H	-0.62706700	2.89545500	-4.34110600
P	1.72636400	-1.59811900	-0.03002600
C	1.35759300	-2.97448800	-1.22252500
C	1.85135700	-2.44850700	1.61868800
C	3.52942500	-1.28958600	-0.37482200
C	0.83235700	-2.60238200	-2.47131000
C	1.57238000	-4.33687000	-0.96428300

C	2.93442400	-3.26544500	1.98770000
C	0.82364700	-2.23909300	2.55122000
C	4.18543400	-0.31772000	0.40095900
C	4.25662400	-1.94192900	-1.38120300
C	0.54692900	-3.56339400	-3.44194700
H	0.63834600	-1.55157400	-2.67289300
C	1.27172700	-5.30024300	-1.93075900
H	1.96795400	-4.65327300	-0.00423400
C	2.97220900	-3.87360800	3.24367900
H	3.75891900	-3.41544200	1.29656100
C	0.85888300	-2.85052600	3.80683100
H	0.00304400	-1.57471000	2.29451600
C	5.52833900	-0.01359600	0.18398500
H	3.63894700	0.21528800	1.17394100
C	5.60287600	-1.63307900	-1.60180700
H	3.77678300	-2.69526200	-1.99718400
C	0.76238400	-4.91670400	-3.17255100
H	0.14444700	-3.25517300	-4.40340700
C	1.93216100	-3.67157600	4.15480000
H	3.81823700	-4.50110000	3.51280900
H	0.05163000	-2.67313600	4.51261700
C	6.24347600	-0.67122300	-0.82127400
H	6.00945800	0.74700000	0.79316300
H	6.14867100	-2.15027100	-2.38716000
H	0.52915600	-5.66742200	-3.92317500
H	1.96543200	-4.14323100	5.13356900
H	7.28907100	-0.43127500	-0.99608300
H	1.43839600	-6.35203300	-1.71115000
H	-3.04164500	6.90055700	-0.01059800
H	5.77470600	4.29235900	1.80623900
H	1.71275500	2.54431800	-5.13971200
C	-3.59251100	0.38430700	-0.78569400
C	-3.37432300	0.65052800	-2.14968400
C	-4.74598000	0.90440800	-0.17949000
C	-4.29218900	1.39493300	-2.88934100
H	-2.47322400	0.27912800	-2.63102500
C	-5.65609800	1.66818600	-0.91744100

H	-4.93925900	0.71580000	0.87148600
C	-5.43621200	1.91111200	-2.27363500
H	-4.10878800	1.58160300	-3.94438000
H	-6.54207100	2.06575000	-0.42860100
H	-6.14715300	2.50022000	-2.84695700
C	-2.75441600	-2.33780700	-0.42769000
C	-3.84140700	-2.63634800	-1.26400000
C	-1.96264200	-3.39992400	0.04026300
C	-4.12404200	-3.95725900	-1.62385700
H	-4.47599800	-1.84012800	-1.63788500
C	-2.25121900	-4.71792500	-0.31025400
H	-1.11339400	-3.19781600	0.68535800
C	-3.33217700	-5.00196100	-1.14822100
H	-4.96980700	-4.16516800	-2.27471200
H	-1.62124000	-5.52125800	0.06139100
H	-3.55252400	-6.02860400	-1.42905800
P	-2.30166700	-0.61093400	0.10687900
C	-2.94428000	-0.62249700	1.85710000
C	-2.38815600	0.27282100	2.78480700
C	-3.96741800	-1.48544100	2.28826100
C	-2.84791800	0.31140500	4.10407500
H	-1.58408100	0.93255900	2.46854000
C	-4.42182200	-1.45004600	3.60804300
H	-4.40904400	-2.19134500	1.59175000
C	-3.86397000	-0.55081200	4.51999100
H	-2.40487900	1.01268000	4.80663400
H	-5.21166100	-2.12742400	3.92298900
H	-4.21692200	-0.52530400	5.54779500

IRC of triphenylphosphonin C–P oxidative -Point9

0 1

P	0.48327700	2.39180500	0.61620400
C	-0.60760700	3.88502900	0.49626000
C	2.14188400	3.09212400	1.03585900
Pd	0.05065500	0.22718900	-0.09977700
C	-1.95447000	3.67729000	0.15141700
C	-0.17433400	5.20293400	0.71174800

C	2.81254900	3.95973800	0.15813800
C	2.79758800	2.68408300	2.20727400
C	0.81039600	2.08378200	-1.33645700
C	-2.82166100	4.75243600	-0.04475900
H	-2.32667600	2.66555100	0.02335000
C	-1.04754200	6.27778200	0.53454700
H	0.85022500	5.39916400	1.00845700
C	4.10891400	4.38900200	0.42646500
H	2.32312700	4.28455400	-0.75350100
C	4.09865700	3.11979400	2.48314200
H	2.29440600	2.01004300	2.89677200
C	2.10158800	1.77924300	-1.83929300
C	-0.16876500	2.42291600	-2.29653700
C	-2.36822300	6.05998900	0.13809700
H	-3.85120500	4.56109100	-0.33565800
H	-0.68813200	7.29076000	0.69903400
C	4.75826400	3.96460500	1.58851600
H	4.61492100	5.04991800	-0.27272100
H	4.59651300	2.79367900	3.39284000
C	2.42115200	1.94915600	-3.18945700
H	2.88606600	1.46981300	-1.15902000
C	0.15293500	2.59049200	-3.64884800
H	-1.18040800	2.64421400	-1.97914900
C	1.45854600	2.39606700	-4.09938500
H	3.43702200	1.74746800	-3.52118700
H	-0.62382300	2.90740300	-4.34125400
P	1.72742800	-1.59944800	-0.03009100
C	1.35777900	-2.97518300	-1.22275800
C	1.85152300	-2.44936500	1.61863700
C	3.53004900	-1.29043700	-0.37465700
C	0.83278700	-2.60273300	-2.47156500
C	1.57217200	-4.33765900	-0.96455400
C	2.93461700	-3.26603400	1.98809100
C	0.82364700	-2.23955900	2.55089800
C	4.18557200	-0.31818500	0.40104100
C	4.25727500	-1.94252700	-1.38113600
C	0.54693800	-3.56367400	-3.44218100

H	0.63975900	-1.55182900	-2.67349200
C	1.27140100	-5.30084000	-1.93114400
H	1.96762200	-4.65419500	-0.00449600
C	2.97223800	-3.87372700	3.24425900
H	3.75923400	-3.41612200	1.29712800
C	0.85874000	-2.85052300	3.80673900
H	0.00294500	-1.57531900	2.29417400
C	5.52831600	-0.01355500	0.18391200
H	3.63889500	0.21492800	1.17379200
C	5.60339400	-1.63322600	-1.60176400
H	3.77760200	-2.69595500	-1.99713000
C	0.76208000	-4.91703400	-3.17288300
H	0.14461800	-3.25526900	-4.40364200
C	1.93200800	-3.67140900	4.15511100
H	3.81826600	-4.50103700	3.51379200
H	0.05143300	-2.67286000	4.51238200
C	6.24362400	-0.67108300	-0.82127800
H	6.00908300	0.74745000	0.79283400
H	6.14935700	-2.15019700	-2.38713700
H	0.52873800	-5.66762200	-3.92359800
H	1.96515600	-4.14268000	5.13406300
H	7.28911100	-0.43073900	-0.99617000
H	1.43794800	-6.35268200	-1.71170700
H	-3.04037900	6.90062400	-0.01339200
H	5.77284100	4.29456500	1.79707600
H	1.71886700	2.57307600	-5.14015200
C	-3.59320000	0.38397800	-0.78510500
C	-3.37475200	0.64934800	-2.14921900
C	-4.74637700	0.90481700	-0.17910800
C	-4.29212600	1.39407700	-2.88915000
H	-2.47397100	0.27716100	-2.63049000
C	-5.65613600	1.66858200	-0.91745100
H	-4.93966900	0.71682300	0.87197400
C	-5.43595400	1.91095500	-2.27369400
H	-4.10847700	1.58037600	-3.94420000
H	-6.54197500	2.06671900	-0.42885300
H	-6.14654300	2.50023500	-2.84726600

C	-2.75508600	-2.33820900	-0.42713800
C	-3.84182200	-2.63674900	-1.26381300
C	-1.96302800	-3.40021000	0.04059200
C	-4.12409700	-3.95761800	-1.62400200
H	-4.47648700	-1.84055700	-1.63761400
C	-2.25119800	-4.71819000	-0.31040200
H	-1.11410400	-3.19818900	0.68614000
C	-3.33202900	-5.00224400	-1.14850000
H	-4.96973400	-4.16558400	-2.27499400
H	-1.62107200	-5.52146800	0.06109200
H	-3.55212800	-6.02886900	-1.42958000
P	-2.30363300	-0.61148400	0.10840100
C	-2.94589900	-0.62294700	1.85834300
C	-2.38947700	0.27249900	2.78574900
C	-3.96881200	-1.48607200	2.28964000
C	-2.84893100	0.31101300	4.10510800
H	-1.58549200	0.93242200	2.46960000
C	-4.42281800	-1.45066200	3.60952400
H	-4.41053700	-2.19201700	1.59322800
C	-3.86477400	-0.55130700	4.52125800
H	-2.40576800	1.01235100	4.80751500
H	-5.21250700	-2.12807800	3.92475700
H	-4.21747700	-0.52581400	5.54914800

IRC of triphenylphosphonin C–P oxidative -Point10

0 1

P	0.47534900	2.38919100	0.64223300
C	-0.60804600	3.88355800	0.49681100
C	2.13935600	3.08768700	1.04046300
Pd	0.05416300	0.23684200	-0.10226900
C	-1.95434200	3.67690400	0.14818200
C	-0.17455100	5.20170700	0.71194400
C	2.80697900	3.95287100	0.15804600
C	2.79963400	2.68264900	2.21062400
C	0.80756600	2.05439200	-1.34488100
C	-2.82089600	4.75234900	-0.04822700
H	-2.32710800	2.66553500	0.01908600

C	-1.04697900	6.27687200	0.53314100
H	0.84935800	5.39760800	1.01104100
C	4.10345500	4.38474000	0.42266800
H	2.31432800	4.27469700	-0.75288900
C	4.10112300	3.11961900	2.48182600
H	2.29837500	2.01121900	2.90403000
C	2.10213700	1.76519700	-1.84918300
C	-0.16884500	2.40667600	-2.30357400
C	-2.36754000	6.05980100	0.13592700
H	-3.85009400	4.56138900	-0.34063900
H	-0.68713200	7.28966900	0.69784000
C	4.75669300	3.96407400	1.58398700
H	4.60674500	5.04481100	-0.27926700
H	4.60174800	2.79605700	3.39091500
C	2.42454100	1.95379200	-3.19691800
H	2.88716800	1.45133700	-1.17148300
C	0.15558400	2.59436500	-3.65320000
H	-1.18192100	2.62136200	-1.98580500
C	1.46238200	2.40784000	-4.10379100
H	3.44223900	1.76101200	-3.52859700
H	-0.62018400	2.91993200	-4.34280000
P	1.72844200	-1.60077100	-0.03018900
C	1.35797300	-2.97584000	-1.22300000
C	1.85164600	-2.45010000	1.61858600
C	3.53059300	-1.29116300	-0.37453600
C	0.83317000	-2.60305900	-2.47181000
C	1.57201100	-4.33839100	-0.96481300
C	2.93478300	-3.26650100	1.98842100
C	0.82362000	-2.23996300	2.55061500
C	4.18565500	-0.31855000	0.40108900
C	4.25783500	-1.94303800	-1.38109600
C	0.54693100	-3.56394000	-3.44239700
H	0.64108300	-1.55207300	-2.67411800
C	1.27112000	-5.30139500	-1.93149700
H	1.96737000	-4.65503300	-0.00475200
C	2.97226400	-3.87380700	3.24473200
H	3.75950800	-3.41662800	1.29760400

C	0.85861600	-2.85050800	3.80665900
H	0.00274300	-1.57593900	2.29393700
C	5.52826400	-0.01350000	0.18384000
H	3.63882700	0.21469200	1.17361500
C	5.60383800	-1.63335900	-1.60172100
H	3.77830900	-2.69654600	-1.99710700
C	0.76180900	-4.91734100	-3.17318400
H	0.14475300	-3.25537400	-4.40385700
C	1.93187900	-3.67125600	4.15535500
H	3.81829300	-4.50096100	3.51460000
H	0.05127100	-2.67261200	4.51218700
C	6.24373100	-0.67096600	-0.82126500
H	6.00870900	0.74787800	0.79252800
H	6.14995600	-2.15013900	-2.38710300
H	0.52837500	-5.66781100	-3.92398400
H	1.96492400	-4.14221000	5.13445600
H	7.28913000	-0.43028900	-0.99621100
H	1.43756500	-6.35328200	-1.71222400
H	-3.03938400	6.90066600	-0.01562600
H	5.77107500	4.29667800	1.78926000
H	1.72442100	2.59867400	-5.14164800
C	-3.59374000	0.38370800	-0.78460700
C	-3.37506600	0.64832600	-2.14883200
C	-4.74666300	0.90517000	-0.17877800
C	-4.29202900	1.39334700	-2.88898000
H	-2.47461000	0.27541300	-2.63009700
C	-5.65613400	1.66888700	-0.91745300
H	-4.93994100	0.71771700	0.87239900
C	-5.43569900	1.91079500	-2.27373700
H	-4.10816300	1.57935000	-3.94403200
H	-6.54186500	2.06749000	-0.42905900
H	-6.14599700	2.50020900	-2.84752100
C	-2.75568300	-2.33859100	-0.42668100
C	-3.84220100	-2.63711400	-1.26366800
C	-1.96335600	-3.40047300	0.04084900
C	-4.12415900	-3.95794700	-1.62413700
H	-4.47691900	-1.84093800	-1.63739200

C	-2.25118100	-4.71843700	-0.31054000
H	-1.11470800	-3.19851500	0.68678000
C	-3.33191000	-5.00250000	-1.14874000
H	-4.96968200	-4.16597200	-2.27524600
H	-1.62093100	-5.52166900	0.06082400
H	-3.55180200	-6.02911100	-1.43002000
P	-2.30553100	-0.61204600	0.10985900
C	-2.94737500	-0.62335000	1.85947400
C	-2.39064800	0.27222500	2.78657700
C	-3.97006400	-1.48665100	2.29087300
C	-2.84981900	0.31066400	4.10601400
H	-1.58677500	0.93239500	2.47062600
C	-4.42370300	-1.45121400	3.61083800
H	-4.41187600	-2.19262500	1.59454200
C	-3.86547600	-0.55174200	4.52236700
H	-2.40653800	1.01206800	4.80826800
H	-5.21326400	-2.12865100	3.92633700
H	-4.21795900	-0.52625500	5.55033100

IRC of triphenylphosphonin C−P oxidative -Point11

0 1

P	0.46733800	2.38720700	0.66921100
C	-0.60842200	3.88211800	0.49740300
C	2.13696400	3.08359700	1.04459300
Pd	0.05741800	0.24596500	-0.10436000
C	-1.95425400	3.67653700	0.14530600
C	-0.17477200	5.20060200	0.71208800
C	2.80189800	3.94669300	0.15802100
C	2.80152000	2.68129900	2.21357300
C	0.80509900	2.02427400	-1.35630300
C	-2.82024100	4.75225000	-0.05118500
H	-2.32749900	2.66551100	0.01512900
C	-1.04648900	6.27604000	0.53186500
H	0.84851700	5.39624500	1.01340500
C	4.09849300	4.38092600	0.41945100
H	2.30633800	4.26596400	-0.75222200
C	4.10332600	3.11936300	2.48068600

H	2.30187200	2.01240600	2.91055700
C	2.10320400	1.75163100	-1.85995000
C	-0.16879500	2.39169600	-2.31160000
C	-2.36697800	6.05964200	0.13406900
H	-3.84913900	4.56163500	-0.34492000
H	-0.68621700	7.28867200	0.69671900
C	4.75527100	3.96358100	1.58007700
H	4.59933800	5.04034200	-0.28485100
H	4.60632300	2.79810300	3.38928700
C	2.42823900	1.95832400	-3.20490000
H	2.88824800	1.43348200	-1.18417000
C	0.15818300	2.59859400	-3.65819500
H	-1.18300400	2.60011200	-1.99282000
C	1.46601800	2.41849100	-4.10858800
H	3.44760500	1.77434800	-3.53667100
H	-0.61631700	2.93280900	-4.34516300
P	1.72941400	-1.60209300	-0.03032700
C	1.35817900	-2.97647300	-1.22325000
C	1.85173200	-2.45073300	1.61853200
C	3.53107200	-1.29178600	-0.37445400
C	0.83351500	-2.60337100	-2.47204400
C	1.57188700	-4.33908500	-0.96506300
C	2.93492600	-3.26687100	1.98869900
C	0.82357100	-2.24031800	2.55036000
C	4.18569500	-0.31883800	0.40111100
C	4.25832400	-1.94348700	-1.38107400
C	0.54691700	-3.56419500	-3.44260000
H	0.64233000	-1.55231400	-2.67475900
C	1.27086900	-5.30191900	-1.93182700
H	1.96718400	-4.65580900	-0.00500400
C	2.97228500	-3.87385600	3.24512000
H	3.75974500	-3.41700300	1.29800700
C	0.85850500	-2.85048400	3.80658600
H	0.00245200	-1.57657300	2.29378500
C	5.52819100	-0.01343500	0.18377100
H	3.63874900	0.21455300	1.17342100
C	5.60422600	-1.63348400	-1.60167500

H	3.77893000	-2.69706100	-1.99710400
C	0.76156500	-4.91763100	-3.17346300
H	0.14486600	-3.25548400	-4.40405700
C	1.93176600	-3.67111200	4.15554700
H	3.81831500	-4.50087700	3.51526900
H	0.05113400	-2.67238500	4.51201800
C	6.24380700	-0.67086700	-0.82124000
H	6.00833500	0.74828300	0.79224400
H	6.15048800	-2.15010000	-2.38705500
H	0.52805200	-5.66799200	-3.92434100
H	1.96472300	-4.14179900	5.13477200
H	7.28913000	-0.42990200	-0.99621800
H	1.43722400	-6.35384800	-1.71271000
H	-3.03855700	6.90070500	-0.01752300
H	5.76942000	4.29864700	1.78248400
H	1.72944500	2.62158900	-5.14373700
C	-3.59416100	0.38348600	-0.78417500
C	-3.37529700	0.64742200	-2.14849900
C	-4.74686400	0.90548200	-0.17848500
C	-4.29191300	1.39270700	-2.88882500
H	-2.47517000	0.27383300	-2.62980900
C	-5.65610300	1.66912400	-0.91744800
H	-4.94011100	0.71851700	0.87277900
C	-5.43544800	1.91063100	-2.27376800
H	-4.10785300	1.57846800	-3.94387500
H	-6.54174300	2.06811500	-0.42922800
H	-6.14549900	2.50015300	-2.84773600
C	-2.75623300	-2.33896300	-0.42628900
C	-3.84255700	-2.63745600	-1.26354900
C	-1.96364500	-3.40072000	0.04105800
C	-4.12422600	-3.95825600	-1.62426500
H	-4.47731200	-1.84128400	-1.63720100
C	-2.25116600	-4.71867200	-0.31067000
H	-1.11523300	-3.19880500	0.68731500
C	-3.33181200	-5.00273700	-1.14895300
H	-4.96964300	-4.16634000	-2.27547900
H	-1.62080900	-5.52186500	0.06057900

H	-3.55152100	-6.02933500	-1.43040600
P	-2.30737000	-0.61263000	0.11126700
C	-2.94874000	-0.62372000	1.86051700
C	-2.39170700	0.27198700	2.78732000
C	-3.97120800	-1.48719000	2.29199200
C	-2.85061600	0.31034800	4.10682300
H	-1.58797100	0.93246900	2.47165100
C	-4.42450500	-1.45171600	3.61202500
H	-4.41309800	-2.19318400	1.59572900
C	-3.86610300	-0.55213500	4.52335700
H	-2.40722000	1.01182200	4.80891900
H	-5.21395600	-2.12916100	3.92776900
H	-4.21838900	-0.52664600	5.55138600

IRC of triphenylphosphonin C–P oxidative -Point12

0 1

P	0.45932300	2.38576500	0.69665500
C	-0.60876700	3.88067600	0.49806000
C	2.13464300	3.07972800	1.04837600
Pd	0.06049700	0.25469700	-0.10615700
C	-1.95421400	3.67618500	0.14272300
C	-0.17500700	5.19957100	0.71222400
C	2.79716100	3.94102300	0.15807900
C	2.80326900	2.68000700	2.21624400
C	0.80297400	1.99354700	-1.37021000
C	-2.81966600	4.75214900	-0.05378900
H	-2.32790000	2.66549000	0.01143500
C	-1.04605100	6.27526000	0.53069200
H	0.84767900	5.39500900	1.01565600
C	4.09389500	4.37741900	0.41665100
H	2.29894500	4.25811300	-0.75147100
C	4.10532300	3.11905300	2.47967400
H	2.30501800	2.01359900	2.91657500
C	2.10465700	1.73846300	-1.87127900
C	-0.16863600	2.37773200	-2.32022300
C	-2.36649500	6.05950700	0.13240500
H	-3.84829300	4.56185600	-0.34873800

H	-0.68536100	7.28773700	0.69566200
C	4.75396300	3.96309500	1.57659900
H	4.59248200	5.03631100	-0.28975600
H	4.61040300	2.79992500	3.38787900
C	2.43212700	1.96280800	-3.21310600
H	2.88924400	1.41597900	-1.19693900
C	0.16072400	2.60309100	-3.66347300
H	-1.18376800	2.58002600	-1.99997700
C	1.46947600	2.42832600	-4.11352100
H	3.45302300	1.78749200	-3.54505100
H	-0.61234400	2.94586500	-4.34791300
P	1.73035200	-1.60342500	-0.03050700
C	1.35840000	-2.97709800	-1.22351000
C	1.85178700	-2.45128700	1.61847400
C	3.53150300	-1.29232800	-0.37440600
C	0.83383400	-2.60367800	-2.47227100
C	1.57179200	-4.33975800	-0.96530900
C	2.93504900	-3.26716900	1.98893700
C	0.82350200	-2.24063600	2.55012200
C	4.18569900	-0.31906600	0.40111200
C	4.25876400	-1.94389600	-1.38106000
C	0.54689900	-3.56444400	-3.44279700
H	0.64351900	-1.55256000	-2.67541000
C	1.27063700	-5.30242600	-1.93214200
H	1.96704700	-4.65654800	-0.00525600
C	2.97229900	-3.87388200	3.24544500
H	3.75995500	-3.41727900	1.29835700
C	0.85840100	-2.85045500	3.80651600
H	0.00208400	-1.57722600	2.29369800
C	5.52810000	-0.01336300	0.18370400
H	3.63865600	0.21449700	1.17320300
C	5.60457600	-1.63360700	-1.60162300
H	3.77949400	-2.69752700	-1.99711300
C	0.76134100	-4.91791200	-3.17372700
H	0.14496600	-3.25559900	-4.40425000
C	1.93166300	-3.67097200	4.15570200
H	3.81833200	-4.50078300	3.51583300

H	0.05101100	-2.67217300	4.51186400
C	6.24386000	-0.67077900	-0.82120300
H	6.00795600	0.74867800	0.79197500
H	6.15097500	-2.15007900	-2.38699100
H	0.52775700	-5.66816800	-3.92468000
H	1.96454400	-4.14142800	5.13503200
H	7.28911700	-0.42955700	-0.99619900
H	1.43690300	-6.35439400	-1.71317400
H	-3.03782400	6.90075100	-0.01925400
H	5.76786300	4.30046600	1.77643600
H	1.73402400	2.64243000	-5.14615900
C	-3.59449200	0.38329900	-0.78378600
C	-3.37546900	0.64659700	-2.14820000
C	-4.74700400	0.90576400	-0.17821600
C	-4.29178400	1.39212400	-2.88868100
H	-2.47567600	0.27236500	-2.62959100
C	-5.65604900	1.66931300	-0.91743700
H	-4.94020600	0.71925500	0.87313200
C	-5.43519800	1.91046400	-2.27379000
H	-4.10754600	1.57767800	-3.94372400
H	-6.54160900	2.06863900	-0.42937000
H	-6.14503300	2.50007500	-2.84792200
C	-2.75675600	-2.33933400	-0.42593600
C	-3.84290100	-2.63778500	-1.26344600
C	-1.96390900	-3.40096100	0.04123500
C	-4.12429700	-3.95855400	-1.62438900
H	-4.47768200	-1.84160900	-1.63702600
C	-2.25115300	-4.71890100	-0.31079300
H	-1.11570500	-3.19907200	0.68777500
C	-3.33172500	-5.00296300	-1.14915100
H	-4.96961000	-4.16669700	-2.27570500
H	-1.62069900	-5.52205900	0.06034700
H	-3.55126600	-6.02954900	-1.43076000
P	-2.30917400	-0.61324400	0.11264700
C	-2.95003400	-0.62407100	1.86150100
C	-2.39269500	0.27176900	2.78800500
C	-3.97228300	-1.48770400	2.29303500

C	-2.85135300	0.31005000	4.10756700
H	-1.58912300	0.93263000	2.47269200
C	-4.42525400	-1.45218500	3.61312500
H	-4.41424700	-2.19371200	1.59683100
C	-3.86667900	-0.55249900	4.52426800
H	-2.40784100	1.01160100	4.80949700
H	-5.21460500	-2.12963000	3.92910100
H	-4.21878600	-0.52700600	5.55235600

IRC of triphenylphosphonin C–P oxidative -Point13

0 1

P	0.45133400	2.38474900	0.72423900
C	-0.60911200	3.87921200	0.49881400
C	2.13232700	3.07598400	1.05195500
Pd	0.06346700	0.26317000	-0.10773500
C	-1.95421500	3.67584500	0.14037000
C	-0.17526700	5.19858000	0.71239500
C	2.79263000	3.93569300	0.15824200
C	2.80491200	2.67875200	2.21875500
C	0.80117200	1.96238200	-1.38605800
C	-2.81914400	4.75204800	-0.05616700
H	-2.32833200	2.66548000	0.00794600
C	-1.04564900	6.27451400	0.52959500
H	0.84682100	5.39385200	1.01789200
C	4.08953300	4.37409600	0.41413700
H	2.29196100	4.25092200	-0.75060700
C	4.10717000	3.11870900	2.47875400
H	2.30793200	2.01480000	2.92229200
C	2.10637600	1.72555200	-1.88300600
C	-0.16836600	2.36451900	-2.32920300
C	-2.36605600	6.05938800	0.13084800
H	-3.84751100	4.56206800	-0.35228200
H	-0.68454500	7.28684400	0.69464700
C	4.75273700	3.96259100	1.57340400
H	4.58597100	5.03254000	-0.29421900
H	4.61414800	2.80160200	3.38662200
C	2.43611200	1.96727500	-3.22139600

H	2.89015700	1.39855000	-1.20982000
C	0.16323100	2.60778400	-3.66882800
H	-1.18428800	2.56075100	-2.00722600
C	1.47280000	2.43763000	-4.11847500
H	3.45843000	1.80050200	-3.55351700
H	-0.60832500	2.95904300	-4.35073400
P	1.73127000	-1.60478000	-0.03073300
C	1.35864000	-2.97772900	-1.22378200
C	1.85181800	-2.45178200	1.61840800
C	3.53189800	-1.29281200	-0.37438700
C	0.83413800	-2.60399000	-2.47249600
C	1.57171900	-4.34042600	-0.96555700
C	2.93515700	-3.26741400	1.98914600
C	0.82341500	-2.24093200	2.54989100
C	4.18567100	-0.31924700	0.40109400
C	4.25917300	-1.94428300	-1.38105000
C	0.54688300	-3.56469400	-3.44299500
H	0.64467000	-1.55281700	-2.67607200
C	1.27041300	-5.30293000	-1.93244900
H	1.96694900	-4.65727100	-0.00551500
C	2.97230600	-3.87388600	3.24572500
H	3.76014500	-3.41748300	1.29866900
C	0.85829800	-2.85042000	3.80644500
H	0.00164900	-1.57790500	2.29365700
C	5.52799200	-0.01328100	0.18363700
H	3.63853800	0.21452100	1.17294600
C	5.60490200	-1.63373100	-1.60156000
H	3.78002200	-2.69796500	-1.99712700
C	0.76112800	-4.91819300	-3.17398400
H	0.14506100	-3.25572100	-4.40444200
C	1.93156400	-3.67083100	4.15582900
H	3.81834300	-4.50067800	3.51632300
H	0.05089300	-2.67197200	4.51171600
C	6.24389500	-0.67069700	-0.82115400
H	6.00756300	0.74907300	0.79171300
H	6.15143600	-2.15007300	-2.38690800
H	0.52747500	-5.66834600	-3.92500900

H	1.96437900	-4.14107900	5.13525200
H	7.28909100	-0.42923800	-0.99615800
H	1.43658600	-6.35493700	-1.71362700
H	-3.03713400	6.90080400	-0.02093600
H	5.76638200	4.30214400	1.77085500
H	1.73827300	2.66190200	-5.14871300
C	-3.59475800	0.38313800	-0.78342100
C	-3.37560000	0.64581700	-2.14792000
C	-4.74710200	0.90602700	-0.17795800
C	-4.29164400	1.39157300	-2.88854100
H	-2.47614800	0.27095600	-2.62941700
C	-5.65597800	1.66947000	-0.91742100
H	-4.94024900	0.71996000	0.87347100
C	-5.43494500	1.91029200	-2.27380600
H	-4.10723900	1.57693900	-3.94357500
H	-6.54146400	2.06910000	-0.42949200
H	-6.14458300	2.49998000	-2.84809100
C	-2.75727400	-2.33971400	-0.42560300
C	-3.84324300	-2.63811100	-1.26334900
C	-1.96416200	-3.40120300	0.04139300
C	-4.12437000	-3.95884900	-1.62451300
H	-4.47804600	-1.84192500	-1.63685600
C	-2.25114000	-4.71913000	-0.31091400
H	-1.11614400	-3.19932700	0.68818600
C	-3.33164500	-5.00318500	-1.14934200
H	-4.96957900	-4.16705400	-2.27592900
H	-1.62059500	-5.52225600	0.06012100
H	-3.55102400	-6.02975900	-1.43110100
P	-2.31096400	-0.61389800	0.11402200
C	-2.95129600	-0.62441500	1.86245000
C	-2.39364600	0.27155900	2.78865500
C	-3.97332600	-1.48820700	2.29403500
C	-2.85205600	0.30976200	4.10827100
H	-1.59026700	0.93285600	2.47375800
C	-4.42597500	-1.45263700	3.61417700
H	-4.41536300	-2.19422400	1.59788600
C	-3.86722700	-0.55284800	4.52513300

H	-2.40842500	1.01139600	4.81002300
H	-5.21523300	-2.13007600	3.93038100
H	-4.21916200	-0.52734500	5.55327600

IRC of triphenylphosphonin C–P oxidative -Point14

0 1

P	0.44337900	2.38406200	0.75174900
C	-0.60947500	3.87772100	0.49970000
C	2.12996600	3.07230700	1.05547600
Pd	0.06638400	0.27149700	-0.10914600
C	-1.95424400	3.67551400	0.13819900
C	-0.17556100	5.19761100	0.71264200
C	2.78819100	3.93057200	0.15853100
C	2.80647700	2.67751900	2.22121200
C	0.79967600	1.93094800	-1.40337400
C	-2.81865100	4.75194700	-0.05841700
H	-2.32877800	2.66548000	0.00460500
C	-1.04527400	6.27379000	0.52854900
H	0.84592200	5.39274400	1.02020400
C	4.08529600	4.37085500	0.41181000
H	2.28521200	4.24419700	-0.74960000
C	4.10891900	3.11833900	2.47790100
H	2.31071800	2.01600900	2.92788600
C	2.10827100	1.71274800	-1.89505900
C	-0.16798100	2.35181600	-2.33839800
C	-2.36564000	6.05927700	0.12932800
H	-3.84675600	4.56227100	-0.35570700
H	-0.68376000	7.28598200	0.69365400
C	4.75156000	3.96205200	1.57037500
H	4.57963500	5.02888500	-0.29842100
H	4.61769300	2.80319300	3.38546300
C	2.44013400	1.97173700	-3.22971900
H	2.89099700	1.38089200	-1.22295600
C	0.16573100	2.61261500	-3.67415000
H	-1.18461900	2.54200600	-2.01461500
C	1.47603800	2.44664100	-4.12340900
H	3.46379000	1.81338600	-3.56198100

H	-0.60430700	2.97228100	-4.35345600
P	1.73217500	-1.60616400	-0.03100900
C	1.35890100	-2.97838000	-1.22407200
C	1.85182800	-2.45223500	1.61833100
C	3.53226900	-1.29325500	-0.37439300
C	0.83443700	-2.60431500	-2.47272400
C	1.57166200	-4.34110400	-0.96581200
C	2.93525300	-3.26761900	1.98933100
C	0.82331100	-2.24121400	2.54966000
C	4.18561300	-0.31938900	0.40105500
C	4.25956800	-1.94466400	-1.38103800
C	0.54687000	-3.56495200	-3.44319800
H	0.64579700	-1.55309300	-2.67675200
C	1.27019200	-5.30344400	-1.93275700
H	1.96687900	-4.65799700	-0.00578200
C	2.97230800	-3.87387200	3.24597200
H	3.76032300	-3.41763300	1.29895500
C	0.85819200	-2.85038100	3.80636900
H	0.00115200	-1.57861500	2.29363900
C	5.52786500	-0.01318700	0.18356900
H	3.63837600	0.21462700	1.17262800
C	5.60521600	-1.63385900	-1.60148500
H	3.78053600	-2.69839600	-1.99714000
C	0.76092300	-4.91848100	-3.17424100
H	0.14515700	-3.25585400	-4.40463900
C	1.93146800	-3.67068500	4.15593700
H	3.81834900	-4.50055800	3.51676300
H	0.05077300	-2.67177800	4.51156600
C	6.24391700	-0.67061800	-0.82109300
H	6.00714700	0.74948200	0.79144900
H	6.15188800	-2.15008100	-2.38680400
H	0.52719700	-5.66853400	-3.92533500
H	1.96422200	-4.14073800	5.13544600
H	7.28905600	-0.42893100	-0.99609600
H	1.43626300	-6.35548900	-1.71407800
H	-3.03645700	6.90086000	-0.02266100
H	5.76495700	4.30369200	1.76553000

H	1.74229200	2.68052900	-5.15131900
C	-3.59498000	0.38298900	-0.78306200
C	-3.37570500	0.64505500	-2.14764600
C	-4.74717100	0.90628200	-0.17770200
C	-4.29149500	1.39103500	-2.88840200
H	-2.47660500	0.26956200	-2.62926500
C	-5.65589300	1.66960800	-0.91739900
H	-4.94025800	0.72065300	0.87380700
C	-5.43468700	1.91011500	-2.27381800
H	-4.10692900	1.57621900	-3.94342600
H	-6.54130700	2.06952600	-0.42960200
H	-6.14413800	2.49987200	-2.84825100
C	-2.75780000	-2.34010800	-0.42527200
C	-3.84359200	-2.63844400	-1.26325100
C	-1.96441200	-3.40145100	0.04154200
C	-4.12444700	-3.95915000	-1.62463900
H	-4.47841600	-1.84224500	-1.63667800
C	-2.25112600	-4.71936600	-0.31103600
H	-1.11656500	-3.19957700	0.68856700
C	-3.33156800	-5.00341000	-1.14953300
H	-4.96954800	-4.16741800	-2.27615800
H	-1.62049100	-5.52246000	0.05989200
H	-3.55078400	-6.02997200	-1.43144400
P	-2.31276100	-0.61459900	0.11541300
C	-2.95256000	-0.62476400	1.86338700
C	-2.39459100	0.27134600	2.78928800
C	-3.97436700	-1.48871000	2.29502100
C	-2.85274700	0.30947600	4.10895600
H	-1.59142800	0.93312300	2.47484300
C	-4.42668800	-1.45308200	3.61521500
H	-4.41648100	-2.19473600	1.59892800
C	-3.86776500	-0.55319000	4.52598000
H	-2.40899200	1.01120100	4.81051900
H	-5.21585500	-2.13051100	3.93164800
H	-4.21952900	-0.52767500	5.55417700

IRC of triphenylphosphonin C−P oxidative -Point15

0 1

P	0.43547100	2.38363600	0.77903200
C	-0.60986500	3.87620900	0.50075200
C	2.12752400	3.06866700	1.05906800
Pd	0.06929300	0.27976700	-0.11042500
C	-1.95428100	3.67518900	0.13617800
C	-0.17589800	5.19665600	0.71300700
C	2.78374800	3.92555700	0.15896800
C	2.80798700	2.67630000	2.22370300
C	0.79845400	1.89938200	-1.42177100
C	-2.81816600	4.75184000	-0.06062000
H	-2.32918900	2.66547700	0.00136700
C	-1.04492200	6.27308700	0.52753800
H	0.84496400	5.39167300	1.02267000
C	4.08109800	4.36761600	0.40959400
H	2.27853900	4.23778200	-0.74841600
C	4.11060900	3.11795100	2.47710000
H	2.31345700	2.01722400	2.93349300
C	2.11027100	1.69990200	-1.90742800
C	-0.16748500	2.33941100	-2.34775000
C	-2.36523000	6.05916500	0.12779100
H	-3.84599300	4.56246000	-0.35912800
H	-0.68300900	7.28515000	0.69266300
C	4.75040600	3.96145700	1.56742400
H	4.57334800	5.02523300	-0.30249700
H	4.62114400	2.80473500	3.38436100
C	2.44414800	1.97618900	-3.23806500
H	2.89177200	1.36283000	-1.23643800
C	0.16823800	2.61753300	-3.67938900
H	-1.18477500	2.52364300	-2.02214800
C	1.47922300	2.45554100	-4.12831200
H	3.46908300	1.82619500	-3.57037900
H	-0.60031200	2.98558000	-4.35594400
P	1.73307200	-1.60758300	-0.03133700
C	1.35918400	-2.97906000	-1.22438200
C	1.85182000	-2.45266100	1.61824100
C	3.53262500	-1.29367200	-0.37442300

C	0.83473800	-2.60466300	-2.47296300
C	1.57161700	-4.34180400	-0.96607800
C	2.93534000	-3.26779300	1.98949800
C	0.82318900	-2.24149200	2.54942000
C	4.18552600	-0.31949800	0.40099300
C	4.25995900	-1.94505100	-1.38102200
C	0.54686500	-3.56522600	-3.44341300
H	0.64691100	-1.55339800	-2.67745800
C	1.26996700	-5.30397700	-1.93307100
H	1.96683000	-4.65874000	-0.00606300
C	2.97230400	-3.87383800	3.24619700
H	3.76049400	-3.41774400	1.29922300
C	0.85808200	-2.85033900	3.80628400
H	0.00060000	-1.57936300	2.29362600
C	5.52771700	-0.01307800	0.18349700
H	3.63815200	0.21481800	1.17223100
C	5.60553000	-1.63399600	-1.60139400
H	3.78105400	-2.69883600	-1.99714900
C	0.76071900	-4.91878700	-3.17450400
H	0.14526000	-3.25600300	-4.40484700
C	1.93137000	-3.67053000	4.15603000
H	3.81835300	-4.50042000	3.51716800
H	0.05064600	-2.67158900	4.51140600
C	6.24392900	-0.67053800	-0.82101900
H	6.00670000	0.74991500	0.79117400
H	6.15234500	-2.15010500	-2.38667600
H	0.52691400	-5.66873900	-3.92566400
H	1.96406800	-4.14039300	5.13562100
H	7.28901300	-0.42862500	-0.99601300
H	1.43592300	-6.35606100	-1.71453200
H	-3.03577100	6.90091100	-0.02449900
H	5.76356600	4.30511200	1.76030500
H	1.74616400	2.69880700	-5.15386700
C	-3.59517300	0.38284400	-0.78269800
C	-3.37579800	0.64428800	-2.14736700
C	-4.74722200	0.90653400	-0.17744100
C	-4.29133900	1.39049000	-2.88825800

H	-2.47705900	0.26815100	-2.62911500
C	-5.65579500	1.66973800	-0.91737200
H	-4.94024600	0.72134900	0.87415000
C	-5.43442000	1.90993100	-2.27382500
H	-4.10661300	1.57549100	-3.94327200
H	-6.54113900	2.06993800	-0.42970300
H	-6.14368800	2.49975100	-2.84840700
C	-2.75834800	-2.34052500	-0.42492900
C	-3.84395700	-2.63879100	-1.26314500
C	-1.96466800	-3.40171400	0.04169100
C	-4.12452700	-3.95946500	-1.62476900
H	-4.47880400	-1.84257800	-1.63648500
C	-2.25111200	-4.71961400	-0.31116000
H	-1.11698200	-3.19983100	0.68893100
C	-3.33148900	-5.00364500	-1.14972900
H	-4.96951600	-4.16779800	-2.27639600
H	-1.62038300	-5.52267700	0.05965300
H	-3.55053700	-6.03019400	-1.43179900
P	-2.31457800	-0.61535100	0.11683600
C	-2.95385500	-0.62512800	1.86432700
C	-2.39555400	0.27112100	2.78991600
C	-3.97543200	-1.48922500	2.29601600
C	-2.85344300	0.30918700	4.10963800
H	-1.59262700	0.93340300	2.47593100
C	-4.42741200	-1.45353200	3.61626500
H	-4.41762700	-2.19525900	1.59998400
C	-3.86830500	-0.55353400	4.52683200
H	-2.40955500	1.01100800	4.81100000
H	-5.21648500	-2.13094800	3.93293700
H	-4.21989300	-0.52800300	5.55508500

IRC of triphenylphosphonin C–P oxidative -Point16

0 1

P	0.42763700	2.38343000	0.80595700
C	-0.61030000	3.87470300	0.50203500
C	2.12497700	3.06504700	1.06283700
Pd	0.07223400	0.28805100	-0.11158800

C	-1.95431000	3.67486700	0.13429000
C	-0.17629100	5.19572100	0.71354500
C	2.77922300	3.92057000	0.15957200
C	2.80945400	2.67509200	2.22630300
C	0.79746000	1.86775000	-1.44096700
C	-2.81767100	4.75172000	-0.06284200
H	-2.32949100	2.66545200	-0.00180700
C	-1.04459600	6.27240800	0.52655300
H	0.84392300	5.39063900	1.02537400
C	4.07686700	4.36431000	0.40742700
H	2.27178700	4.23153100	-0.74701800
C	4.11226900	3.11754700	2.47634100
H	2.31620800	2.01845200	2.93922900
C	2.11232500	1.68690900	-1.92011400
C	-0.16688300	2.32713900	-2.35722400
C	-2.36481400	6.05904400	0.12618600
H	-3.84519300	4.56262700	-0.36265600
H	-0.68230000	7.28435500	0.69165800
C	4.74924800	3.96078600	1.56448100
H	4.56700600	5.02148500	-0.30655500
H	4.62458500	2.80625800	3.38328200
C	2.44812700	1.98061600	-3.24645500
H	2.89248500	1.34419600	-1.25039500
C	0.17075600	2.62249100	-3.68452800
H	-1.18475800	2.50551700	-2.02981000
C	1.48238100	2.46446700	-4.13318400
H	3.47429600	1.83891500	-3.57872500
H	-0.59637000	2.99889900	-4.35815900
P	1.73396400	-1.60903700	-0.03172300
C	1.35949100	-2.97977700	-1.22471700
C	1.85179600	-2.45306900	1.61813200
C	3.53297000	-1.29407600	-0.37447500
C	0.83505000	-2.60504000	-2.47321900
C	1.57158200	-4.34253700	-0.96636000
C	2.93542100	-3.26794200	1.98965000
C	0.82304700	-2.24177200	2.54916200
C	4.18540600	-0.31957600	0.40090300

C	4.26036100	-1.94545400	-1.38099800
C	0.54687000	-3.56552200	-3.44364600
H	0.64802500	-1.55373700	-2.67819400
C	1.26973500	-5.30453900	-1.93339600
H	1.96679500	-4.65951400	-0.00636200
C	2.97229600	-3.87378500	3.24640500
H	3.76066100	-3.41782300	1.29948000
C	0.85796200	-2.85029300	3.80618600
H	-0.00000700	-1.58015400	2.29359800
C	5.52754500	-0.01294900	0.18341700
H	3.63785300	0.21509700	1.17173500
C	5.60585300	-1.63414300	-1.60128500
H	3.78159000	-2.69930100	-1.99714600
C	0.76051300	-4.91911700	-3.17477800
H	0.14537400	-3.25617400	-4.40507200
C	1.93126900	-3.67036200	4.15611000
H	3.81835600	-4.50026000	3.51755200
H	0.05050700	-2.67140500	4.51122800
C	6.24393400	-0.67045300	-0.82093100
H	6.00621500	0.75038500	0.79088000
H	6.15282100	-2.15014500	-2.38651700
H	0.52661700	-5.66896700	-3.92600100
H	1.96391600	-4.14003500	5.13578300
H	7.28896300	-0.42831200	-0.99590600
H	1.43555900	-6.35666500	-1.71499700
H	-3.03505900	6.90094800	-0.02652600
H	5.76219000	4.30639500	1.75504700
H	1.74994400	2.71704200	-5.15634300
C	-3.59535500	0.38269000	-0.78231500
C	-3.37588700	0.64349500	-2.14707200
C	-4.74726500	0.90678900	-0.17716800
C	-4.29117500	1.38992400	-2.88810600
H	-2.47752100	0.26669200	-2.62895000
C	-5.65568700	1.66986800	-0.91734000
H	-4.94022600	0.72206200	0.87450500
C	-5.43414100	1.90973700	-2.27383000
H	-4.10628800	1.57473100	-3.94311100

H	-6.54095900	2.07035500	-0.42980200
H	-6.14322400	2.49961900	-2.84856500
C	-2.75892900	-2.34096900	-0.42456100
C	-3.84434300	-2.63916100	-1.26302500
C	-1.96493700	-3.40199700	0.04184600
C	-4.12461000	-3.95980000	-1.62490300
H	-4.47922100	-1.84293300	-1.63626800
C	-2.25109600	-4.71987900	-0.31129000
H	-1.11740200	-3.20009500	0.68928900
C	-3.33140600	-5.00389700	-1.14993700
H	-4.96948100	-4.16820100	-2.27664600
H	-1.62026600	-5.52291000	0.05939800
H	-3.55027400	-6.03043200	-1.43217700
P	-2.31642500	-0.61615900	0.11830600
C	-2.95520800	-0.62551700	1.86528600
C	-2.39655700	0.27087400	2.79055000
C	-3.97654400	-1.48976000	2.29704200
C	-2.85415800	0.30888700	4.11033100
H	-1.59387800	0.93366700	2.47700500
C	-4.42816400	-1.45399700	3.61735000
H	-4.41882800	-2.19580600	1.60107600
C	-3.86886300	-0.55388700	4.52770700
H	-2.41013000	1.01081100	4.81148000
H	-5.21713800	-2.13140000	3.93427500
H	-4.22026200	-0.52833600	5.55601900

IRC of triphenylphosphonin C–P oxidative -Point17

0 1

P	0.41991200	2.38342000	0.83239600
C	-0.61081500	3.87323700	0.50364000
C	2.12230400	3.06143700	1.06687600
Pd	0.07524500	0.29639800	-0.11264700
C	-1.95432400	3.67454500	0.13253200
C	-0.17676000	5.19481700	0.71431700
C	2.77454600	3.91554600	0.16036400
C	2.81088300	2.67389500	2.22908000
C	0.79665400	1.83613400	-1.46076400

C	-2.81715600	4.75158300	-0.06514400
H	-2.32962800	2.66538200	-0.00493500
C	-1.04430200	6.27176200	0.52558700
H	0.84277800	5.38964600	1.02840300
C	4.07254200	4.36087700	0.40526000
H	2.26482300	4.22533200	-0.74537200
C	4.11392000	3.11713000	2.47561800
H	2.31901700	2.01969800	2.94519900
C	2.11438900	1.67364800	-1.93317300
C	-0.16618700	2.31483100	-2.36684100
C	-2.36438300	6.05891100	0.12446600
H	-3.84432900	4.56276700	-0.36640100
H	-0.68164500	7.28360900	0.69061600
C	4.74806600	3.96001500	1.56148700
H	4.56052600	5.01755600	-0.31068500
H	4.62808100	2.80778400	3.38220300
C	2.45204500	1.98501600	-3.25489700
H	2.89317200	1.32495900	-1.26489900
C	0.17328600	2.62745800	-3.68955300
H	-1.18453900	2.48753900	-2.03751400
C	1.48553000	2.47354400	-4.13802400
H	3.47943100	1.85166600	-3.58696700
H	-0.59248700	3.01231100	-4.36000200
P	1.73484900	-1.61052400	-0.03217100
C	1.35982400	-2.98054100	-1.22508000
C	1.85175500	-2.45346800	1.61799900
C	3.53331100	-1.29447900	-0.37455000
C	0.83538600	-2.60545100	-2.47349800
C	1.57155500	-4.34331200	-0.96666200
C	2.93549500	-3.26807100	1.98978800
C	0.82288300	-2.24206300	2.54887800
C	4.18525200	-0.31962200	0.40077700
C	4.26078300	-1.94588200	-1.38096100
C	0.54689100	-3.56584800	-3.44390200
H	0.64916800	-1.55410800	-2.67895500
C	1.26949100	-5.30514100	-1.93373900
H	1.96676800	-4.66033000	-0.00668000

C	2.97228300	-3.87370900	3.24660400
H	3.76082700	-3.41787900	1.29972900
C	0.85782900	-2.85024600	3.80606800
H	-0.00066500	-1.58099500	2.29353200
C	5.52734600	-0.01279200	0.18332500
H	3.63746700	0.21546500	1.17112900
C	5.60619500	-1.63430400	-1.60115200
H	3.78216200	-2.69980700	-1.99712400
C	0.76030300	-4.91947900	-3.17507000
H	0.14550700	-3.25637200	-4.40532100
C	1.93116400	-3.67017600	4.15618000
H	3.81836000	-4.50007100	3.51792500
H	0.05034800	-2.67122600	4.51102500
C	6.24393500	-0.67035900	-0.82082800
H	6.00568100	0.75090700	0.79055800
H	6.15333200	-2.15020400	-2.38631800
H	0.52630100	-5.66922500	-3.92635200
H	1.96376100	-4.13965500	5.13593800
H	7.28890900	-0.42798300	-0.99577300
H	1.43516500	-6.35731100	-1.71547700
H	-3.03430900	6.90096600	-0.02881800
H	5.76081800	4.30752200	1.74964700
H	1.75370400	2.73570600	-5.15861600
C	-3.59554000	0.38251500	-0.78190300
C	-3.37598300	0.64265600	-2.14675200
C	-4.74730900	0.90705200	-0.17687800
C	-4.29100400	1.38931900	-2.88794300
H	-2.47800300	0.26515600	-2.62875500
C	-5.65557000	1.67000600	-0.91730300
H	-4.94021200	0.72280300	0.87488100
C	-5.43384700	1.90953200	-2.27383400
H	-4.10595100	1.57391200	-3.94294100
H	-6.54076600	2.07079500	-0.42990400
H	-6.14273700	2.49947400	-2.84873300
C	-2.75955200	-2.34144900	-0.42415600
C	-3.84475900	-2.63956400	-1.26288400
C	-1.96522500	-3.40230700	0.04201300

C	-4.12469700	-3.96016400	-1.62504500
H	-4.47967700	-1.84332400	-1.63601700
C	-2.25107700	-4.72016900	-0.31143000
H	-1.11783500	-3.20037600	0.68964900
C	-3.33131400	-5.00417500	-1.15016300
H	-4.96944100	-4.16863500	-2.27691200
H	-1.62013500	-5.52316600	0.05911900
H	-3.54998600	-6.03069300	-1.43259300
P	-2.31830800	-0.61702600	0.11983400
C	-2.95664300	-0.62594200	1.86627700
C	-2.39762500	0.27059300	2.79120300
C	-3.97772600	-1.49032800	2.29811700
C	-2.85491200	0.30857000	4.11104900
H	-1.59520100	0.93388800	2.47804900
C	-4.42896000	-1.45448700	3.61849300
H	-4.42010600	-2.19638800	1.60222500
C	-3.86945300	-0.55425900	4.52862500
H	-2.41073300	1.01060200	4.81197200
H	-5.21782700	-2.13187800	3.93569000
H	-4.22064700	-0.52868300	5.55700200

IRC of triphenylphosphonin C−P oxidative -Point18

0 1

P	0.41231100	2.38358000	0.85820500
C	-0.61146500	3.87183500	0.50572100
C	2.11944500	3.05780800	1.07135000
Pd	0.07837700	0.30486000	-0.11359800
C	-1.95432900	3.67421400	0.13091300
C	-0.17734400	5.19394900	0.71544000
C	2.76959600	3.91037800	0.16140500
C	2.81228200	2.67270300	2.23216300
C	0.79607800	1.80480100	-1.48098900
C	-2.81660400	4.75142800	-0.06761800
H	-2.32957000	2.66525400	-0.00804600
C	-1.04404700	6.27115500	0.52463600
H	0.84145900	5.38867300	1.03197900
C	4.06801400	4.35721700	0.40302800

H	2.25742500	4.21895600	-0.74339600
C	4.11559700	3.11670100	2.47493400
H	2.32197000	2.02099000	2.95162200
C	2.11645000	1.66007600	-1.94665700
C	-0.16536200	2.30235600	-2.37661300
C	-2.36391900	6.05876100	0.12255500
H	-3.84334100	4.56289000	-0.37060400
H	-0.68105300	7.28292500	0.68949800
C	4.74682400	3.95910600	1.55835600
H	4.55373400	5.01324600	-0.31508000
H	4.63176500	2.80934900	3.38108200
C	2.45589100	1.98934600	-3.26350600
H	2.89394700	1.30497600	-1.28027400
C	0.17584300	2.63236300	-3.69451700
H	-1.18412100	2.46941700	-2.04537800
C	1.48871400	2.48294800	-4.14289800
H	3.48447600	1.86440800	-3.59526900
H	-0.58866800	3.02574600	-4.36151400
P	1.73572700	-1.61204200	-0.03269100
C	1.36019200	-2.98136600	-1.22548100
C	1.85169900	-2.45386900	1.61783100
C	3.53365500	-1.29489200	-0.37464800
C	0.83576600	-2.60590700	-2.47381300
C	1.57153400	-4.34414900	-0.96699400
C	2.93556500	-3.26818300	1.98991500
C	0.82269000	-2.24237700	2.54855000
C	4.18505500	-0.31962600	0.40060300
C	4.26124600	-1.94635000	-1.38090500
C	0.54693900	-3.56620900	-3.44419300
H	0.65039500	-1.55451400	-2.67974000
C	1.26923200	-5.30579600	-1.93411100
H	1.96674200	-4.66121700	-0.00702700
C	2.97226600	-3.87360500	3.24679800
H	3.76100100	-3.41791200	1.29998000
C	0.85767500	-2.85019700	3.80591900
H	-0.00139200	-1.58191700	2.29339000
C	5.52710800	-0.01259100	0.18321600

H	3.63696000	0.21596500	1.17035900
C	5.60657300	-1.63447900	-1.60098200
H	3.78280800	-2.70039000	-1.99706100
C	0.76008800	-4.91988200	-3.17539100
H	0.14568200	-3.25660300	-4.40561100
C	1.93104800	-3.66996500	4.15624100
H	3.81836700	-4.49983600	3.51830700
H	0.05015200	-2.67105600	4.51077700
C	6.24393600	-0.67024500	-0.82069900
H	6.00506900	0.75152300	0.79018700
H	6.15391200	-2.15029100	-2.38605300
H	0.52595600	-5.66952200	-3.92672800
H	1.96359700	-4.13923100	5.13609100
H	7.28885500	-0.42761500	-0.99559700
H	1.43472400	-6.35801700	-1.71599100
H	-3.03347000	6.90096300	-0.03157600
H	5.75944200	4.30843800	1.74388000
H	1.75751700	2.75520000	-5.16073000
C	-3.59574800	0.38230400	-0.78144000
C	-3.37610000	0.64173700	-2.14639000
C	-4.74736500	0.90733300	-0.17656000
C	-4.29082200	1.38865200	-2.88776000
H	-2.47854000	0.26345400	-2.62851000
C	-5.65544400	1.67016500	-0.91726300
H	-4.94022000	0.72360200	0.87529100
C	-5.43353000	1.90931500	-2.27383900
H	-4.10559400	1.57298300	-3.94276000
H	-6.54055600	2.07129500	-0.43001600
H	-6.14220800	2.49931900	-2.84892200
C	-2.76023700	-2.34197500	-0.42369700
C	-3.84521800	-2.64001300	-1.26271200
C	-1.96554300	-3.40265700	0.04220000
C	-4.12478600	-3.96057000	-1.62520000
H	-4.48020100	-1.84376800	-1.63570900
C	-2.25105200	-4.72049300	-0.31158800
H	-1.11829900	-3.20068800	0.69002900
C	-3.33120300	-5.00448800	-1.15042400

H	-4.96938900	-4.16911900	-2.27721100
H	-1.61997400	-5.52345200	0.05879200
H	-3.54964500	-6.03098700	-1.43308300
P	-2.32024100	-0.61795800	0.12144000
C	-2.95820100	-0.62642100	1.86732100
C	-2.39880000	0.27026100	2.79189500
C	-3.97901800	-1.49094800	2.29927400
C	-2.85573600	0.30821900	4.11181700
H	-1.59663900	0.93403600	2.47906400
C	-4.42983100	-1.45502400	3.61973000
H	-4.42151400	-2.19703300	1.60347700
C	-3.87010200	-0.55466900	4.52961800
H	-2.41140000	1.01036400	4.81250700
H	-5.21857700	-2.13240500	3.93723300
H	-4.22106900	-0.52907000	5.55806900

IRC of triphenylphosphonin C−P oxidative -Point19

0 1

P	0.40484900	2.38387700	0.88299800
C	-0.61243900	3.87058500	0.50874700
C	2.11625900	3.05420100	1.07667800
Pd	0.08176800	0.31359800	-0.11441200
C	-1.95434100	3.67387100	0.12955700
C	-0.17812700	5.19313800	0.71713800
C	2.76416100	3.90489600	0.16288500
C	2.81364100	2.67152500	2.23579000
C	0.79591900	1.77458500	-1.50132400
C	-2.81598000	4.75125600	-0.07040400
H	-2.32933200	2.66505000	-0.01090600
C	-1.04383900	6.27062000	0.52366900
H	0.83987200	5.38772900	1.03634100
C	4.06309400	4.35312100	0.40069700
H	2.24942100	4.21218900	-0.74092900
C	4.11733300	3.11623500	2.47431100
H	2.32520500	2.02228900	2.95875200
C	2.11850500	1.64592200	-1.96097600
C	-0.16432100	2.28940300	-2.38681000

C	-2.36339400	6.05858800	0.12034000
H	-3.84216500	4.56299100	-0.37547600
H	-0.68053600	7.28234400	0.68820600
C	4.74544300	3.95796600	1.55500600
H	4.54638800	5.00829500	-0.31983600
H	4.63577200	2.81093100	3.37986900
C	2.45961400	1.99355800	-3.27233000
H	2.89513800	1.28464100	-1.29698500
C	0.17847100	2.63712300	-3.69935600
H	-1.18335800	2.45116800	-2.05369200
C	1.49199900	2.49299600	-4.14769800
H	3.48938200	1.87717600	-3.60339800
H	-0.58498800	3.03910800	-4.36231700
P	1.73660100	-1.61359600	-0.03332000
C	1.36061700	-2.98228700	-1.22593400
C	1.85162500	-2.45427900	1.61761300
C	3.53401400	-1.29533400	-0.37476500
C	0.83622300	-2.60643300	-2.47418000
C	1.57152900	-4.34508200	-0.96736900
C	2.93563000	-3.26827100	1.99003500
C	0.82245400	-2.24272300	2.54815500
C	4.18479600	-0.31956400	0.40036300
C	4.26178500	-1.94687200	-1.38080900
C	0.54703200	-3.56662500	-3.44453600
H	0.65175100	-1.55497200	-2.68052400
C	1.26895700	-5.30653600	-1.93453000
H	1.96671800	-4.66221100	-0.00741500
C	2.97224200	-3.87345600	3.24699900
H	3.76118700	-3.41792300	1.30024300
C	0.85748800	-2.85014300	3.80572500
H	-0.00219500	-1.58293900	2.29311400
C	5.52681500	-0.01231500	0.18309000
H	3.63628800	0.21664500	1.16937400
C	5.60701900	-1.63466400	-1.60075100
H	3.78357500	-2.70107900	-1.99693100
C	0.75986900	-4.92034700	-3.17575600
H	0.14591500	-3.25688100	-4.40595600

C	1.93091500	-3.66971100	4.15629600
H	3.81837600	-4.49953800	3.51871400
H	0.04990100	-2.67089600	4.51046500
C	6.24394500	-0.67009200	-0.82052300
H	6.00435300	0.75227400	0.78976200
H	6.15460100	-2.15039600	-2.38569300
H	0.52557500	-5.66987700	-3.92714500
H	1.96341500	-4.13874300	5.13625000
H	7.28880800	-0.42718200	-0.99534600
H	1.43422800	-6.35881500	-1.71655500
H	-3.03251300	6.90092900	-0.03494200
H	5.75798600	4.30905800	1.73756600
H	1.76149800	2.77632700	-5.16219700
C	-3.59601900	0.38202000	-0.78088700
C	-3.37626000	0.64068900	-2.14595300
C	-4.74745800	0.90764400	-0.17619500
C	-4.29062200	1.38788900	-2.88754100
H	-2.47917100	0.26151500	-2.62818000
C	-5.65531100	1.67036600	-0.91721600
H	-4.94029300	0.72447100	0.87574900
C	-5.43317900	1.90908100	-2.27384300
H	-4.10520200	1.57189800	-3.94255000
H	-6.54033400	2.07188800	-0.43015300
H	-6.14161700	2.49915200	-2.84914300
C	-2.76102500	-2.34257100	-0.42313600
C	-3.84574000	-2.64053600	-1.26249200
C	-1.96590700	-3.40306400	0.04242400
C	-4.12487300	-3.96104200	-1.62538000
H	-4.48082000	-1.84429700	-1.63532300
C	-2.25101200	-4.72086700	-0.31177600
H	-1.11880000	-3.20103900	0.69043200
C	-3.33106100	-5.00485700	-1.15073700
H	-4.96931400	-4.16967300	-2.27756000
H	-1.61976500	-5.52378000	0.05839500
H	-3.54922900	-6.03133300	-1.43367400
P	-2.32226300	-0.61898300	0.12318100
C	-2.95997900	-0.62699100	1.86846300

C	-2.40016700	0.26983800	2.79266700
C	-3.98049900	-1.49165500	2.30057500
C	-2.85668700	0.30781300	4.11268100
H	-1.59826100	0.93401900	2.48003300
C	-4.43083500	-1.45564100	3.62113200
H	-4.42312400	-2.19777600	1.60489200
C	-3.87086200	-0.55514300	4.53074500
H	-2.41217500	1.01007400	4.81312300
H	-5.21943600	-2.13301900	3.93898500
H	-4.22156500	-0.52951700	5.55928200

IRC of triphenylphosphonin C–P oxidative -Point20

0 1

P	0.39739500	2.38416500	0.90732200
C	-0.61354200	3.86938100	0.51208100
C	2.11290100	3.05060800	1.08234200
Pd	0.08537700	0.32248700	-0.11516500
C	-1.95440900	3.67353200	0.12829400
C	-0.17907200	5.19236500	0.71924800
C	2.75847500	3.89927900	0.16456200
C	2.81487600	2.67038700	2.23974000
C	0.79598900	1.74489700	-1.52159500
C	-2.81532700	4.75108200	-0.07343700
H	-2.32910300	2.66483700	-0.01370800
C	-1.04371800	6.27011300	0.52277600
H	0.83807600	5.38681700	1.04126700
C	4.05799000	4.34876000	0.39828400
H	2.24106600	4.20521200	-0.73822800
C	4.11902700	3.11573300	2.47375600
H	2.32836800	2.02366700	2.96627200
C	2.12067800	1.63185700	-1.97549900
C	-0.16317100	2.27650800	-2.39709500
C	-2.36284200	6.05842100	0.11783100
H	-3.84088700	4.56308700	-0.38083000
H	-0.68013600	7.28180700	0.68696900
C	4.74398000	3.95660000	1.55151500
H	4.53883500	5.00293000	-0.32482200

H	4.63986300	2.81252200	3.37866500
C	2.46337400	1.99777100	-3.28141200
H	2.89648700	1.26437600	-1.31395100
C	0.18112900	2.64186900	-3.70432900
H	-1.18249900	2.43292800	-2.06209700
C	1.49533500	2.50328600	-4.15262700
H	3.49428000	1.88976400	-3.61187500
H	-0.58137200	3.05227100	-4.36326600
P	1.73746600	-1.61517600	-0.03402000
C	1.36107700	-2.98327300	-1.22644300
C	1.85152900	-2.45470900	1.61734000
C	3.53437800	-1.29578900	-0.37491000
C	0.83674200	-2.60703000	-2.47461200
C	1.57153300	-4.34608500	-0.96778500
C	2.93568800	-3.26834700	1.99013700
C	0.82217800	-2.24310500	2.54768900
C	4.18448600	-0.31945000	0.40006000
C	4.26238700	-1.94744700	-1.38067500
C	0.54717500	-3.56711200	-3.44493900
H	0.65318400	-1.55549800	-2.68137800
C	1.26867900	-5.30734800	-1.93498800
H	1.96668400	-4.66327300	-0.00783500
C	2.97220900	-3.87326800	3.24719800
H	3.76138100	-3.41791700	1.30050500
C	0.85725800	-2.85009300	3.80547300
H	-0.00304600	-1.58401400	2.29274300
C	5.52647300	-0.01197200	0.18294100
H	3.63552000	0.21741000	1.16827100
C	5.60752600	-1.63487200	-1.60045600
H	3.78444500	-2.70186600	-1.99673900
C	0.75966400	-4.92088600	-3.17616800
H	0.14620700	-3.25722700	-4.40636500
C	1.93075700	-3.66942300	4.15633100
H	3.81839000	-4.49917300	3.51914100
H	0.04959300	-2.67074500	4.51008000
C	6.24396000	-0.66990500	-0.82030800
H	6.00354900	0.75313200	0.78929500

H	6.15539000	-2.15054600	-2.38522700
H	0.52519200	-5.67030700	-3.92760200
H	1.96320700	-4.13819500	5.13640100
H	7.28876700	-0.42669800	-0.99503100
H	1.43370500	-6.35968700	-1.71714600
H	-3.03145400	6.90090000	-0.03890000
H	5.75652400	4.30933000	1.73092100
H	1.76549700	2.79779400	-5.16377600
C	-3.59635300	0.38166300	-0.78027300
C	-3.37645600	0.63951300	-2.14546000
C	-4.74759400	0.90795900	-0.17580100
C	-4.29041100	1.38701700	-2.88730500
H	-2.47984400	0.25939500	-2.62776900
C	-5.65517700	1.67059100	-0.91717900
H	-4.94042900	0.72538700	0.87624100
C	-5.43280100	1.90881300	-2.27386200
H	-4.10477800	1.57066100	-3.94232600
H	-6.54009900	2.07255900	-0.43032400
H	-6.14096400	2.49896300	-2.84940800
C	-2.76188400	-2.34324000	-0.42250900
C	-3.84631500	-2.64113600	-1.26223000
C	-1.96630900	-3.40353600	0.04267600
C	-4.12495700	-3.96158500	-1.62558300
H	-4.48151200	-1.84490800	-1.63487300
C	-2.25095800	-4.72130200	-0.31200000
H	-1.11935000	-3.20145200	0.69087400
C	-3.33088200	-5.00529000	-1.15111200
H	-4.96922000	-4.17030000	-2.27795200
H	-1.61951400	-5.52416100	0.05793500
H	-3.54873400	-6.03173700	-1.43437400
P	-2.32436600	-0.62008400	0.12501300
C	-2.96191100	-0.62764700	1.86968500
C	-2.40169000	0.26933900	2.79351100
C	-3.98213000	-1.49245100	2.30197700
C	-2.85777700	0.30733700	4.11362300
H	-1.60003800	0.93391700	2.48105300
C	-4.43196600	-1.45634400	3.62264600

H	-4.42488200	-2.19861900	1.60641800
C	-3.87174400	-0.55569500	4.53197400
H	-2.41308100	1.00972200	4.81380600
H	-5.22041000	-2.13372800	3.94086200
H	-4.22216200	-0.53004200	5.56060300

IRC of triphenylphosphonin C–P oxidative -Point21

0 1

P	0.38998700	2.38444000	0.93062500
C	-0.61498200	3.86827500	0.51620200
C	2.10915500	3.04703700	1.08883500
Pd	0.08936200	0.33165700	-0.11580300
C	-1.95457000	3.67316300	0.12722500
C	-0.18037100	5.19163600	0.72216100
C	2.75222300	3.89334100	0.16669800
C	2.81589800	2.66933900	2.24437400
C	0.79655800	1.71665600	-1.54166600
C	-2.81463600	4.75086500	-0.07696400
H	-2.32885200	2.66455700	-0.01635100
C	-1.04379800	6.26964700	0.52200300
H	0.83580500	5.38593500	1.04737700
C	4.05242300	4.34390100	0.39575800
H	2.23196400	4.19771700	-0.73501800
C	4.12064100	3.11522900	2.47336200
H	2.33153900	2.02520700	2.97466200
C	2.12303000	1.61784400	-1.99057300
C	-0.16175900	2.26350300	-2.40772700
C	-2.36227400	6.05822000	0.11478600
H	-3.83940700	4.56312300	-0.38718100
H	-0.68000200	7.28133800	0.68580800
C	4.74229100	3.95490100	1.54779400
H	4.53070000	4.99677100	-0.33024600
H	4.64415000	2.81422300	3.37748900
C	2.46716600	2.00200700	-3.29085100
H	2.89831900	1.24441600	-1.33174800
C	0.18390100	2.64650700	-3.70944900
H	-1.18139200	2.41457700	-2.07100400

C	1.49883400	2.51415000	-4.15768500
H	3.49916300	1.90228300	-3.62060700
H	-0.57783500	3.06511400	-4.36413000
P	1.73832700	-1.61678400	-0.03483900
C	1.36162300	-2.98436600	-1.22703700
C	1.85141000	-2.45516300	1.61698700
C	3.53477100	-1.29625400	-0.37507300
C	0.83740400	-2.60773200	-2.47515100
C	1.57159600	-4.34719900	-0.96827500
C	2.93575200	-3.26837200	1.99024100
C	0.82182100	-2.24355600	2.54709300
C	4.18407200	-0.31922100	0.39969600
C	4.26314800	-1.94807300	-1.38044100
C	0.54747000	-3.56769700	-3.44545700
H	0.65479300	-1.55612400	-2.68232200
C	1.26847300	-5.30826700	-1.93553000
H	1.96667200	-4.66445100	-0.00831300
C	2.97216900	-3.87298100	3.24742700
H	3.76162400	-3.41783900	1.30081700
C	0.85693600	-2.85006000	3.80512100
H	-0.00400900	-1.58522900	2.29216200
C	5.52603000	-0.01145600	0.18282400
H	3.63452800	0.21836100	1.16697500
C	5.60818400	-1.63504400	-1.59999300
H	3.78557700	-2.70280100	-1.99641200
C	0.75957100	-4.92152700	-3.17668100
H	0.14669200	-3.25766700	-4.40690400
C	1.93054600	-3.66906600	4.15634900
H	3.81842500	-4.49864600	3.51965600
H	0.04914500	-2.67064200	4.50954700
C	6.24400100	-0.66957700	-0.81995200
H	6.00254100	0.75425100	0.78882900
H	6.15642900	-2.15068000	-2.38451100
H	0.52492900	-5.67083800	-3.92816200
H	1.96293600	-4.13753600	5.13655600
H	7.28874800	-0.42601200	-0.99451200
H	1.43323000	-6.36066900	-1.71781800

H	-3.03025600	6.90083100	-0.04395100
H	5.75495400	4.30909500	1.72364300
H	1.76968100	2.82043500	-5.16516500
C	-3.59680900	0.38115700	-0.77955500
C	-3.37670300	0.63809900	-2.14487200
C	-4.74783800	0.90825100	-0.17538900
C	-4.29015500	1.38593200	-2.88706100
H	-2.48059200	0.25691500	-2.62720700
C	-5.65506700	1.67081000	-0.91721100
H	-4.94073400	0.72634600	0.87675100
C	-5.43236900	1.90845000	-2.27395400
H	-4.10425400	1.56912300	-3.94210100
H	-6.53988800	2.07330800	-0.43063200
H	-6.14019700	2.49868600	-2.84981400
C	-2.76286800	-2.34404300	-0.42176800
C	-3.84695500	-2.64189300	-1.26192900
C	-1.96676100	-3.40412100	0.04296700
C	-4.12497100	-3.96227400	-1.62588700
H	-4.48232500	-1.84570100	-1.63434300
C	-2.25082100	-4.72184100	-0.31231900
H	-1.11997300	-3.20195900	0.69138300
C	-3.33056000	-5.00584500	-1.15165400
H	-4.96900700	-4.17108800	-2.27850600
H	-1.61911500	-5.52462300	0.05731600
H	-3.54798600	-6.03225600	-1.43535800
P	-2.32661000	-0.62132200	0.12700300
C	-2.96414200	-0.62847400	1.87104100
C	-2.40354700	0.26868200	2.79449400
C	-3.98403100	-1.49344600	2.30353400
C	-2.85917600	0.30670500	4.11471200
H	-1.60215100	0.93363200	2.48215400
C	-4.43334400	-1.45726500	3.62432700
H	-4.42689300	-2.19968400	1.60810900
C	-3.87289400	-0.55644500	4.53336500
H	-2.41431200	1.00922600	4.81463500
H	-5.22159500	-2.13468700	3.94292500
H	-4.22301000	-0.53078600	5.56209400

IRC of triphenylphosphonin C−P oxidative -Point22

0 1

P	0.38364300	2.39234000	0.95543500
C	-0.61570100	3.87491900	0.52341800
C	2.10612300	3.05115500	1.09841700
Pd	0.09477500	0.34868300	-0.11393600
C	-1.95378000	3.68048300	0.12868300
C	-0.18090700	5.19858400	0.72819900
C	2.74659100	3.89465500	0.17153300
C	2.81774900	2.67600900	2.25196000
C	0.79858000	1.69754800	-1.55896800
C	-2.81280700	4.75837100	-0.07860200
H	-2.32763500	2.67196000	-0.01645600
C	-1.04291700	6.27689100	0.52374600
H	0.83419000	5.39267200	1.05695400
C	4.04762500	4.34597700	0.39537700
H	2.22335500	4.19730600	-0.72907300
C	4.12325300	3.12221100	2.47541800
H	2.33566100	2.03460800	2.98618200
C	2.12653400	1.61156400	-2.00370100
C	-0.15912200	2.25811500	-2.41622300
C	-2.36054600	6.06572900	0.11363600
H	-3.83665000	4.57090500	-0.39208700
H	-0.67894400	7.28858900	0.68717600
C	4.74155200	3.96025600	1.54612000
H	4.52329100	4.99722900	-0.33381100
H	4.64962800	2.82351400	3.37867100
C	2.47192300	2.01373800	-3.29821600
H	2.90159500	1.23264400	-1.34772900
C	0.18772200	2.65860600	-3.71228200
H	-1.17906600	2.40395900	-2.07793100
C	1.50339000	2.53293400	-4.16045400
H	3.50494900	1.92212100	-3.62717800
H	-0.57344100	3.08517100	-4.36250200
P	1.74012400	-1.61084600	-0.03337900
C	1.36311800	-2.97800000	-1.22528700

C	1.85221700	-2.44805600	1.61895400
C	3.53612900	-1.28921400	-0.37290100
C	0.83906000	-2.60099800	-2.47337000
C	1.57251800	-4.34085800	-0.96636200
C	2.93674700	-3.26080500	1.99272300
C	0.82237700	-2.23642500	2.54879900
C	4.18454800	-0.31135200	0.40156200
C	4.26495800	-1.94131300	-1.37773900
C	0.54870200	-3.56086300	-3.44361900
H	0.65746100	-1.54930600	-2.68095300
C	1.26906100	-5.30175400	-1.93363200
H	1.96751300	-4.65815700	-0.00638000
C	2.97306100	-3.86503400	3.25006900
H	3.76281800	-3.41018100	1.30353100
C	0.85752700	-2.84237500	3.80710500
H	-0.00406200	-1.57889100	2.29381400
C	5.52648400	-0.00330100	0.18498000
H	3.63436500	0.22704400	1.16780600
C	5.60989400	-1.62781200	-1.59703700
H	3.78781900	-2.69645500	-1.99353000
C	0.76030800	-4.91475200	-3.17477500
H	0.14818500	-3.25069200	-4.40511800
C	1.93126100	-3.66101500	4.15876400
H	3.81940700	-4.49042200	3.52262800
H	0.04959200	-2.66287700	4.51132800
C	6.24501800	-0.66172200	-0.81719300
H	6.00237000	0.76310100	0.79056900
H	6.15859100	-2.14348600	-2.38120000
H	0.52548800	-5.66396700	-3.92628800
H	1.96359100	-4.12912700	5.13913600
H	7.28970900	-0.41777700	-0.99154700
H	1.43351100	-6.35421700	-1.71601500
H	-3.02776600	6.90848600	-0.04756400
H	5.75446000	4.31568300	1.71805900
H	1.77490400	2.85135600	-5.16399000
C	-3.59642100	0.38817700	-0.77617400
C	-3.37608000	0.64407000	-2.14164800

C	-4.74716200	0.91628400	-0.17236200
C	-4.28893100	1.39228000	-2.88424800
H	-2.48053400	0.26164200	-2.62398700
C	-5.65393500	1.67883200	-0.91469300
H	-4.94015400	0.73513100	0.87988500
C	-5.43089600	1.91573300	-2.27151900
H	-4.10275400	1.57487000	-3.93933400
H	-6.53862100	2.08199100	-0.42843800
H	-6.13832700	2.50606600	-2.84775900
C	-2.76310100	-2.33734400	-0.41834100
C	-3.84683400	-2.63514800	-1.25896300
C	-1.96638800	-3.39720000	0.04583600
C	-4.12414200	-3.95544700	-1.62363900
H	-4.48240700	-1.83899900	-1.63110900
C	-2.24979100	-4.71486100	-0.31015900
H	-1.11974000	-3.19495400	0.69442700
C	-3.32933500	-4.99887800	-1.14973000
H	-4.96790900	-4.16436000	-2.27656400
H	-1.61774400	-5.51755500	0.05906700
H	-3.54624400	-6.02524000	-1.43399400
P	-2.32804300	-0.61506000	0.13169000
C	-2.96567300	-0.62179500	1.87508600
C	-2.40467900	0.27553800	2.79814200
C	-3.98523500	-1.48690600	2.30783200
C	-2.85979800	0.31362800	4.11848200
H	-1.60352300	0.94079500	2.48583500
C	-4.43397900	-1.45062200	3.62876900
H	-4.42822400	-2.19323300	1.61256600
C	-3.87326300	-0.54962500	4.53748700
H	-2.41474300	1.01628900	4.81812300
H	-5.22203000	-2.12808200	3.94777300
H	-4.22305200	-0.52395200	5.56632200

IRC of triphenylphosphonin C–P oxidative -Point23

0 1

P	0.37550000	2.38500600	0.97405400
C	-0.61863200	3.86653200	0.52658900

C	2.10084100	3.04018000	1.10386600
Pd	0.09878500	0.35076600	-0.11686300
C	-1.95497800	3.67274100	0.12555300
C	-0.18354700	5.19040700	0.73022400
C	2.73858500	3.88023000	0.17168500
C	2.81749400	2.66769100	2.25529600
C	0.79932200	1.66531900	-1.58063800
C	-2.81265900	4.75088700	-0.08570100
H	-2.32841300	2.66430100	-0.02112100
C	-1.04383600	6.26907700	0.52066300
H	0.83037400	5.38417100	1.06286400
C	4.04066500	4.33185300	0.38950900
H	2.21218500	4.18077100	-0.72780700
C	4.12402300	3.11383100	2.47246700
H	2.33785800	2.02923600	2.99371400
C	2.12835400	1.59034600	-2.02233800
C	-0.15808300	2.23782400	-2.42985500
C	-2.36036800	6.05822300	0.10686000
H	-3.83540200	4.56378200	-0.40300300
H	-0.67961200	7.28077600	0.68358400
C	4.73891900	3.94956900	1.53881400
H	4.51372800	4.98084000	-0.34340400
H	4.65364200	2.81749900	3.37462500
C	2.47467600	2.00995300	-3.31112700
H	2.90346800	1.20619000	-1.36945300
C	0.18963700	2.65531600	-3.72025300
H	-1.17833300	2.37858200	-2.09010700
C	1.50599400	2.53669600	-4.16845200
H	3.50857100	1.92589800	-3.63945000
H	-0.57121300	3.08942500	-4.36585400
P	1.73988000	-1.62018500	-0.03703000
C	1.36258600	-2.98703400	-1.22858600
C	1.85099900	-2.45622300	1.61585700
C	3.53549200	-1.29755000	-0.37581200
C	0.83875800	-2.60970400	-2.47667800
C	1.57123300	-4.34993800	-0.96940700
C	2.93571200	-3.26851100	1.99016500

C	0.82092600	-2.24453500	2.54545700
C	4.18301700	-0.31872300	0.39818900
C	4.26480200	-1.95009700	-1.37999100
C	0.54778700	-3.56950200	-3.44677800
H	0.65831700	-1.55791900	-2.68475200
C	1.26728900	-5.31069400	-1.93662000
H	1.96604800	-4.66728400	-0.00936400
C	2.97196400	-3.87227900	3.24771400
H	3.76194200	-3.41788900	1.30117800
C	0.85615300	-2.84984500	3.80408400
H	-0.00611200	-1.58779600	2.29038800
C	5.52494300	-0.01044400	0.18188000
H	3.63217600	0.22062100	1.16329200
C	5.60963700	-1.63615900	-1.59907200
H	3.78809900	-2.70576000	-1.99548500
C	0.75868300	-4.92346300	-3.17776300
H	0.14745500	-3.25921800	-4.40830900
C	1.93002600	-3.66808400	4.15621000
H	3.81839500	-4.49739800	3.52059800
H	0.04809900	-2.67020700	4.50812200
C	6.24406000	-0.66932700	-0.81957200
H	6.00022400	0.75672700	0.78693700
H	6.15876900	-2.15201800	-2.38280100
H	0.52341800	-5.67261800	-3.92919100
H	1.96233600	-4.13576000	5.13678200
H	7.28869900	-0.42506200	-0.99377000
H	1.43119400	-6.36323500	-1.71899100
H	-3.02654100	6.90119800	-0.05754100
H	5.75235600	4.30569800	1.70616200
H	1.77805000	2.86742200	-5.16785900
C	-3.59820200	0.37989400	-0.77736500
C	-3.37766300	0.63452500	-2.14304700
C	-4.74846600	0.90939500	-0.17389300
C	-4.28977800	1.38323800	-2.88609000
H	-2.48279800	0.25059200	-2.62539200
C	-5.65465300	1.67206200	-0.91676500
H	-4.94149000	0.72922000	0.87851300

C	-5.43132200	1.90798700	-2.27372200
H	-4.10335900	1.56506800	-3.94125300
H	-6.53902500	2.07623000	-0.43079000
H	-6.13823700	2.49856500	-2.85033700
C	-2.76556200	-2.34594000	-0.41947600
C	-3.84896800	-2.64367200	-1.26053700
C	-1.96821100	-3.40559900	0.04403600
C	-4.12556400	-3.96386300	-1.62601400
H	-4.48481500	-1.84755800	-1.63228700
C	-2.25093800	-4.72318100	-0.31276900
H	-1.12170100	-3.20330600	0.69281500
C	-3.33031400	-5.00717500	-1.15255200
H	-4.96916100	-4.17283100	-2.27913000
H	-1.61856100	-5.52580400	0.05602400
H	-3.54676400	-6.03347500	-1.43737000
P	-2.33163200	-0.62410500	0.13180900
C	-2.96948600	-0.63039300	1.87459200
C	-2.40798200	0.26709400	2.79721200
C	-3.98875800	-1.49555000	2.30772400
C	-2.86246700	0.30533500	4.11771300
H	-1.60701900	0.93255400	2.48484500
C	-4.43680500	-1.45910400	3.62885900
H	-4.43199400	-2.20195700	1.61268900
C	-3.87568500	-0.55794900	4.53719200
H	-2.41708800	1.00812200	4.81701100
H	-5.22467100	-2.13652600	3.94838700
H	-4.22501700	-0.53220200	5.56618000

IRC of triphenylphosphonin C–P oxidative -Point24

0 1

P	0.36852500	2.38536700	0.99377200
C	-0.62086700	3.86600000	0.53286100
C	2.09627400	3.03705500	1.11243400
Pd	0.10440200	0.36064300	-0.11731000
C	-1.95523000	3.67278900	0.12491600
C	-0.18552000	5.19000600	0.73563200
C	2.73124400	3.87305700	0.17452300

C	2.81794600	2.66727300	2.26170400
C	0.80167000	1.64293900	-1.59917000
C	-2.81131000	4.75122900	-0.09111100
H	-2.32823400	2.66443000	-0.02331800
C	-1.04384800	6.26906900	0.52024000
H	0.82705500	5.38337600	1.07268000
C	4.03457900	4.32443600	0.38566900
H	2.20149200	4.17119600	-0.72381500
C	4.12573900	3.11292200	2.47199300
H	2.34079500	2.03204700	3.00454500
C	2.13142000	1.57724500	-2.03890600
C	-0.15573100	2.22562900	-2.44117400
C	-2.35897100	6.05853100	0.10179000
H	-3.83273800	4.56451000	-0.41288500
H	-0.67944000	7.28077200	0.68276400
C	4.73730200	3.94565600	1.53343600
H	4.50508500	4.97062200	-0.35137000
H	4.65879900	2.81907500	3.37295900
C	2.47838000	2.01353400	-3.32207300
H	2.90680200	1.18798500	-1.38933900
C	0.19258300	2.65945400	-3.72598700
H	-1.17632700	2.36138200	-2.10019300
C	1.50959200	2.54814600	-4.17425700
H	3.51301000	1.93654400	-3.64988400
H	-0.56816800	3.10065200	-4.36689600
P	1.74053300	-1.62195400	-0.03851500
C	1.36294900	-2.98862500	-1.22963700
C	1.85068900	-2.45682100	1.61496200
C	3.53580400	-1.29840800	-0.37650800
C	0.83943900	-2.61102000	-2.47778900
C	1.57070300	-4.35158000	-0.97009900
C	2.93559800	-3.26860500	1.98987300
C	0.82036500	-2.24506300	2.54429300
C	4.18233800	-0.31843600	0.39688600
C	4.26572000	-1.95159700	-1.37981400
C	0.54778500	-3.57079700	-3.44767700
H	0.66025700	-1.55913700	-2.68640300

C	1.26619200	-5.31224500	-1.93718900
H	1.96529800	-4.66894200	-0.00996700
C	2.97180000	-3.87182500	3.24767100
H	3.76200900	-3.41799800	1.30111800
C	0.85567400	-2.84965100	3.80328000
H	-0.00727100	-1.58915000	2.28906100
C	5.52426400	-0.00992900	0.18090700
H	3.63076600	0.22195500	1.16073200
C	5.61046300	-1.63721300	-1.59863300
H	3.78954500	-2.70794900	-1.99487500
C	0.75780400	-4.92483100	-3.17837700
H	0.14774300	-3.26042600	-4.40929200
C	1.92971300	-3.66742300	4.15594700
H	3.81834200	-4.49661500	3.52093600
H	0.04747700	-2.66986800	4.50710300
C	6.24407700	-0.66944300	-0.81963000
H	5.99885400	0.75814800	0.78532800
H	6.16013800	-2.15339800	-2.38175700
H	0.52207300	-5.67395900	-3.92968200
H	1.96201100	-4.13458900	5.13675600
H	7.28866800	-0.42483600	-0.99361800
H	1.42946900	-6.36486200	-1.71947000
H	-3.02388600	6.90174300	-0.06650900
H	5.75149200	4.30201100	1.69570800
H	1.78210800	2.89126800	-5.16937000
C	-3.59921300	0.37909700	-0.77572100
C	-3.37844000	0.63226600	-2.14164600
C	-4.74888200	0.91030700	-0.17264800
C	-4.28967900	1.38154500	-2.88522900
H	-2.48433300	0.24657900	-2.62394900
C	-5.65432800	1.67319800	-0.91614900
H	-4.94197600	0.73125000	0.87993400
C	-5.43068400	1.90791300	-2.27327300
H	-4.10301200	1.56239700	-3.94050600
H	-6.53831000	2.07860200	-0.43051200
H	-6.13698400	2.49877100	-2.85034800
C	-2.76737700	-2.34708800	-0.41777900

C	-3.85046900	-2.64474400	-1.25927600
C	-1.96928800	-3.40655300	0.04489700
C	-4.12624000	-3.96480500	-1.62573300
H	-4.48665600	-1.84867700	-1.63053700
C	-2.25123800	-4.72403400	-0.31288100
H	-1.12287400	-3.20422400	0.69381400
C	-3.33044000	-5.00799200	-1.15288800
H	-4.96963300	-4.17382000	-2.27908900
H	-1.61841600	-5.52657700	0.05530900
H	-3.54630200	-6.03420800	-1.43844300
P	-2.33446700	-0.62569800	0.13476500
C	-2.97268100	-0.63155200	1.87694700
C	-2.41065800	0.26608500	2.79912800
C	-3.99168500	-1.49671900	2.31051400
C	-2.86447100	0.30450700	4.11980600
H	-1.60987000	0.93169200	2.48664500
C	-4.43900200	-1.46009300	3.63186300
H	-4.43519500	-2.20322100	1.61573500
C	-3.87744400	-0.55879100	4.53980000
H	-2.41875200	1.00741600	4.81875300
H	-5.22668200	-2.13747500	3.95193000
H	-4.22630000	-0.53297300	5.56894600

IRC of triphenylphosphonin C–P oxidative -Point25

0 1

P	0.36160600	2.38593800	1.01225100
C	-0.62354800	3.86578000	0.53968600
C	2.09132400	3.03446300	1.12165800
Pd	0.11086800	0.37077500	-0.11777100
C	-1.95564500	3.67302100	0.12418100
C	-0.18809300	5.18986100	0.74206500
C	2.72364800	3.86587400	0.17776500
C	2.81779800	2.66735800	2.26882600
C	0.80469800	1.62319300	-1.61674900
C	-2.80990700	4.75174100	-0.09741100
H	-2.32812800	2.66472300	-0.02569100
C	-1.04428000	6.26928900	0.52019500

H	0.82294100	5.38281300	1.08405700
C	4.02844500	4.31634200	0.38182900
H	2.19054500	4.16145400	-0.71944200
C	4.12707000	3.11197400	2.47190100
H	2.34299500	2.03559700	3.01614600
C	2.13486400	1.56516600	-2.05545500
C	-0.15292400	2.21453500	-2.45236900
C	-2.35760700	6.05901400	0.09597600
H	-3.82977700	4.56538300	-0.42431900
H	-0.67984000	7.28100900	0.68257400
C	4.73557800	3.94099000	1.52803800
H	4.49663400	4.95922300	-0.35957500
H	4.66359200	2.82061800	3.37163900
C	2.48216300	2.01685800	-3.33331100
H	2.91062200	1.17098700	-1.40928300
C	0.19569300	2.66343400	-3.73190600
H	-1.17383800	2.34568600	-2.11028200
C	1.51324900	2.55918000	-4.18033800
H	3.51735900	1.94610900	-3.66079700
H	-0.56516600	3.11100400	-4.36826500
P	1.74113300	-1.62368600	-0.04029900
C	1.36337000	-2.99031200	-1.23093800
C	1.85027400	-2.45738800	1.61380400
C	3.53612000	-1.29925000	-0.37732900
C	0.84031200	-2.61252700	-2.47923200
C	1.57015600	-4.35331600	-0.97092100
C	2.93542100	-3.26855500	1.98943900
C	0.81961200	-2.24562400	2.54278400
C	4.18147200	-0.31793600	0.39536500
C	4.26686700	-1.95325900	-1.37948100
C	0.54801700	-3.57234900	-3.44885600
H	0.66241800	-1.56055100	-2.68845100
C	1.26512200	-5.31396000	-1.93784000
H	1.96442900	-4.67063600	-0.01063700
C	2.97155300	-3.87114300	3.24753100
H	3.76207700	-3.41793100	1.30098600
C	0.85496900	-2.84942300	3.80216600

H	-0.00863700	-1.59059900	2.28728000
C	5.52341000	-0.00914400	0.17987000
H	3.62902700	0.22354600	1.15782400
C	5.61153500	-1.63837500	-1.59788600
H	3.79137700	-2.71047800	-1.99401300
C	0.75707300	-4.92644600	-3.17914900
H	0.14835500	-3.26195000	-4.41061200
C	1.92923900	-3.66658600	4.15550800
H	3.81825600	-4.49549900	3.52127200
H	0.04655600	-2.66954100	4.50570400
C	6.24413200	-0.66943800	-0.81949900
H	5.99716700	0.75997400	0.78359200
H	6.16192500	-2.15501900	-2.38019600
H	0.52090400	-5.67559600	-3.93028800
H	1.96150700	-4.13317400	5.13658600
H	7.28868600	-0.42444400	-0.99315900
H	1.42771400	-6.36663800	-1.71992700
H	-3.02108400	6.90245100	-0.07685300
H	5.75074300	4.29698800	1.68493800
H	1.78604600	2.91394900	-5.17127900
C	-3.60046000	0.37803000	-0.77373800
C	-3.37927200	0.62961200	-2.13990200
C	-4.74950600	0.91117700	-0.17122400
C	-4.28947400	1.37947000	-2.88419800
H	-2.48587300	0.24207800	-2.62200000
C	-5.65402100	1.67437200	-0.91551300
H	-4.94279600	0.73334100	0.88153000
C	-5.42992300	1.90768100	-2.27281300
H	-4.10244400	1.55920800	-3.93959400
H	-6.53759400	2.08120000	-0.43033600
H	-6.13548000	2.49884700	-2.85047600
C	-2.76947100	-2.34852000	-0.41575100
C	-3.85219900	-2.64612000	-1.25774900
C	-1.97051300	-3.40777300	0.04591500
C	-4.12693400	-3.96602000	-1.62545000
H	-4.48882700	-1.85012500	-1.62840500
C	-2.25147500	-4.72512700	-0.31309700

H	-1.12421700	-3.20540500	0.69500100
C	-3.33042700	-5.00905600	-1.15342200
H	-4.97007500	-4.17508000	-2.27911000
H	-1.61808600	-5.52755700	0.05434600
H	-3.54552600	-6.03516100	-1.43993700
P	-2.33757900	-0.62756800	0.13812600
C	-2.97639700	-0.63305600	1.87968400
C	-2.41396100	0.26474500	2.80148200
C	-3.99512800	-1.49827000	2.31365000
C	-2.86717100	0.30332600	4.12231800
H	-1.61333800	0.93050300	2.48890700
C	-4.44178200	-1.46150100	3.63520100
H	-4.43883700	-2.20489000	1.61910400
C	-3.87987200	-0.56003900	4.54278200
H	-2.42117600	1.00636900	4.82094400
H	-5.22925700	-2.13888900	3.95575500
H	-4.22829400	-0.53417800	5.57207200

IRC of triphenylphosphonin C−P oxidative -Point26

0 1

P	0.35480400	2.38679800	1.02911100
C	-0.62663100	3.86597800	0.54677300
C	2.08603400	3.03257100	1.13131400
Pd	0.11833700	0.38092000	-0.11831200
C	-1.95614700	3.67361400	0.12295100
C	-0.19126600	5.19005300	0.74952600
C	2.71600500	3.85877300	0.18123400
C	2.81693500	2.66812400	2.27655000
C	0.80850600	1.60651300	-1.63308500
C	-2.80832900	4.75263500	-0.10495400
H	-2.32802700	2.66537800	-0.02876700
C	-1.04510700	6.26984800	0.52063400
H	0.81799000	5.38251200	1.09713700
C	4.02253900	4.30742500	0.37786500
H	2.17962200	4.15169700	-0.71488700
C	4.12794800	3.11096800	2.47215500
H	2.34419300	2.04017700	3.02840200

C	2.13873400	1.55432300	-2.07183500
C	-0.14956200	2.20510000	-2.46306700
C	-2.35617100	6.05985600	0.08929600
H	-3.82634500	4.56666000	-0.43781100
H	-0.68081300	7.28157200	0.68333900
C	4.73389800	3.93533500	1.52254700
H	4.48879500	4.94636400	-0.36815500
H	4.66784000	2.82208700	3.37069100
C	2.48596500	2.01974300	-3.34490400
H	2.91496600	1.15519700	-1.42926100
C	0.19895800	2.66742000	-3.73785900
H	-1.17071000	2.33221600	-2.11989300
C	1.51685600	2.56954100	-4.18675900
H	3.52149000	1.95410800	-3.67246600
H	-0.56221500	3.12064600	-4.36983500
P	1.74162500	-1.62535900	-0.04253800
C	1.36378500	-2.99210900	-1.23261100
C	1.84968300	-2.45788300	1.61223700
C	3.53639900	-1.30010100	-0.37841100
C	0.84136800	-2.61429700	-2.48117000
C	1.56944500	-4.35515200	-0.97190100
C	2.93511000	-3.26831800	1.98872800
C	0.81859500	-2.24616200	2.54077800
C	4.18035700	-0.31716300	0.39340000
C	4.26824400	-1.95525600	-1.37899900
C	0.54844200	-3.57428500	-3.45042000
H	0.66484700	-1.56224000	-2.69114100
C	1.26390300	-5.31589500	-1.93854000
H	1.96325100	-4.67232800	-0.01137400
C	2.97115200	-3.87016600	3.24717100
H	3.76207200	-3.41765800	1.30064700
C	0.85396400	-2.84908700	3.80059600
H	-0.01026900	-1.59207700	2.28488100
C	5.52233600	-0.00808300	0.17857300
H	3.62686200	0.22555200	1.15424800
C	5.61287300	-1.63987700	-1.59680100
H	3.79361200	-2.71358900	-1.99282900

C	0.75635900	-4.92842700	-3.18008200
H	0.14928800	-3.26395900	-4.41240400
C	1.92853100	-3.66549200	4.15476100
H	3.81806400	-4.49397400	3.52149300
H	0.04526200	-2.66914200	4.50377500
C	6.24422100	-0.66945000	-0.81925000
H	5.99509900	0.76228200	0.78145700
H	6.16418300	-2.15723000	-2.37798600
H	0.51974800	-5.67768700	-3.93096700
H	1.96075300	-4.13141600	5.13615100
H	7.28875900	-0.42406400	-0.99244200
H	1.42568300	-6.36861700	-1.72024900
H	-3.01798700	6.90353200	-0.08867900
H	5.75032800	4.29018100	1.67379500
H	1.78965800	2.93488300	-5.17383600
C	-3.60195400	0.37666900	-0.77121400
C	-3.38015600	0.62650000	-2.13761700
C	-4.75031200	0.91207100	-0.16942400
C	-4.28913400	1.37695900	-2.88282200
H	-2.48742100	0.23698900	-2.61933000
C	-5.65365800	1.67569100	-0.91467400
H	-4.94392500	0.73560400	0.88350400
C	-5.42897000	1.90732900	-2.27217100
H	-4.10162700	1.55539900	-3.93834700
H	-6.53676300	2.08421600	-0.43008400
H	-6.13362500	2.49885200	-2.85056500
C	-2.77194500	-2.35029500	-0.41320400
C	-3.85431400	-2.64783100	-1.25571000
C	-1.97196900	-3.40933900	0.04719400
C	-4.12782100	-3.96752400	-1.62496300
H	-4.49150600	-1.85192000	-1.62558000
C	-2.25175100	-4.72652700	-0.31335800
H	-1.12577900	-3.20696400	0.69644500
C	-3.33041800	-5.01039900	-1.15405100
H	-4.97070100	-4.17660100	-2.27895000
H	-1.61765000	-5.52882700	0.05312500
H	-3.54458500	-6.03635400	-1.44178600

P	-2.34101000	-0.62978600	0.14208900
C	-2.98071500	-0.63496900	1.88299600
C	-2.41799100	0.26301200	2.80448000
C	-3.99920500	-1.50024300	2.31730500
C	-2.87071300	0.30173800	4.12544300
H	-1.61751200	0.92892300	2.49185700
C	-4.44530900	-1.46335500	3.63902700
H	-4.44302900	-2.20700400	1.62295800
C	-3.88314700	-0.56172600	4.54630900
H	-2.42452300	1.00492500	4.82379300
H	-5.23258600	-2.14077600	3.95999500
H	-4.23120900	-0.53583500	5.57571800

IRC of triphenylphosphonin C–P oxidative -Point27

0 1

P	0.34815300	2.38805800	1.04410900
C	-0.63005400	3.86671000	0.55370000
C	2.08048200	3.03153600	1.14111900
Pd	0.12686800	0.39084500	-0.11897300
C	-1.95669800	3.67472900	0.12089200
C	-0.19500500	5.19069500	0.75772500
C	2.70858300	3.85202500	0.18486100
C	2.81525100	2.66963100	2.28468900
C	0.81309400	1.59308400	-1.64789700
C	-2.80658000	4.75408500	-0.11380900
H	-2.32789700	2.66656900	-0.03295100
C	-1.04635300	6.27087100	0.52156700
H	0.81224100	5.38257000	1.11157800
C	4.01710500	4.29790200	0.37400600
H	2.16914700	4.14233500	-0.71027400
C	4.12823700	3.10990000	2.47286200
H	2.34414100	2.04580900	3.04100500
C	2.14301700	1.54481500	-2.08779100
C	-0.14561100	2.19775900	-2.47284400
C	-2.35471200	6.06121100	0.08187900
H	-3.82245800	4.56853300	-0.45336800
H	-0.68240000	7.28256900	0.68521200

C	4.73231300	3.92876000	1.51727200
H	4.48194900	4.93231900	-0.37673900
H	4.67123000	2.82336600	3.37029300
C	2.48970100	2.02193200	-3.35679900
H	2.91981100	1.14063300	-1.44906500
C	0.20234600	2.67149800	-3.74362600
H	-1.16684100	2.32161200	-2.12847100
C	1.52028500	2.57883400	-4.19351600
H	3.52526800	1.96005300	-3.68500700
H	-0.55931200	3.12972600	-4.37140800
P	1.74198500	-1.62689700	-0.04535600
C	1.36416200	-2.99395600	-1.23475700
C	1.84886200	-2.45820900	1.61014000
C	3.53662800	-1.30092600	-0.37984800
C	0.84262900	-2.61632600	-2.48374500
C	1.56850500	-4.35701700	-0.97306400
C	2.93459700	-3.26780400	1.98762800
C	0.81724600	-2.24657200	2.53813300
C	4.17895600	-0.31604700	0.39086000
C	4.26987600	-1.95764600	-1.37836600
C	0.54910800	-3.57664800	-3.45247000
H	0.66759100	-1.56421200	-2.69467600
C	1.26249400	-5.31802900	-1.93927400
H	1.96165400	-4.67391000	-0.01216900
C	2.97049900	-3.86881500	3.24647200
H	3.76193500	-3.41709500	1.30000300
C	0.85255700	-2.84855200	3.79842100
H	-0.01222000	-1.59347000	2.28170400
C	5.52102500	-0.00672100	0.17694400
H	3.62419300	0.22811400	1.14978700
C	5.61452600	-1.64183400	-1.59531400
H	3.79629300	-2.71737600	-1.99129300
C	0.75568200	-4.93080600	-3.18120200
H	0.15063500	-3.26654500	-4.41480100
C	1.92747100	-3.66406200	4.15356900
H	3.81766000	-4.49196900	3.52149500
H	0.04348200	-2.66857800	4.50115200

C	6.24436800	-0.66955300	-0.81885300
H	5.99261400	0.76513200	0.77881600
H	6.16699800	-2.16022600	-2.37498000
H	0.51864300	-5.68030000	-3.93171500
H	1.95960800	-4.12924800	5.13530700
H	7.28893200	-0.42381600	-0.99138900
H	1.42330800	-6.37076600	-1.72035800
H	-3.01468100	6.90515100	-0.10163400
H	5.75027900	4.28160400	1.66279500
H	1.79274700	2.95334000	-5.17723700
C	-3.60362100	0.37499000	-0.76802500
C	-3.38095200	0.62299700	-2.13463600
C	-4.75127200	0.91289100	-0.16714800
C	-4.28851700	1.37407400	-2.88095100
H	-2.48878300	0.23146000	-2.61575100
C	-5.65320200	1.67706300	-0.91353400
H	-4.94537800	0.73788200	0.88593600
C	-5.42773700	1.90683400	-2.27123000
H	-4.10037300	1.55109200	-3.93659600
H	-6.53581300	2.08750700	-0.42967900
H	-6.13133100	2.49876000	-2.85050300
C	-2.77480800	-2.35247100	-0.41004500
C	-3.85687400	-2.64990000	-1.25301000
C	-1.97366500	-3.41133400	0.04877700
C	-4.12900900	-3.96932900	-1.62412800
H	-4.49475900	-1.85406600	-1.62186400
C	-2.25211600	-4.72830000	-0.31363300
H	-1.12753800	-3.20901600	0.69815700
C	-3.33051100	-5.01205300	-1.15469500
H	-4.97165700	-4.17836600	-2.27842300
H	-1.61715700	-5.53047100	0.05163200
H	-3.54361000	-6.03780900	-1.44392100
P	-2.34471600	-0.63242100	0.14676600
C	-2.98563800	-0.63737100	1.88698000
C	-2.42281300	0.26081400	2.80825200
C	-4.00394100	-1.50272300	2.32150600
C	-2.87526600	0.29967200	4.12927800

H	-1.62245600	0.92690200	2.49566800
C	-4.44971300	-1.46573300	3.64333500
H	-4.44775200	-2.20964800	1.62729900
C	-3.88746700	-0.56392300	4.55040600
H	-2.42902000	1.00301600	4.82742700
H	-5.23682100	-2.14321200	3.96458800
H	-4.23532000	-0.53800600	5.57988300

IRC of triphenylphosphonin C–P oxidative -Point28

0 1

P	0.34170100	2.38981000	1.05702100
C	-0.63369400	3.86806400	0.55993400
C	2.07479800	3.03143100	1.15071600
Pd	0.13642200	0.40030100	-0.11975200
C	-1.95725800	3.67650600	0.11772400
C	-0.19917700	5.19188000	0.76613700
C	2.70169000	3.84596800	0.18861100
C	2.81268800	2.67179600	2.29297100
C	0.81839600	1.58281300	-1.66100200
C	-2.80470700	4.75624900	-0.12385000
H	-2.32772900	2.66845200	-0.03853600
C	-1.04798000	6.27246300	0.52288700
H	0.80588100	5.38307500	1.12666100
C	4.01236300	4.28821600	0.37066900
H	2.15964100	4.13388900	-0.70571600
C	4.12778400	3.10875300	2.47418100
H	2.34265100	2.05225300	3.05347000
C	2.14765300	1.53663600	-2.10307700
C	-0.14110000	2.19272800	-2.48132900
C	-2.35329500	6.06322500	0.07398300
H	-3.81822900	4.57118100	-0.47062300
H	-0.68455600	7.28408700	0.68815500
C	4.73081200	3.92154300	1.51272700
H	4.47641600	4.91776300	-0.38464900
H	4.67340500	2.82428800	3.37068700
C	2.49326500	2.02319200	-3.36890300
H	2.92509900	1.12735800	-1.46841700

C	0.20578600	2.67568200	-3.74898000
H	-1.16219000	2.31427600	-2.13550000
C	1.52338800	2.58668900	-4.20057400
H	3.52856100	1.96359400	-3.69843800
H	-0.55649600	3.13833900	-4.37275700
P	1.74220200	-1.62820500	-0.04887300
C	1.36447800	-2.99576300	-1.23747800
C	1.84776000	-2.45824700	1.60739300
C	3.53680000	-1.30167300	-0.38174300
C	0.84412300	-2.61856900	-2.48709000
C	1.56728300	-4.35881000	-0.97444400
C	2.93380200	-3.26692300	1.98603200
C	0.81550200	-2.24670900	2.53470500
C	4.17726000	-0.31451600	0.38761900
C	4.27177900	-1.96045900	-1.37760300
C	0.55007400	-3.57943200	-3.45511100
H	0.67069500	-1.56642900	-2.69924700
C	1.26087400	-5.32029600	-1.94004500
H	1.95953900	-4.67523900	-0.01302900
C	2.96946500	-3.86702100	3.24531600
H	3.76159800	-3.41616500	1.29896100
C	0.85063500	-2.84769100	3.79549000
H	-0.01452500	-1.59460500	2.27758400
C	5.51949300	-0.00505800	0.17492300
H	3.62097600	0.23137400	1.14423400
C	5.61653900	-1.64435200	-1.59337500
H	3.79943800	-2.72187600	-1.98940800
C	0.75508100	-4.93356600	-3.18255100
H	0.15249800	-3.26973900	-4.41794000
C	1.92591200	-3.66221400	4.15178900
H	3.81688800	-4.48944300	3.52117200
H	0.04109000	-2.66770900	4.49766900
C	6.24462000	-0.66984000	-0.81827800
H	5.98972300	0.76854200	0.77559000
H	6.17044100	-2.16417700	-2.37106300
H	0.51765700	-5.68344500	-3.93255300
H	1.95788200	-4.12660700	5.13390200

H	7.28927300	-0.42385500	-0.98991800
H	1.42054600	-6.37301100	-1.72020500
H	-3.01131300	6.90745900	-0.11509600
H	5.75049800	4.27162700	1.65279900
H	1.79510100	2.96865100	-5.18162500
C	-3.60531900	0.37298700	-0.76406600
C	-3.38143300	0.61928300	-2.13080500
C	-4.75234000	0.91344900	-0.16431500
C	-4.28740900	1.37099800	-2.87841000
H	-2.48965100	0.22582100	-2.61108100
C	-5.65262500	1.67829500	-0.91199100
H	-4.94717600	0.73984300	0.88887100
C	-5.42611300	1.90618900	-2.26983900
H	-4.09840000	1.54662400	-3.93412800
H	-6.53479200	2.09073800	-0.42903500
H	-6.12849500	2.49856300	-2.85012200
C	-2.77800200	-2.35508100	-0.40621200
C	-3.85989400	-2.65230700	-1.24951400
C	-1.97557700	-3.41383100	0.05068200
C	-4.13061900	-3.97140000	-1.62277200
H	-4.49857300	-1.85651000	-1.61708900
C	-2.25264700	-4.73050600	-0.31387000
H	-1.12941900	-3.21168300	0.70011100
C	-3.33085900	-5.01402600	-1.15522200
H	-4.97312200	-4.18030100	-2.27729400
H	-1.61670700	-5.53258100	0.04988700
H	-3.54284000	-6.03952100	-1.44617900
P	-2.34858600	-0.63553200	0.15223800
C	-2.99108800	-0.64033000	1.89169100
C	-2.42843400	0.25810700	2.81287900
C	-4.00928000	-1.50579200	2.32623400
C	-2.88095400	0.29709200	4.13386600
H	-1.62817500	0.92442200	2.50047000
C	-4.45505900	-1.46869700	3.64806100
H	-4.45287700	-2.21291600	1.63207600
C	-3.89299100	-0.56666700	4.55503900
H	-2.43487000	1.00062600	4.83192200

H	-5.24205300	-2.14626300	3.96941100
H	-4.24088200	-0.54070700	5.58450100

IRC of triphenylphosphonin C−P oxidative -Point29

0 1

P	0.33551900	2.39206100	1.06765600
C	-0.63738000	3.87004700	0.56498900
C	2.06914100	3.03217800	1.15977100
Pd	0.14680100	0.40904200	-0.12060400
C	-1.95778500	3.67899900	0.11333000
C	-0.20355400	5.19362300	0.77412200
C	2.69557700	3.84088400	0.19248900
C	2.80926400	2.67439700	2.30112300
C	0.82426600	1.57530000	-1.67240000
C	-2.80277200	4.75919200	-0.13478300
H	-2.32753500	2.67108900	-0.04556200
C	-1.04985800	6.27465300	0.52433300
H	0.79923200	5.38404800	1.14146000
C	4.00841100	4.27895100	0.36834000
H	2.15153500	4.12677400	-0.70128400
C	4.12647300	3.10753800	2.47628400
H	2.33968400	2.05904100	3.06530000
C	2.15253600	1.52964300	-2.11755200
C	-0.13614000	2.18983800	-2.48837600
C	-2.35195800	6.06595300	0.06587200
H	-3.81383600	4.57468500	-0.48893900
H	-0.68710100	7.28614800	0.69184300
C	4.72930500	3.91415300	1.50949400
H	4.47232200	4.90360600	-0.39111300
H	4.67408600	2.82473300	3.37210800
C	2.49656000	2.02345700	-3.38109200
H	2.93072700	1.11534800	-1.48710900
C	0.20917800	2.67990300	-3.75377700
H	-1.15684400	2.31005900	-2.14076600
C	1.52605400	2.59298500	-4.20783900
H	3.53128400	1.96477300	-3.71263000
H	-0.55383700	3.14651800	-4.37371100

P	1.74228500	-1.62919300	-0.05316900
C	1.36472700	-2.99742200	-1.24084900
C	1.84634600	-2.45789000	1.60391200
C	3.53693000	-1.30229300	-0.38416800
C	0.84588400	-2.62092800	-2.49130200
C	1.56574600	-4.36041800	-0.97609100
C	2.93264800	-3.26561700	1.98387200
C	0.81332000	-2.24641700	2.53038700
C	4.17530200	-0.31253300	0.38359300
C	4.27396700	-1.96369400	-1.37674200
C	0.55140000	-3.58254900	-3.45843600
H	0.67420600	-1.56879800	-2.70496800
C	1.25903400	-5.32259300	-1.94090000
H	1.95683800	-4.67619100	-0.01398700
C	2.96790600	-3.86474100	3.24363100
H	3.76099300	-3.41484300	1.29747200
C	0.84809100	-2.84636000	3.79168700
H	-0.01719000	-1.59529300	2.27238300
C	5.51779500	-0.00312400	0.17247300
H	3.61723800	0.23542500	1.13744800
C	5.61894900	-1.64750400	-1.59097000
H	3.80304400	-2.72707600	-1.98721000
C	0.75459800	-4.93661700	-3.18419700
H	0.15497300	-3.27346700	-4.42193000
C	1.92369400	-3.65986500	4.14931800
H	3.81556400	-4.48640000	3.52046800
H	0.03797300	-2.66635700	4.49319000
C	6.24503700	-0.67040600	-0.81750700
H	5.98649900	0.77247100	0.77173400
H	6.17455000	-2.16920100	-2.36618100
H	0.51685400	-5.68704000	-3.93355000
H	1.95536400	-4.12342900	5.13182800
H	7.28986200	-0.42433700	-0.98797200
H	1.41737000	-6.37524600	-1.71981800
H	-3.00801800	6.91052000	-0.12845200
H	5.75075800	4.26097100	1.64476000
H	1.79660900	2.98069600	-5.18695300

C	-3.60687000	0.37066400	-0.75929500
C	-3.38133800	0.61560900	-2.12601900
C	-4.75346000	0.91349900	-0.16088900
C	-4.28556600	1.36802100	-2.87503600
H	-2.48969000	0.22049100	-2.60520700
C	-5.65190500	1.67914700	-0.90995400
H	-4.94933400	0.74104700	0.89230000
C	-5.42397200	1.90543000	-2.26784500
H	-4.09538800	1.54249600	-3.93073100
H	-6.53377500	2.09346600	-0.42807300
H	-6.12501400	2.49831700	-2.84922700
C	-2.78141200	-2.35813300	-0.40170700
C	-3.86333700	-2.65499000	-1.24514500
C	-1.97765200	-3.41688500	0.05289900
C	-4.13277300	-3.97366700	-1.62073000
H	-4.50286300	-1.85914800	-1.61116600
C	-2.25344500	-4.73319000	-0.31400100
H	-1.13131900	-3.21507600	0.70223900
C	-3.33165900	-5.01629800	-1.15546300
H	-4.97528500	-4.18228500	-2.27532900
H	-1.61645900	-5.53524600	0.04795500
H	-3.54259700	-6.04146700	-1.44831700
P	-2.35244700	-0.63914800	0.15850800
C	-2.99690200	-0.64388100	1.89711400
C	-2.43477600	0.25490300	2.81835500
C	-4.01505700	-1.50950200	2.33142500
C	-2.88780200	0.29403800	4.13916200
H	-1.63460200	0.92151900	2.50628400
C	-4.46129000	-1.47226900	3.65310100
H	-4.45817600	-2.21689200	1.63721400
C	-3.89975800	-0.56992800	4.56011500
H	-2.44217500	0.99783100	4.83724600
H	-5.24823200	-2.14995700	3.97432200
H	-4.24802100	-0.54387500	5.58944700

IRC of triphenylphosphonin C−P oxidative -Point30

0 1

P	0.32971700	2.39471800	1.07604500
C	-0.64091400	3.87258500	0.56873200
C	2.06364900	3.03350700	1.16819300
Pd	0.15749800	0.41688100	-0.12151400
C	-1.95824900	3.68216000	0.10778600
C	-0.20783200	5.19586000	0.78134800
C	2.69031400	3.83672300	0.19651900
C	2.80509700	2.67722100	2.30909600
C	0.83051300	1.56980900	-1.68239900
C	-2.80082300	4.76287500	-0.14644100
H	-2.32733900	2.67443700	-0.05391400
C	-1.05173800	6.27738700	0.52560200
H	0.79268600	5.38542300	1.15558200
C	4.00518900	4.27045600	0.36724400
H	2.14489800	4.12085900	-0.69697500
C	4.12430300	3.10638400	2.47928700
H	2.33540700	2.06584800	3.07641500
C	2.15759700	1.52367600	-2.13118900
C	-0.13092200	2.18831100	-2.49436100
C	-2.35064300	6.06935900	0.05751600
H	-3.80943300	4.57902100	-0.50807600
H	-0.68968900	7.28869400	0.69581300
C	4.72769200	3.90704700	1.50784200
H	4.46953400	4.89036000	-0.39585300
H	4.67326400	2.82488300	3.37469200
C	2.49962600	2.02312800	-3.39309700
H	2.93666900	1.10457000	-1.50499200
C	0.21245600	2.68405800	-3.75809600
H	-1.15112300	2.30769500	-2.14488000
C	1.52835200	2.59821900	-4.21508500
H	3.53357900	1.96452300	-3.72706300
H	-0.55138000	3.15432600	-4.37430500
P	1.74228600	-1.62984700	-0.05821900
C	1.36497600	-2.99887200	-1.24489900
C	1.84464400	-2.45713000	1.59970900
C	3.53707700	-1.30276500	-0.38711900
C	0.84802000	-2.62327600	-2.49641100

C	1.56389600	-4.36180000	-0.97807100
C	2.93111800	-3.26391500	1.98119900
C	0.81071500	-2.24562500	2.52516900
C	4.17315600	-0.31004000	0.37875500
C	4.27650400	-1.96738300	-1.37577700
C	0.55317000	-3.58583000	-3.46251100
H	0.67832800	-1.57117400	-2.71187200
C	1.25695100	-5.32483700	-1.94193900
H	1.95352400	-4.67678300	-0.01511000
C	2.96574600	-3.86198100	3.24147800
H	3.76011000	-3.41320400	1.29560500
C	0.84488200	-2.84445900	3.78701700
H	-0.02017700	-1.59544100	2.26607900
C	5.51601900	-0.00090900	0.16957100
H	3.61304700	0.24043700	1.12934800
C	5.62182800	-1.65135600	-1.58809700
H	3.80718800	-2.73305500	-1.98466100
C	0.75424900	-4.93981200	-3.18624000
H	0.15819500	-3.27751300	-4.42684800
C	1.92073100	-3.65695900	4.14619500
H	3.81358300	-4.48287300	3.51948400
H	0.03406800	-2.66437300	4.48768900
C	6.24571000	-0.67130600	-0.81654600
H	5.98302100	0.77697500	0.76719800
H	6.17940500	-2.17542900	-2.36031000
H	0.51622500	-5.69091100	-3.93482700
H	1.95192900	-4.11963600	5.12913600
H	7.29080200	-0.42535200	-0.98554900
H	1.41369000	-6.37741100	-1.71932300
H	-3.00476500	6.91430800	-0.14178500
H	5.75088000	4.25035000	1.63904300
H	1.79748300	2.99066400	-5.19270400
C	-3.60808400	0.36808200	-0.75371000
C	-3.38048300	0.61217200	-2.12025100
C	-4.75452100	0.91291000	-0.15684100
C	-4.28281700	1.36539700	-2.87073500
H	-2.48871400	0.21571400	-2.59813400

C	-5.65098000	1.67949300	-0.90734100
H	-4.95175900	0.74124400	0.89622900
C	-5.42120500	1.90465600	-2.26512100
H	-4.09113800	1.53909500	-3.92628300
H	-6.53275700	2.09543500	-0.42668900
H	-6.12078600	2.49816600	-2.84763600
C	-2.78483600	-2.36154300	-0.39659000
C	-3.86710300	-2.65781200	-1.23985500
C	-1.97975900	-3.42046800	0.05537500
C	-4.13554000	-3.97599400	-1.61783900
H	-4.50750800	-1.86180500	-1.60402000
C	-2.25454900	-4.73632800	-0.31396300
H	-1.13304200	-3.21920300	0.70441600
C	-3.33305000	-5.01879300	-1.15524500
H	-4.97829700	-4.18414300	-2.27227300
H	-1.61650500	-5.53849200	0.04589800
H	-3.54314600	-6.04357200	-1.45007700
P	-2.35603700	-0.64318300	0.16551200
C	-3.00280200	-0.64799100	1.90319900
C	-2.44165900	0.25131200	2.82460900
C	-4.02097300	-1.51386000	2.33701800
C	-2.89569700	0.29065800	4.14507200
H	-1.64159300	0.91835100	2.51303800
C	-4.46817500	-1.47640300	3.65836800
H	-4.46329800	-2.22163600	1.64268000
C	-3.90763100	-0.57358700	4.56552700
H	-2.45090600	0.99483800	4.84329700
H	-5.25511400	-2.15426800	3.97923800
H	-4.25666200	-0.54736000	5.59459600

IRC of triphenylphosphonin C–P oxidative -Point31

0 1

P	0.32440900	2.39763800	1.08173800
C	-0.64426400	3.87551000	0.57096500
C	2.05844300	3.03542900	1.17584400
Pd	0.16875800	0.42380400	-0.12230000
C	-1.95873200	3.68567400	0.10193800

C	-0.21188200	5.19848600	0.78676400
C	2.68603500	3.83404000	0.20100900
C	2.80027300	2.67988100	2.31669300
C	0.83698900	1.56682700	-1.69067900
C	-2.79903800	4.76691700	-0.15756700
H	-2.32733700	2.67814100	-0.06208000
C	-1.05358400	6.28049700	0.52598200
H	0.78651600	5.38725400	1.16703800
C	4.00264200	4.26361100	0.36822100
H	2.14005100	4.11695300	-0.69257100
C	4.12121400	3.10516100	2.48349100
H	2.32996000	2.07174100	3.08620500
C	2.16255500	1.51869400	-2.14393500
C	-0.12558900	2.18844200	-2.49892900
C	-2.34948700	6.07313000	0.04943400
H	-3.80537000	4.58368600	-0.52570900
H	-0.69221500	7.29161600	0.69869500
C	4.72580300	3.90081100	1.50866000
H	4.46792400	4.87951500	-0.39754700
H	4.67078800	2.82428400	3.37874300
C	2.50225200	2.02177400	-3.40512400
H	2.94251800	1.09505500	-1.52200800
C	0.21546400	2.68763300	-3.76201900
H	-1.14500600	2.30805400	-2.14713600
C	1.53009700	2.60165300	-4.22261900
H	3.53520900	1.96219800	-3.74208500
H	-0.54926400	3.16086000	-4.37481700
P	1.74220100	-1.63002300	-0.06398400
C	1.36505900	-2.99990600	-1.24959500
C	1.84261700	-2.45586300	1.59479700
C	3.53724600	-1.30311700	-0.39060100
C	0.85023400	-2.62537700	-2.50229600
C	1.56177700	-4.36272100	-0.98048600
C	2.92907400	-3.26185900	1.97798800
C	0.80767100	-2.24412900	2.51904800
C	4.17103300	-0.30744600	0.37331700
C	4.27916500	-1.97122700	-1.37495600

C	0.55519400	-3.58899000	-3.46728900
H	0.68244200	-1.57335800	-2.71963100
C	1.25476200	-5.32674200	-1.94333600
H	1.94972300	-4.67678400	-0.01655500
C	2.96276500	-3.85884600	3.23880400
H	3.75879100	-3.41136700	1.29333700
C	0.84092600	-2.84183300	3.78145900
H	-0.02340700	-1.59475300	2.25856800
C	5.51435500	0.00117300	0.16637000
H	3.60877800	0.24562600	1.12040700
C	5.62494700	-1.65565300	-1.58503500
H	3.81144500	-2.73916400	-1.98221600
C	0.75407200	-4.94283400	-3.18878600
H	0.16182900	-3.28157100	-4.43256200
C	1.91682900	-3.65349300	4.14236900
H	3.81062600	-4.47910300	3.51812900
H	0.02933700	-2.66152800	4.48116600
C	6.24660500	-0.67263200	-0.81548400
H	5.97967300	0.78131900	0.76232200
H	6.18459300	-2.18232000	-2.35394400
H	0.51589800	-5.69469100	-3.93656000
H	1.94731600	-4.11527800	5.12574600
H	7.29204800	-0.42701400	-0.98278300
H	1.40981600	-6.37919400	-1.71900600
H	-3.00184000	6.91845300	-0.15407000
H	5.75048700	4.24073400	1.63708600
H	1.79749500	2.99724400	-5.19957500
C	-3.60904700	0.36511900	-0.74752200
C	-3.37878600	0.60926900	-2.11360400
C	-4.75572100	0.91131000	-0.15237500
C	-4.27907600	1.36350400	-2.86550800
H	-2.48650400	0.21206500	-2.58994700
C	-5.65004100	1.67903000	-0.90423900
H	-4.95476600	0.73973900	0.90037800
C	-5.41787000	1.90392600	-2.26166700
H	-4.08545700	1.53713500	-3.92071200
H	-6.53205200	2.09606900	-0.42496900

H	-6.11588900	2.49820000	-2.84527300
C	-2.78844400	-2.36547500	-0.39100300
C	-3.87122800	-2.66092000	-1.23393500
C	-1.98217000	-3.42472600	0.05813600
C	-4.13902400	-3.97852300	-1.61429700
H	-4.51238400	-1.86460500	-1.59612500
C	-2.25628400	-4.74004800	-0.31365700
H	-1.13493700	-3.22425200	0.70678500
C	-3.33530000	-5.02164000	-1.15454200
H	-4.98218400	-4.18601800	-2.26842100
H	-1.61729200	-5.54244600	0.04398100
H	-3.54484200	-6.04596800	-1.45131200
P	-2.35952200	-0.64784900	0.17297700
C	-3.00876800	-0.65265100	1.90969700
C	-2.44893100	0.24735400	2.83130400
C	-4.02691700	-1.51884500	2.34292400
C	-2.90433700	0.28705600	4.15129500
H	-1.64898500	0.91484700	2.52030300
C	-4.47544300	-1.48104100	3.66382700
H	-4.46818100	-2.22715000	1.64843900
C	-3.91626200	-0.57752500	4.57112500
H	-2.46066000	0.99178300	4.84967700
H	-5.26236800	-2.15914500	3.98423600
H	-4.26633900	-0.55098700	5.59983200

N(*para*–H–phenyl)$_3$

0 1

C	0.15379600	-1.41344100	-0.00003200
C	1.14726300	0.83998900	0.00018200
C	-1.30082500	0.57346300	-0.00016700
C	-0.67079000	-2.22123700	0.80075000
C	1.13255800	-2.02543000	-0.80076200
C	2.25941300	0.52987200	0.80058100
C	1.18724800	1.99395300	-0.80008000
C	-1.58936700	1.68916300	0.80323800
C	-2.31888700	0.03372900	-0.80377900
C	-0.52255800	-3.60713400	0.79036600

H	-1.42488400	-1.75647200	1.42785100
C	1.28546100	-3.41080800	-0.78997600
H	1.76926800	-1.40981800	-1.42809800
C	3.38535500	1.35141600	0.78992300
H	2.23437300	-0.35569200	1.42753700
C	2.31042900	2.81929900	-0.78957800
H	0.33535100	2.23742700	-1.42688800
C	-2.86384100	2.25347600	0.79266300
H	-0.81074500	2.10831300	1.43251300
C	-3.59524000	0.59377900	-0.79343900
H	-2.10285000	-0.82384100	-1.43293900
C	0.45790600	-4.21185500	0.00033500
H	-1.16986600	-4.21554100	1.41673300
H	2.04833100	-3.86617100	-1.41622400
C	3.41835000	2.50303500	0.00012100
H	4.23622900	1.09510700	1.41588900
H	2.32284400	3.70788300	-1.41548700
C	-3.87644900	1.70878700	-0.00047000
H	-3.06821800	3.11654100	1.42103800
H	-4.37006500	0.16237600	-1.42196600
N	0.00023700	-0.00006000	0.00011400
H	-4.87044000	2.14692700	-0.00062300
H	4.29477100	3.14480000	0.00012200
H	0.57530500	-5.29175900	0.00049000

N(*para*–H–phenyl)$_2$(*para*–Cl–phenyl)

0 1

C	0.76189300	-0.00001000	-0.00002100
C	-1.36913500	-1.23160900	0.00108100
C	-1.36911500	1.23161100	-0.00110800
C	1.47956200	0.92613100	-0.77600200
C	1.47955300	-0.92615100	0.77596800
C	-0.95530200	-2.29681200	-0.81530100
C	-2.49978900	-1.39803900	0.81717900
C	-2.49970400	1.39811600	-0.81728000
C	-0.95532500	2.29674300	0.81538500
C	2.87225500	0.93439300	-0.77066700

H	0.94139900	1.64358200	-1.38661300
C	2.87224600	-0.93440700	0.77065500
H	0.94138300	-1.64360700	1.38656800
C	-1.65304800	-3.50357800	-0.80369000
H	-0.08762200	-2.17250500	-1.45549200
C	-3.20176400	-2.60231000	0.80806900
H	-2.82246700	-0.58079500	1.45438600
C	-3.20166100	2.60239800	-0.80813400
H	-2.82234400	0.58092100	-1.45456900
C	-1.65305200	3.50352100	0.80381100
H	-0.08769400	2.17237300	1.45562900
C	3.56362200	-0.00000500	0.00000000
H	3.41735800	1.65247400	-1.37425800
H	3.41734300	-1.65248600	1.37425400
C	-2.78194100	-3.66385200	0.00309500
H	-1.31862300	-4.31738400	-1.44177100
H	-4.07462400	-2.71393200	1.44599000
C	-2.78188100	3.66387200	-0.00304800
H	-4.07447100	2.71408300	-1.44611200
H	-1.31866400	4.31727700	1.44197800
N	-0.65574800	-0.00000800	-0.00003700
H	-3.32737600	4.60316800	-0.00393300
H	-3.32745200	-4.60313900	0.00401000
Cl	5.32291800	-0.00000300	0.00001400

N(*para*–H–phenyl) (*para*–Cl–phenyl)$_2$

0 1

C	-1.23087700	-0.12307600	0.00131500
C	-0.00000100	2.00826600	0.00002500
C	1.23087900	-0.12307100	-0.00123900
C	-1.39767800	-1.27798000	-0.78116100
C	-2.30947500	0.32266400	0.78342000
C	-0.86465300	2.71905200	-0.84712400
C	0.86465600	2.71908400	0.84714400
C	2.30940800	0.32261100	-0.78346600
C	1.39773800	-1.27791600	0.78130900
C	-2.60361200	-1.97488800	-0.77548300

H	-0.57796000	-1.63094900	-1.39829300
C	-3.52367600	-0.35958100	0.77818000
H	-2.19467200	1.20953300	1.39783800
C	-0.86763100	4.11310400	-0.83692000
H	-1.53018500	2.17440000	-1.50954200
C	0.86764900	4.11313400	0.83687400
H	1.53017400	2.17445300	1.50959300
C	3.52361100	-0.35963400	-0.77827400
H	2.19455400	1.20943600	-1.39793900
C	2.60367000	-1.97482600	0.77558600
H	0.57806400	-1.63083900	1.39852700
C	-3.66420700	-1.50959200	0.00163400
H	-2.72392000	-2.86500600	-1.38394900
H	-4.35099600	-0.00874700	1.38603700
C	0.00001300	4.81874600	-0.00004100
H	-1.54325100	4.64857100	-1.49867300
H	1.54327000	4.64862600	1.49860500
C	3.66420300	-1.50958500	-0.00165300
H	4.35088100	-0.00884800	-1.38622700
H	2.72403300	-2.86489800	1.38410700
N	-0.00000500	0.58307500	0.00007000
H	0.00002000	5.90484700	-0.00006700
Cl	-5.19203000	-2.38003700	0.00184600
Cl	5.19202500	-2.38003200	-0.00191900

N(*para*–Cl–phenyl)$_3$

0 1

C	0.97090500	1.03740600	-0.00022400
C	-1.38398600	0.32232200	0.00014200
C	0.41268600	-1.35931600	-0.00026600
C	2.11959400	0.94150600	0.80214100
C	0.80001900	2.17742100	-0.80254100
C	-1.87582500	1.36455100	0.80288500
C	-2.28543300	-0.39577400	-0.80245300
C	-0.24188500	-2.30551500	0.80514800
C	1.48289500	-1.78173300	-0.80562800
C	3.07799500	1.95218700	0.79685100

H	2.26197600	0.07059300	1.43353500
C	1.74561400	3.20009800	-0.79689500
H	-0.07833300	2.26235700	-1.43398600
C	-3.23040100	1.68882800	0.79734500
H	-1.19304800	1.92340900	1.43449700
C	-3.64397000	-0.08855100	-0.79712200
H	-1.91951200	-1.19860700	-1.43412600
C	0.15446600	-3.64079600	0.79982000
H	-1.06528600	-1.99271500	1.43888100
C	1.89611200	-3.11188400	-0.80010400
H	1.99327400	-1.06393800	-1.43947400
C	2.88413800	3.08054000	0.00006800
H	3.96222800	1.87132000	1.42014600
H	1.60692300	4.07718400	-1.42010700
C	-4.11023600	0.95681900	0.00001900
H	-3.60281300	2.49472100	1.42085200
H	-4.33388500	-0.64719900	-1.42068500
C	1.22616000	-4.03750000	-0.00003800
H	-0.35555200	-4.36566600	1.42539900
H	2.72311500	-3.43074000	-1.42564100
Cl	-5.82185000	1.35531900	-0.00019700
Cl	1.73700100	-5.71903000	0.00028200
Cl	4.08536900	4.36334000	0.00035500
N	-0.00014500	0.00027400	-0.00023800

N(*para*–H–phenyl)$_2$(*para*–CF$_3$–phenyl)

0 1

C	0.21020000	0.01119100	0.01439700
C	-1.91505200	-1.23382700	0.00806200
C	-1.93441300	1.22384900	-0.00729200
C	0.92728300	1.01308700	-0.66659900
C	0.93231100	-0.97854900	0.70801800
C	-1.53077900	-2.28224500	-0.84260100
C	-3.02026500	-1.40985300	0.85482200
C	-3.03146000	1.38200400	-0.86810800
C	-1.57793700	2.27851600	0.84775000
C	2.31714600	1.02349100	-0.64967200

H	0.38868900	1.78156000	-1.21002400
C	2.32218700	-0.96956500	0.70968900
H	0.39698800	-1.74947600	1.25124400
C	-2.23278400	-3.48668900	-0.83283200
H	-0.68307600	-2.14716200	-1.50701300
C	-3.72743300	-2.61131000	0.84470400
H	-3.31925200	-0.60249200	1.51587000
C	-3.75778200	2.57200700	-0.86751000
H	-3.30914300	0.56989800	-1.53261800
C	-2.29889400	3.47159600	0.82853100
H	-0.73676100	2.15720900	1.52303200
C	3.02699600	0.03229600	0.03515600
H	2.85424100	1.80446400	-1.17831600
H	2.86327400	-1.73355200	1.25864800
C	-3.33628800	-3.65775800	0.00636400
H	-1.92269900	-4.28924400	-1.49677300
H	-4.58112700	-2.73256800	1.50621000
C	-3.39416300	3.62482900	-0.02478500
H	-4.60478300	2.67943500	-1.53992900
H	-2.01014900	4.27915000	1.49602600
N	-1.20160200	0.00076500	0.00522600
H	-3.95818700	4.55309600	-0.03188700
H	-3.88546400	-4.59491300	0.00594400
C	4.52612900	0.00889800	-0.00564000
F	4.99562000	-0.70282700	-1.06039200
F	5.05462700	-0.55518700	1.10511800
F	5.04849300	1.25217300	-0.11713900

N(*para*–H–phenyl) (*para*–CF_3–phenyl)$_2$

0 1

C	-1.23214800	0.29556900	-0.00293700
C	-0.00004300	2.42348000	0.00003200
C	1.23218700	0.29562000	0.00306300
C	-1.38920700	-0.88312900	-0.75449700
C	-2.32754900	0.78035600	0.73248900
C	-0.80383000	3.13107800	-0.90571200
C	0.80369000	3.13123000	0.90570900

C	2.32763200	0.78058300	-0.73217900
C	1.38922800	-0.88324600	0.75438100
C	-2.60299600	-1.56067900	-0.75745800
H	-0.55891100	-1.25890100	-1.34275600
C	-3.54345900	0.10510600	0.71511400
H	-2.22061900	1.68801700	1.31659600
C	-0.80789900	4.52538900	-0.89612100
H	-1.42102000	2.58455600	-1.61207500
C	0.80765000	4.52553900	0.89598300
H	1.42092100	2.58482300	1.61212300
C	3.54355500	0.10534600	-0.71487100
H	2.22074100	1.68836300	-1.31610400
C	2.60302200	-1.56077300	0.75726800
H	0.55890700	-1.25915700	1.34251500
C	-3.68982800	-1.07073400	-0.02599400
H	-2.71402000	-2.46228400	-1.35135400
H	-4.38135200	0.49170800	1.28577100
C	-0.00015300	5.22955800	-0.00010400
H	-1.43552700	5.06185800	-1.60253300
H	1.43523400	5.06212800	1.60234300
C	3.68990100	-1.07065200	0.02598000
H	4.38147100	0.49208400	-1.28539800
H	2.71402000	-2.46250600	1.35097900
N	0.00001300	0.99435700	0.00011400
H	-0.00019700	6.31571600	-0.00015600
C	-4.98132900	-1.83578300	0.00453900
C	4.98138900	-1.83571500	-0.00458700
F	-6.03675800	-1.03576800	0.27645400
F	-5.22975300	-2.45100200	-1.17452000
F	-4.97240400	-2.80529000	0.95127200
F	6.03678800	-1.03579200	-0.27687700
F	4.97228100	-2.80547300	-0.95106400
F	5.22999900	-2.45065000	1.17458600

N(*para*–CF_3–phenyl)$_3$

0 1

C	-1.06843700	0.93909800	-0.00174000

C	-0.25908800	-1.38461500	0.01621800
C	1.34797000	0.47781200	0.01465800
C	-1.01305000	2.10409700	0.78148600
C	-2.20132700	0.70856400	-0.80042100
C	-1.30066000	-1.91011700	0.79948400
C	0.51877900	-2.26118300	-0.75869000
C	2.31414100	-0.13677600	0.82898000
C	1.72772400	1.56274800	-0.79250100
C	-2.06228400	3.01710600	0.75982400
H	-0.14580900	2.29025800	1.40605600
C	-3.25448100	1.61686700	-0.80602400
H	-2.24925300	-0.18023700	-1.42057000
C	-1.56228300	-3.27610500	0.79720100
H	-1.89824900	-1.24519500	1.41396500
C	0.26301500	-3.62835000	-0.74470800
H	1.32261600	-1.86696500	-1.37122200
C	3.62821200	0.31821500	0.82649400
H	2.02877300	-0.96640600	1.46713500
C	3.04045000	2.02350100	-0.78009100
H	0.99124000	2.04205500	-1.42871900
C	-3.19044400	2.77825900	-0.03020100
H	-2.00660600	3.91557800	1.36553400
H	-4.11973600	1.43435400	-1.43484700
C	-0.78039800	-4.14426000	0.02936600
H	-2.36255700	-3.67212900	1.41371000
H	0.87282300	-4.29623500	-1.34417100
C	3.99911900	1.40286600	0.02558900
H	4.36374300	-0.15673700	1.46758500
H	3.32180600	2.86445700	-1.40515300
N	0.00623000	0.01055400	0.01095900
C	-4.35062400	3.73286500	-0.00331200
C	-1.09617100	-5.61279800	-0.00871200
C	5.43108500	1.85720700	-0.00876700
F	-5.25756100	3.39653000	0.94472000
F	-3.95556100	4.99725200	0.26568700
F	-5.01107900	3.75360200	-1.18278100
F	-1.63354300	-6.04206600	1.15515500

F	-1.98855600	-5.91023200	-0.98328400
F	0.00588700	-6.35781100	-0.24899300
F	6.03923000	1.68851100	1.18705400
F	6.15746300	1.16161000	-0.91596600
F	5.53817700	3.16297300	-0.34057100

N(*para*–H–phenyl)$_2$(*para*–NO$_2$–phenyl)

0 1

C	-0.55607200	0.00001700	-0.00000100
C	1.58067500	-1.22642200	0.00058200
C	1.58070700	1.22639600	-0.00057400
C	-1.27884700	1.07299800	0.56831800
C	-1.27887100	-1.07295400	-0.56830500
C	1.27116800	-2.24229200	0.91709500
C	2.63579500	-1.41212900	-0.90390800
C	2.63565700	1.41218200	0.90409700
C	1.27140600	2.24215800	-0.91727500
C	-2.66506600	1.07501100	0.56564000
H	-0.74346200	1.89930300	1.02128500
C	-2.66508800	-1.07492700	-0.56563400
H	-0.74350500	-1.89928100	-1.02125600
C	1.99898500	-3.43162500	0.91434400
H	0.46249800	-2.09449300	1.62618200
C	3.36904800	-2.59800800	-0.88881800
H	2.87558600	-0.62551000	-1.61252100
C	3.36894300	2.59804200	0.88900800
H	2.87528500	0.62563800	1.61284800
C	1.99925400	3.43147300	-0.91452900
H	0.46286800	2.09428700	-1.62649700
C	-3.35419600	0.00005200	-0.00000200
H	-3.22433900	1.88994300	1.00876000
H	-3.22439100	-1.88984400	-1.00874900
C	3.05227500	-3.61449000	0.01517100
H	1.74926900	-4.21162600	1.62842100
H	4.18419200	-2.73060800	-1.59497500
C	3.05237000	3.61441800	-0.01516900
H	4.18395300	2.73071100	1.59530700

H	1.74970100	4.21139400	-1.62874900
N	0.84573800	-0.00000800	0.00000300
H	3.62186100	4.53931600	-0.02044000
H	3.62174000	-4.53940300	0.02043900
N	-4.81121900	0.00005200	-0.00001900
O	-5.38756600	-0.97490600	-0.49030600
O	-5.38765000	0.97496500	0.49028500

N(*para*–H–phenyl) (*para*–NO_2–phenyl)$_2$

0 1

C	1.23338100	0.01885200	-0.00299000
C	0.00007600	2.14108600	0.00003000
C	-1.23350300	0.01894600	0.00288700
C	1.38995400	-1.18943200	0.70586700
C	2.33766000	0.55019000	-0.69852200
C	0.72832600	2.84361500	0.96926800
C	-0.72800200	2.84389600	-0.96913600
C	-2.33802700	0.55076300	0.69767800
C	-1.38988700	-1.18982500	-0.70522400
C	2.60882400	-1.85316400	0.70945700
H	0.55508100	-1.59790300	1.26428700
C	3.56048700	-0.10625700	-0.68937500
H	2.22743600	1.47635600	-1.25118100
C	0.73228900	4.23821200	0.96091300
H	1.28552700	2.29489800	1.72241700
C	-0.73160000	4.23849400	-0.96064900
H	-1.28534900	2.29539200	-1.72233400
C	-3.56085800	-0.10568600	0.68856900
H	-2.22803400	1.47729800	1.24976100
C	-2.60877400	-1.85350800	-0.70880900
H	-0.55485300	-1.59872800	-1.26308100
C	3.68660600	-1.30569600	0.01219700
H	2.74339900	-2.77748300	1.25772200
H	4.41377900	0.28753000	-1.22775600
C	0.00043900	4.94014100	0.00016400
H	1.29944800	4.77594100	1.71543900
H	-1.29861600	4.77644300	-1.71512600

C	-3.68677100	-1.30556400	-0.01225800
H	-4.41428500	0.28847900	1.22645800
H	-2.74318100	-2.77816200	-1.25654800
N	-0.00006200	0.70643000	-0.00005900
H	0.00058300	6.02622000	0.00021300
N	4.97350200	-2.00086300	0.01961100
N	-4.97368800	-2.00069500	-0.01962500
O	5.04489500	-3.06684000	0.63380400
O	5.90973100	-1.47904300	-0.58863500
O	-5.91003200	-1.47847400	0.58809900
O	-5.04496100	-3.06698800	-0.63328700

N(*para*–NO_2–phenyl)$_3$

0 1

C	0.27159100	1.39238000	0.00047100
C	-1.34260500	-0.46144800	0.00042400
C	1.07007400	-0.93247400	0.00012200
C	1.31365900	1.91266100	0.78978500
C	-0.49813100	2.26645600	-0.78891300
C	-2.31403700	0.18087600	0.78994700
C	-1.71498100	-1.56469700	-0.78942700
C	1.00000500	-2.09532100	0.78917100
C	2.21191400	-0.70223900	-0.78903900
C	1.58575200	3.27477500	0.78649800
H	1.90248800	1.24664800	1.41101200
C	-0.23748500	3.63082400	-0.78603200
H	-1.29437200	1.87084000	-1.40999900
C	-3.62973000	-0.26443200	0.78670500
H	-2.03151000	1.02368000	1.41132900
C	-3.02693800	-2.02095500	-0.78655300
H	-0.97434100	-2.05640400	-1.41068000
C	2.04405700	-3.01150100	0.78589500
H	0.12878700	-2.27276100	1.41025500
C	3.26356000	-1.60964700	-0.78618100
H	2.26727900	0.18532600	-1.40983700
C	0.80488700	4.12146100	0.00003100
H	2.37928600	3.69230500	1.39389900

H	-0.81557700	4.31620500	-1.39352000
C	-3.97281300	-1.36374100	-0.00005700
H	-4.38799000	0.21390100	1.39432500
H	-3.33157000	-2.86398900	-1.39438200
C	3.16784300	-2.75775700	-0.00015900
H	2.00912300	-3.90771000	1.39300600
H	4.14625300	-1.45101500	-1.39335400
N	-0.00033700	-0.00058200	0.00045300
N	1.08648100	5.56086800	-0.00036900
N	-5.36018900	-1.83949400	-0.00017600
N	4.27450900	-3.72025100	-0.00024500
O	0.36884000	6.28172600	-0.69388500
O	2.02299400	5.95821900	0.69293800
O	-5.62587300	-2.82137200	-0.69371200
O	-6.17236400	-1.22701300	0.69327100
O	5.25803200	-3.45721500	-0.69245200
O	4.15076700	-4.73086300	0.69186200

N(*para*−H−phenyl)$_2$(*para*−OMe−phenyl)

0 1

C	0.73218800	-0.10044300	0.07672500
C	-1.47675400	-1.17481100	-0.01797700
C	-1.29714800	1.28752600	0.01295500
C	1.53848200	0.65134300	-0.78455300
C	1.35500200	-0.96203700	0.99695300
C	-1.05399900	-2.28625100	-0.76707500
C	-2.68451300	-1.26024500	0.69649800
C	-2.42007500	1.54247200	-0.79348800
C	-0.77714800	2.33128200	0.79768500
C	2.93174400	0.56458300	-0.72917500
H	1.07226700	1.31857400	-1.50295600
C	2.73782800	-1.07128200	1.04234000
H	0.74302500	-1.54898900	1.67482900
C	-1.81903000	-3.45115700	-0.79346100
H	-0.12518400	-2.22973600	-1.32552800
C	-3.45039400	-2.42344500	0.64934800
H	-3.01536900	-0.41228400	1.28742100

C	-3.01013700	2.80503400	-0.80139500
H	-2.82457600	0.74712000	-1.41121600
C	-1.36448400	3.59482400	0.76929800
H	0.08683500	2.14429900	1.42725900
C	3.54040600	-0.30471500	0.18339500
H	3.52409300	1.16653500	-1.40882500
H	3.22339400	-1.73629000	1.74980400
C	-3.02375000	-3.52854600	-0.09125900
H	-1.47416800	-4.29931300	-1.37947500
H	-4.38084000	-2.46918700	1.20962200
C	-2.48650600	3.84158200	-0.02514800
H	-3.87762500	2.98127800	-1.43236900
H	-0.94750200	4.38790100	1.38484700
N	-0.68932300	0.00502900	0.02709800
H	-2.94523600	4.82611300	-0.03961100
H	-3.62021100	-4.43594600	-0.11938800
O	4.88940900	-0.47710100	0.31750700
C	5.74638600	0.27193700	-0.52672300
H	6.76369800	-0.01332800	-0.25188800
H	5.57861200	0.03631300	-1.58642500
H	5.62019800	1.35264800	-0.37551700

N(*para*−H−phenyl) (*para*−OMe−phenyl)$_2$

0 1

C	1.17281600	-0.17386100	0.10868900
C	0.10966200	2.04822700	-0.00247200
C	-1.27562300	0.01103400	0.08339100
C	1.27622000	-1.24090900	1.01941500
C	2.24168200	0.06016100	-0.76416100
C	1.13929400	2.72726200	0.67433800
C	-0.81183800	2.79941800	-0.75400000
C	-2.30327600	0.48456200	0.91967300
C	-1.53595400	-1.10165800	-0.72428400
C	2.40732600	-2.04476600	1.04697900
H	0.45742400	-1.43684100	1.70469600
C	3.39321600	-0.73002900	-0.72609900
H	2.17785000	0.87474500	-1.47896400

C	1.24404200	4.11404700	0.59117500
H	1.85227900	2.16102200	1.26465400
C	-0.70683700	4.18779400	-0.81648000
H	-1.60655600	2.28861500	-1.28780100
C	-3.54796600	-0.12894900	0.93203900
H	-2.11764300	1.34206600	1.55894700
C	-2.77924800	-1.73887400	-0.69977800
H	-0.75485400	-1.47999500	-1.37640900
C	3.48049900	-1.79409500	0.17854500
H	2.48950700	-2.86942800	1.74831700
H	4.20189300	-0.51305700	-1.41488000
C	0.32188600	4.85710700	-0.14993300
H	2.04704600	4.61757000	1.12374700
H	-1.43000100	4.74768100	-1.40427300
C	-3.79748800	-1.25042900	0.12627400
H	-4.34342700	0.23472700	1.57517700
H	-2.94059400	-2.60151800	-1.33641600
N	0.00311700	0.63803400	0.07410500
H	0.40347900	5.93880200	-0.20644000
O	4.55178800	-2.63580400	0.29473900
O	-5.05143000	-1.78673000	0.22333600
C	5.66125900	-2.42525800	-0.56071900
H	6.39192200	-3.19373200	-0.30077800
H	5.38428400	-2.53288000	-1.61837000
H	6.10920500	-1.43387700	-0.40751400
C	-5.35415600	-2.92240100	-0.56737900
H	-6.38817600	-3.18444100	-0.33472800
H	-5.26952300	-2.70376800	-1.64068000
H	-4.70188300	-3.77194500	-0.32288400

N(*para*–OMe–phenyl)$_3$

0 1

C	-0.30541200	1.31870600	0.09918000
C	-0.95180100	-1.05496100	-0.02418300
C	1.42602200	-0.43317500	0.09223200
C	0.34020300	2.21406500	0.97251100
C	-1.31265800	1.81901300	-0.73522600

C	-2.11754900	-0.97816500	0.74818800
C	-0.80410500	-2.14779400	-0.89847200
C	1.85819900	-1.52463100	0.86902900
C	2.38175700	0.26727700	-0.65409200
C	-0.00591300	3.55791900	0.99763500
H	1.12058800	1.84585700	1.63098600
C	-1.68202900	3.16592800	-0.69787700
H	-1.82019200	1.14629300	-1.41938100
C	-3.11782300	-1.94820700	0.64837300
H	-2.24827800	-0.14566600	1.43250900
C	-1.78354500	-3.12769300	-0.98484600
H	0.09000300	-2.22480100	-1.50905700
C	3.19336500	-1.90268800	0.88448600
H	1.13456600	-2.07797400	1.45927500
C	3.73132100	-0.09329900	-0.62369800
H	2.06942900	1.10935700	-1.26364800
C	-1.02461100	4.04769300	0.16666100
H	0.49221100	4.24943400	1.67033200
H	-2.46983700	3.51227100	-1.35728400
C	-2.95370100	-3.03549800	-0.21703400
H	-4.00720700	-1.84992000	1.26072700
H	-1.66978600	-3.97217000	-1.65767400
C	4.14557300	-1.18822200	0.14220600
H	3.52732000	-2.74589500	1.48138000
H	4.44038000	0.47810200	-1.21215300
N	0.05559000	-0.05597300	0.07064400
O	-1.29658000	5.38429800	0.27818400
O	-3.86102300	-4.04563300	-0.38648300
O	5.43497900	-1.63640300	0.23576700
C	-2.31300400	5.92762000	-0.54464900
H	-3.28815800	5.46163700	-0.34658900
H	-2.36569300	6.98977600	-0.29717100
H	-2.07449500	5.81665200	-1.61143900
C	-5.05765500	-3.99909100	0.36934400
H	-5.63000300	-4.88366100	0.08276500
H	-4.85745700	-4.03256400	1.44911300
H	-5.64588600	-3.09904300	0.14301300

C	6.43179700	-0.95633400	-0.50539200
H	7.37078700	-1.47031200	-0.29021200
H	6.23516200	-1.00020300	-1.58549400
H	6.51780100	0.09576300	-0.20049500

N(*para*–H–phenyl)$_2$(*para*–Me–phenyl)

0 1

C	1.06814800	0.00569700	0.00048000
C	-1.05631200	-1.23572200	-0.00306100
C	-1.06746200	1.22916700	0.00101600
C	1.78341100	0.88110100	-0.83067500
C	1.78784700	-0.86098600	0.83753200
C	-0.60559100	-2.31048300	-0.78795700
C	-2.20895400	-1.40623500	0.78237300
C	-2.22008200	1.39000500	-0.78646100
C	-0.62829500	2.30693700	0.78828700
C	3.17652400	0.88924200	-0.81418700
H	1.24259600	1.55845700	-1.48429500
C	3.18068900	-0.85476000	0.82928600
H	1.24992600	-1.53658200	1.49535800
C	-1.28860900	-3.52544900	-0.77759300
H	0.28014500	-2.18606500	-1.40267500
C	-2.89507700	-2.61939800	0.77204400
H	-2.56076200	-0.58459600	1.39802400
C	-2.91745400	2.59673400	-0.77588900
H	-2.56302000	0.56595400	-1.40389900
C	-1.32255300	3.51553300	0.77820600
H	0.25742200	2.18993500	1.40449300
C	3.90559700	0.01864900	0.00695200
H	3.70738000	1.58058500	-1.46526100
H	3.71501000	-1.53436700	1.48992800
C	-2.43934000	-3.68854700	-0.00285800
H	-0.92435200	-4.34490400	-1.39192200
H	-3.78451000	-2.73187900	1.38672400
C	-2.47319400	3.66899500	0.00137100
H	-3.80667500	2.70181000	-1.39218600
H	-0.96714000	4.33748700	1.39437000

N	-0.35505800	-0.00010700	-0.00119600
H	-3.01547400	4.61017700	0.00151300
H	-2.97286700	-4.63471600	-0.00282000
C	5.41638100	0.00324000	-0.01199500
H	5.82717300	-0.27857700	0.96379900
H	5.80182900	-0.71836100	-0.74539800
H	5.82468800	0.98407900	-0.27860900

N(*para*–H–phenyl) (*para*–Me–phenyl)$_2$

0 1

C	-1.23044400	-0.37781500	-0.00277900
C	-0.00000500	1.75543900	-0.00001700
C	1.23045100	-0.37780800	0.00273900
C	-1.39963000	-1.51500000	-0.80814700
C	-2.30494900	0.03964500	0.79844800
C	-0.91296200	2.47031200	-0.79380600
C	0.91293800	2.47030600	0.79379100
C	2.30498700	0.03967800	-0.79843400
C	1.39961400	-1.51501200	0.80808500
C	-2.60504200	-2.21320800	-0.79933600
H	-0.58332300	-1.84648500	-1.44219700
C	-3.51055800	-0.65788300	0.78197100
H	-2.19207300	0.91624100	1.42859100
C	-0.91475300	3.86404100	-0.78360700
H	-1.61735300	1.92680600	-1.41541900
C	0.91470400	3.86403500	0.78363200
H	1.61734100	1.92679700	1.41538900
C	3.51059900	-0.65784000	-0.78192800
H	2.19212700	0.91628800	-1.42856100
C	2.60503300	-2.21321100	0.79930400
H	0.58328700	-1.84652300	1.44209600
C	-3.68610400	-1.80192800	-0.00824800
H	-2.71133300	-3.08982500	-1.43498900
H	-4.32884000	-0.31066000	1.40937000
C	-0.00003100	4.57149800	0.00002300
H	-1.62848400	4.39893500	-1.40501200
H	1.62842400	4.39892500	1.40505200

C	3.68612300	-1.80190500	0.00827000
H	4.32890400	-0.31059700	-1.40928500
H	2.71130200	-3.08984300	1.43494100
N	0.00000300	0.33504700	-0.00004100
H	-0.00004100	5.65776600	0.00003800
C	-4.98262900	-2.57784100	0.01243500
H	-4.98433400	-3.33781300	0.80602300
H	-5.84107200	-1.92143900	0.19294100
H	-5.15198400	-3.10045200	-0.93541100
C	4.98265300	-2.57781000	-0.01238300
H	4.98434800	-3.33784000	-0.80591500
H	5.84108600	-1.92141500	-0.19295300
H	5.15203100	-3.10035200	0.93549800

N(*para*–Me–phenyl)$_3$

0 1

C	1.23182100	0.70970900	-0.00169100
C	-0.00158200	-1.42066400	-0.00184600
C	-1.23033700	0.71260800	-0.00159700
C	1.40471400	1.85363300	-0.79679500
C	2.30380100	0.28546800	0.79994800
C	0.90008900	-2.14158000	-0.80035600
C	-0.90152000	-2.13752900	0.80316400
C	-2.30856000	0.28713900	-0.79389900
C	-1.39868100	1.85514200	0.79686300
C	2.61120900	2.55000900	-0.77944200
H	0.58758400	2.19703300	-1.42336000
C	3.51019400	0.98142100	0.79207500
H	2.18470800	-0.58999900	1.43050500
C	0.90098500	-3.53466900	-0.78314300
H	1.60320800	-1.60492100	-1.42952900
C	-0.90105800	-3.53020100	0.79521500
H	-1.59813600	-1.59717200	1.43641100
C	-3.51545100	0.98239200	-0.77649900
H	-2.19731200	-0.59379600	-1.41821900
C	-2.60554000	2.55069100	0.78892200
H	-0.58048500	2.19266200	1.42521900

C	3.69187300	2.12756300	0.00612700
H	2.71717800	3.43583400	-1.40227100
H	4.32372000	0.63312700	1.42518700
C	-0.00174900	-4.25995500	0.00570600
H	1.61301700	-4.06877400	-1.40887200
H	-1.60674800	-4.06106700	1.43095500
C	-3.68979600	2.13170200	0.00625600
H	-4.33611100	0.62866500	-1.39719200
H	-2.71047500	3.43127100	1.41937200
N	-0.00014700	0.00077700	-0.00382000
C	5.01141500	2.86366200	-0.01222100
H	5.52512200	2.79018100	0.95285500
H	5.69108600	2.45342500	-0.77193100
H	4.87507600	3.92632200	-0.24081900
C	-0.02329200	-5.77078600	-0.01278700
H	0.96108300	-6.18314200	-0.25971500
H	-0.32567200	-6.17977500	0.95779500
H	-0.73206500	-6.15443000	-0.75966500
C	-4.98815900	2.90454200	-0.01321500
H	-4.99450300	3.66163100	-0.80957500
H	-5.84562300	2.24537900	-0.18834700
H	-5.15587800	3.43031500	0.93322400

N(*para*–H–phenyl)$_2$(*para*–NMe$_2$–phenyl)

0 1

C	-0.42510800	-0.02387200	0.01884600
C	1.72086700	-1.22068700	0.04032400
C	1.67788000	1.24778100	-0.04385000
C	-1.15320900	0.75893600	0.92355000
C	-1.14243400	-0.82834900	-0.87561500
C	1.25604700	-2.29714500	0.81606000
C	2.89754400	-1.38930500	-0.71128300
C	2.86359200	1.45472100	0.68373300
C	1.16068800	2.30982800	-0.80626600
C	-2.54417300	0.74623600	0.93306200
H	-0.62154900	1.39714400	1.62324200
C	-2.53270300	-0.86595400	-0.85799800

H	-0.60186000	-1.43585700	-1.59552700
C	1.94956000	-3.50591700	0.83359500
H	0.35010700	-2.17833600	1.40145500
C	3.59204900	-2.59682500	-0.67360300
H	3.26045500	-0.57065000	-1.32426800
C	3.51578800	2.68520800	0.63520600
H	3.26671500	0.64757500	1.28674600
C	1.81223200	3.54148100	-0.83457100
H	0.24746800	2.16161400	-1.37333700
C	-3.27720200	-0.08297000	0.05372700
H	-3.05726400	1.38072900	1.64585700
H	-3.03713400	-1.50326900	-1.57445800
C	3.12396700	-3.66562200	0.09461300
H	1.57264400	-4.32470400	1.44141800
H	4.49889200	-2.70547400	-1.26330200
C	2.99582900	3.73930800	-0.11982000
H	4.43047400	2.82317400	1.20637000
H	1.39517800	4.34842800	-1.43194500
N	1.00290200	0.00172400	0.00353500
H	3.50368500	4.69911300	-0.14918500
H	3.66461200	-4.60757500	0.11561000
N	-4.66943300	-0.13643800	0.09284300
C	-5.37903600	-0.80353300	-0.98509800
H	-5.19892400	-0.34460900	-1.97159700
H	-5.09233500	-1.85993000	-1.04717000
H	-6.45150100	-0.76783400	-0.78176400
C	-5.39125900	0.86468500	0.85911600
H	-6.46245300	0.66388800	0.78858400
H	-5.11834400	0.81808800	1.91989100
H	-5.20866000	1.89347200	0.50637300

N(*para*–H–phenyl) (*para*–NMe$_2$–phenyl)$_2$

0 1

C	1.22563500	0.14251400	-0.00418700
C	0.00015900	2.28334400	-0.00010200
C	-1.22578100	0.14274400	0.00370000
C	1.42998800	-0.92719800	0.87752600

C	2.26065200	0.45974500	-0.89420400
C	1.02658200	3.00450100	0.63943000
C	-1.02609700	3.00491700	-0.63943900
C	-2.26116700	0.46076500	0.89310400
C	-1.43000200	-0.92757100	-0.87725500
C	2.61317200	-1.65843200	0.86657900
H	0.64701000	-1.19134200	1.58216300
C	3.45640600	-0.25179400	-0.89639700
H	2.13210400	1.28576400	-1.58740500
C	1.02493400	4.39766500	0.62974600
H	1.82122400	2.46510400	1.14396200
C	-1.02411200	4.39807700	-0.62941000
H	-1.82087600	2.46583500	-1.14410000
C	-3.45688500	-0.25074700	0.89551100
H	-2.13291100	1.28740600	1.58561700
C	-2.61324100	-1.65880000	-0.86607900
H	-0.64693000	-1.19233300	-1.58155700
C	3.66270400	-1.34571000	-0.02617600
H	2.71731700	-2.47354600	1.57276700
H	4.22739800	0.04535000	-1.59727300
C	0.00050200	5.10868400	0.00025400
H	1.82836600	4.93067100	1.13256500
H	-1.82741400	4.93140200	-1.13209700
C	-3.66292000	-1.34550700	0.02621300
H	-4.22820100	0.04716100	1.59571800
H	-2.71720400	-2.47426600	-1.57189700
N	-0.00003500	0.87071000	-0.00028100
H	0.00064100	6.19496400	0.00039100
N	4.84183800	-2.09342100	-0.05777700
N	-4.84204100	-2.09316900	0.05807500
C	5.97746000	-1.57749100	-0.80217200
H	6.33038500	-0.59941600	-0.43351200
H	6.80349200	-2.28868400	-0.73069600
H	5.73111700	-1.46829900	-1.86471900
C	5.11943900	-3.00779000	1.03642000
H	4.34604600	-3.78166300	1.10534300
H	6.06941900	-3.51259900	0.84693900

H	5.18431700	-2.50515300	2.01621800
C	-5.97766100	-1.57722100	0.80242400
H	-6.33129500	-0.59964900	0.43311500
H	-6.80331000	-2.28896000	0.73186800
H	-5.73095400	-1.46706200	1.86477500
C	-5.11948000	-3.00792200	-1.03578900
H	-4.34609900	-3.78187700	-1.10426900
H	-6.06955900	-3.51258800	-0.84639700
H	-5.18412800	-2.50569500	-2.01582600

N(*para*–NMe$_2$–phenyl)$_3$

0 1

C	-1.25790800	-0.68284600	-0.07540100
C	0.03769200	1.41187800	-0.04393200
C	1.20302400	-0.75395100	-0.06333900
C	-1.45318000	-1.83206800	-0.86259100
C	-2.34152400	-0.22495200	0.68487400
C	-0.79128200	2.17803000	-0.87564900
C	0.91562100	2.09904500	0.80628200
C	2.28817800	-0.37353700	-0.86574300
C	1.36200100	-1.88863400	0.74550000
C	-2.67449700	-2.49205700	-0.87892200
H	-0.63731100	-2.20125400	-1.47620800
C	-3.57069100	-0.88483800	0.66338900
H	-2.22107500	0.65632800	1.30736900
C	-0.75200900	3.56872800	-0.85550400
H	-1.48719600	1.67613900	-1.54116700
C	0.97770700	3.48883000	0.81459000
H	1.56220100	1.53390700	1.47093900
C	3.48164300	-1.08889400	-0.85780500
H	2.19984100	0.50535900	-1.49718000
C	2.54393500	-2.62241100	0.74083600
H	0.54534800	-2.20188100	1.38900400
C	-3.76976400	-2.03841000	-0.11537800
H	-2.79053900	-3.35330600	-1.52978200
H	-4.36995700	-0.49863900	1.28593400
C	0.14950700	4.26821900	-0.02308300

H	-1.42563000	4.10760600	-1.51137700
H	1.67415500	3.96448600	1.49506800
C	3.64027200	-2.24845000	-0.06734500
H	4.28985600	-0.74024600	-1.48980000
H	2.60972800	-3.48801300	1.38947100
N	-0.00878200	-0.00977500	-0.06075800
N	-5.01768300	-2.70298400	-0.19110200
N	0.23106600	5.66461100	-0.03981300
N	4.82023300	-2.99948500	-0.09501700
C	-0.81883200	6.41451400	-0.70702600
H	-0.59206500	7.48121700	-0.64103500
H	-0.86631700	6.15598200	-1.77101400
H	-1.81894600	6.24568200	-0.27215500
C	0.93838100	6.33328000	1.03847000
H	0.50402100	6.13523300	2.03331700
H	1.99063400	6.02757000	1.06355800
H	0.91694900	7.41147800	0.86360200
C	-6.14628300	-2.07976800	0.47606500
H	-6.08080500	-2.10659100	1.58005500
H	-6.23966200	-1.03585400	0.16250500
H	-7.06179500	-2.60438800	0.18302700
C	-5.01322900	-4.15398400	-0.03403700
H	-5.96358900	-4.55999200	-0.39813400
H	-4.21159300	-4.60707400	-0.61838300
H	-4.88636900	-4.46666800	1.01864500
C	5.99809700	-2.42010000	-0.71683000
H	5.81862100	-2.21756900	-1.77897800
H	6.32203100	-1.47814900	-0.24201300
H	6.82162600	-3.13545300	-0.65639400
C	5.03874900	-3.98908600	0.94555000
H	4.25996100	-4.75998600	0.92017300
H	5.99525600	-4.48660700	0.76912500
H	5.05514700	-3.55712400	1.96081600

N(*para*–Cl–phenyl)$_2$(*para*–CF$_3$–phenyl)

0 1

C	0.91173900	0.02351900	0.01464600

C	-1.20202200	-1.23872100	0.00697100
C	-1.24255800	1.21764700	-0.00053200
C	1.61757900	1.00106200	-0.70948100
C	1.63857800	-0.93018500	0.74984700
C	-0.79333000	-2.28940000	-0.82954300
C	-2.31741800	-1.42752500	0.83779000
C	-2.35933100	1.36681100	-0.83764900
C	-0.87395800	2.28384400	0.83504000
C	3.00776200	1.02387400	-0.69321900
H	1.07177400	1.74038100	-1.28564000
C	3.02882200	-0.91068200	0.75016700
H	1.10844200	-1.68079100	1.32609400
C	-1.47357100	-3.50496200	-0.82773900
H	0.06167000	-2.15288600	-1.48371200
C	-3.01343800	-2.63419900	0.82995200
H	-2.64060400	-0.62485200	1.49270900
C	-3.09534000	2.54950400	-0.83695900
H	-2.65220100	0.55215800	-1.49199900
C	-1.59449200	3.47593200	0.82609200
H	-0.01847100	2.17807800	1.49422000
C	3.72404500	0.06764100	0.03299100
H	3.53917300	1.78566800	-1.25435000
H	3.57667100	-1.64604100	1.33034900
C	-2.58437800	-3.66996000	-0.00005800
H	-1.15329400	-4.31304500	-1.47676800
H	-3.87423900	-2.77456500	1.47500800
C	-2.70574500	3.60143700	-0.00786600
H	-3.95688000	2.65912000	-1.48698200
H	-1.30483000	4.29602600	1.47443800
N	-0.50382400	0.00143200	0.00681100
C	5.22483300	0.05492900	-0.00683500
F	5.69669700	-0.69317100	-1.03367500
F	5.75548500	-0.46164000	1.12486400
F	5.73525400	1.29715600	-0.16596300
Cl	-3.45233500	-5.19735300	-0.00396600
Cl	-3.62437200	5.09889400	-0.01307900

N(*para*–Cl–phenyl) (*para*–CF_3–phenyl)$_2$

0 1

C	1.24338700	-0.22734400	0.00764100
C	-0.02067300	1.88093700	0.00243100
C	-1.22119200	-0.26372400	0.01592000
C	1.42307400	-1.38759900	0.78139200
C	2.32151400	0.25405400	-0.75428200
C	0.80719200	2.60809900	0.87095300
C	-0.87040800	2.57739500	-0.87009500
C	-2.31137300	0.19337000	0.77662800
C	-1.36586800	-1.44081100	-0.73858600
C	2.64440300	-2.05192300	0.78090600
H	0.60454600	-1.76021500	1.38797200
C	3.54544300	-0.40695700	-0.73979800
H	2.19568100	1.14690100	-1.35738500
C	0.79544700	4.00110200	0.86257700
H	1.46291400	2.07959000	1.55545500
C	-0.90116100	3.97015200	-0.86982400
H	-1.50966900	2.02500800	-1.55132100
C	-3.51361600	-0.50533500	0.77504900
H	-2.20886600	1.09352800	1.37323800
C	-2.56630700	-2.14315400	-0.72499700
H	-0.53529900	-1.80110800	-1.33612100
C	3.71483000	-1.56511800	0.02388600
H	2.77412500	-2.93993000	1.39111000
H	4.37087200	-0.02359400	-1.33042900
C	-0.06332700	4.67563200	-0.00567400
H	1.43702200	4.55897800	1.53625200
H	-1.55951200	4.50419900	-1.54662700
C	-3.64873300	-1.67989100	0.02866900
H	-4.34389200	-0.14850900	1.37580900
H	-2.66410500	-3.05240300	-1.30900400
N	0.00065600	0.45599500	0.00669800
Cl	-0.08989700	6.43145600	-0.01089000
C	5.01513100	-2.31624200	-0.01052300
C	-4.96420300	-2.40401300	-0.00684800
F	5.27808400	-2.92024600	1.17074800

F	6.05871900	-1.50570600	-0.29523800
F	5.00928500	-3.29103300	-0.95120600
F	-5.64011500	-2.27485300	1.15726600
F	-5.77575400	-1.92904800	-0.98228600
F	-4.80594200	-3.72588600	-0.24186800

N(*para*–Cl–phenyl)$_2$(*para*–NO$_2$–phenyl)

0 1

C	-1.24594400	-0.00153500	0.00009600
C	0.89219500	-1.22506800	-0.00160600
C	0.88951100	1.22632100	0.00158300
C	-1.96659100	1.04634200	0.61240100
C	-1.96483000	-1.05052000	-0.61239700
C	0.56324400	-2.25568600	0.89156500
C	1.96633800	-1.40428500	-0.88522000
C	1.96317300	1.40800000	0.88526700
C	0.55817400	2.25618200	-0.89157000
C	-3.35358000	1.04808900	0.60920800
H	-1.43133500	1.85318300	1.09976800
C	-3.35181400	-1.05458500	-0.60922600
H	-1.42825100	-1.85640200	-1.09987800
C	1.28228000	-3.44888600	0.89234500
H	-0.25871300	-2.12180400	1.58751700
C	2.70075000	-2.58808400	-0.87717500
H	2.22710300	-0.61294900	-1.58064700
C	2.69491800	2.59344600	0.87718500
H	2.22569400	0.61726700	1.58072500
C	1.27450700	3.45101000	-0.89237100
H	-0.26351400	2.12042400	-1.58748200
C	-4.03985600	-0.00383600	0.00002800
H	-3.91401900	1.84356000	1.08496600
H	-3.91092500	-1.85094300	-1.08504100
C	2.35087700	-3.60715700	0.00911300
H	1.02529400	-4.24377700	1.58424000
H	3.53028300	-2.72400200	-1.56272900
C	2.34276300	3.61168900	-0.00916200
H	3.52413000	2.73126400	1.56274700

H	1.01571100	4.24531900	-1.58426100
N	0.16017400	-0.00016900	0.00002600
N	-5.49951400	-0.00496100	0.00003300
O	-6.07325500	-0.95926900	-0.53015400
O	-6.07450300	0.94852800	0.53023700
Cl	3.26690400	-5.10432100	0.01501400
Cl	3.25540700	5.11091400	-0.01509500

N(*para*–Cl–phenyl) (*para*–NO_2–phenyl)$_2$

0 1

C	1.23326100	-0.54151000	-0.00270800
C	0.00007400	1.58056500	-0.00005100
C	-1.23337500	-0.54137300	0.00257900
C	1.38855600	-1.74007500	0.72165100
C	2.33334700	-0.02498100	-0.71479000
C	0.76202300	2.28770100	0.94004100
C	-0.76177600	2.28786600	-0.94010300
C	-2.33345100	-0.02460400	0.71448300
C	-1.38872800	-1.74008500	-0.72154700
C	2.60451400	-2.40960700	0.72526600
H	0.55528800	-2.13687900	1.29088900
C	3.55375100	-0.68665100	-0.70517800
H	2.22297300	0.89290500	-1.28133200
C	0.77135100	3.68090000	0.93721800
H	1.34805200	1.74513200	1.67509800
C	-0.77090100	3.68106600	-0.93720000
H	-1.34788200	1.74542300	-1.67519100
C	-3.55391500	-0.68619400	0.70495000
H	-2.22307900	0.89339800	1.28083400
C	-2.60474500	-2.40950300	-0.72511200
H	-0.55545600	-2.13710100	-1.29062800
C	3.67906500	-1.87628800	0.01257900
H	2.73919500	-3.32713700	1.28478100
H	4.40471800	-0.30477100	-1.25568200
C	0.00027400	4.37004800	0.00003100
H	1.36078800	4.22784400	1.66509100
H	-1.36025400	4.22813900	-1.66504300

C	-3.67927100	-1.87594100	-0.01257600
H	-4.40484600	-0.30412200	1.25537400
H	-2.73946700	-3.32711600	-1.28447600
N	-0.00002000	0.14972300	-0.00010300
N	4.96370500	-2.57770300	0.02025900
N	-4.96400100	-2.57724800	-0.02016400
Cl	0.00039900	6.12338100	0.00008200
O	5.03413000	-3.63479000	0.64908600
O	5.89695400	-2.06854000	-0.60238400
O	-5.89716100	-2.06787200	0.60243300
O	-5.03453900	-3.63437100	-0.64891700

N(*para*–Cl–phenyl)$_2$(*para*–OMe–phenyl)

0 1

C	0.79160000	-1.13460600	0.09367000
C	0.52100900	1.30669100	0.03406300
C	-1.46364600	-0.16077200	0.01485800
C	0.59219400	-2.13900400	1.05641700
C	1.84043200	-1.27965000	-0.81953300
C	1.66791000	1.58409900	0.79770200
C	-0.02241200	2.33271000	-0.75856900
C	-2.32061700	0.71424300	0.70555300
C	-2.03096500	-1.22813300	-0.70232200
C	1.41462800	-3.25632500	1.09357400
H	-0.21631300	-2.03778100	1.77405500
C	2.68637400	-2.39025200	-0.77488600
H	2.00353500	-0.51277900	-1.57079800
C	2.25719200	2.84554200	0.76882400
H	2.09911400	0.80480900	1.41716700
C	0.55305100	3.60089300	-0.77725800
H	-0.89927200	2.13476800	-1.36612800
C	-3.70138300	0.53767200	0.66910500
H	-1.90225200	1.53632000	1.27679400
C	-3.41033400	-1.41928000	-0.72681800
H	-1.38593600	-1.91195000	-1.24378400
C	2.47355300	-3.39046600	0.18148000
H	1.26547100	-4.03667200	1.83321300

H	3.49239100	-2.46713400	-1.49552000
C	1.69412600	3.85174200	-0.01566300
H	3.14109800	3.04962300	1.36397100
H	0.12689000	4.38519700	-1.39402000
C	-4.24179000	-0.53177600	-0.04482900
H	-4.35331700	1.21796100	1.20702600
H	-3.83741000	-2.24590200	-1.28488400
N	-0.05849500	0.01365700	0.05302100
O	3.22917000	-4.51886100	0.31021000
C	4.31221400	-4.70759500	-0.58604000
H	4.77299000	-5.65587200	-0.30364400
H	3.96909800	-4.76768500	-1.62752300
H	5.05475500	-3.90330500	-0.49756300
Cl	2.43017300	5.44913200	-0.04655600
Cl	-5.98508700	-0.76376200	-0.08268800

N(*para*–Cl–phenyl) (*para*–OMe–phenyl)$_2$

0 1

C	0.11711500	1.36284200	-0.12081500
C	1.17506900	-0.86181500	-0.04160100
C	-1.27963200	-0.65710800	-0.09266300
C	-0.64145500	2.11507100	-1.03517900
C	0.95939600	2.04365300	0.76519100
C	2.35648500	-0.46528100	-0.69579000
C	1.18022900	-2.07940500	0.66380100
C	-1.57846200	-1.72890700	-0.95333400
C	-2.28859900	-0.17742300	0.74930900
C	-0.56066700	3.50038300	-1.05374600
H	-1.29972600	1.60232200	-1.72963500
C	1.06367100	3.43658200	0.73677400
H	1.54631500	1.47945100	1.48350600
C	3.50409800	-1.25146500	-0.64018900
H	2.37284200	0.46491800	-1.25355000
C	2.32151400	-2.87622900	0.70809000
H	0.28399800	-2.40184300	1.18276800
C	-2.84083400	-2.30523400	-0.95632900
H	-0.81008400	-2.10865300	-1.61971700

C	-3.56861400	-0.73726900	0.73512600
H	-2.07449600	0.64947000	1.41941800
C	0.29690100	4.17548900	-0.17154900
H	-1.14561000	4.08491000	-1.75709000
H	1.73099000	3.92797900	1.43579500
C	3.48233200	-2.45774500	0.05926700
H	4.40725400	-0.93511800	-1.15165800
H	2.31239100	-3.81164800	1.25792200
C	-3.85091000	-1.81162500	-0.11601800
H	-3.07548100	-3.13300500	-1.61831200
H	-4.32599400	-0.33488400	1.39818100
N	0.01470900	-0.05906800	-0.09399000
Cl	4.93004900	-3.45797700	0.12339200
O	0.30947900	5.53741000	-0.27828900
O	-5.06061200	-2.43993700	-0.20692500
C	1.15322800	6.26878300	0.59457400
H	1.00758500	7.32081000	0.34208000
H	0.88322700	6.10864500	1.64721700
H	2.21003100	6.00538900	0.45156900
C	-6.11836500	-1.97539700	0.61399500
H	-6.97934200	-2.60430500	0.37964400
H	-5.87710800	-2.07549600	1.68095900
H	-6.36653600	-0.92705400	0.39938600

N(*para*–Cl–phenyl)$_2$(*para*–Me–phenyl)

0 1

C	0.00575500	1.69239800	0.00140900
C	1.22882500	-0.44206800	-0.00269000
C	-1.23411800	-0.43292200	0.00271700
C	-0.83468700	2.41148900	-0.86067700
C	0.84881200	2.40297400	0.86826300
C	2.31323600	0.01245300	-0.77193800
C	1.39109300	-1.60601600	0.76780400
C	-1.40586800	-1.59320000	-0.77122000
C	-2.31416900	0.02724300	0.77469600
C	-0.83250500	3.80467300	-0.84488100
H	-1.49220300	1.87505400	-1.53792100

C	0.85438700	3.79605800	0.85889000
H	1.49600700	1.85957100	1.54988600
C	3.52718700	-0.67020800	-0.76676400
H	2.20290000	0.90664100	-1.37640100
C	2.59696700	-2.30289700	0.76198900
H	0.56787500	-1.96580800	1.37620600
C	-2.61686600	-2.28114600	-0.76617400
H	-0.58599900	-1.95713600	-1.38169800
C	-3.53316200	-0.64638400	0.76882700
H	-2.19649700	0.91872600	1.38178700
C	0.01544700	4.52653900	0.00611800
H	-1.49658000	4.34079700	-1.51929900
H	1.51495500	4.32569300	1.54187900
C	3.66270600	-1.82913400	-0.00284700
H	4.35852800	-0.31226000	-1.36494300
H	2.71319500	-3.19971300	1.36137600
C	-3.67815200	-1.80186500	0.00141500
H	-2.74045700	-3.17517700	-1.36824000
H	-4.36113700	-0.28417100	1.36910200
N	-0.00000100	0.26608300	0.00034300
C	0.04316500	6.03702100	-0.01306600
H	0.31813600	6.44549800	0.96542400
H	0.77589300	6.41456300	-0.73930400
H	-0.93125200	6.45307300	-0.29076900
Cl	5.19076200	-2.69984700	-0.00297800
Cl	-5.21262600	-2.66121100	0.00058400

N(*para*–Cl–phenyl) (*para*–Me–phenyl)$_2$

0 1

C	-1.00774400	-1.22813000	0.00104700
C	1.12849400	-0.00436400	-0.00256700
C	-0.99916500	1.23318000	-0.00346600
C	-2.12852900	-1.39663300	0.82813100
C	-0.61443700	-2.29526300	-0.82128400
C	1.84416500	-0.95295100	0.74880000
C	1.85075500	0.94004100	-0.75293700
C	-0.59903000	2.29368300	0.82393000

C	-2.12423300	1.40984100	-0.82323600
C	-2.83526800	-2.59724300	0.82117800
H	-2.44078800	-0.58419100	1.47680500
C	-1.31961900	-3.49640800	-0.80286500
H	0.24849800	-2.18078800	-1.46991000
C	3.23674900	-0.96482500	0.74422800
H	1.30412400	-1.68485400	1.34011200
C	3.24333700	0.94364500	-0.74668900
H	1.31571100	1.67511300	-1.34487200
C	-1.29995400	3.49759900	0.81532600
H	0.26051900	2.16891500	1.47513900
C	-2.82638300	2.61286300	-0.80653300
H	-2.44847400	0.59859900	-1.46751300
C	-2.44768400	-3.67227300	0.01019600
H	-3.69938300	-2.70454900	1.47336200
H	-0.99189400	-4.31005200	-1.44639500
C	3.93177700	-0.01268600	-0.00082600
H	3.77910000	-1.70023400	1.32922600
H	3.79079100	1.67581400	-1.33099800
C	-2.42714400	3.68434100	0.00393600
H	-0.97167300	4.30387800	1.46781000
H	-3.69807800	2.72362600	-1.44800900
N	-0.28743700	0.00003800	-0.00386800
Cl	5.69168800	-0.01798400	0.00012800
C	-3.23213100	-4.96360600	-0.00764700
H	-3.99687000	-4.95805700	-0.79647700
H	-2.58264400	-5.82592200	-0.19435600
H	-3.74951300	-5.13112200	0.94322700
C	-3.16961000	5.00016100	-0.01445000
H	-3.07888800	5.52463700	0.94305500
H	-2.77728200	5.67196100	-0.79027400
H	-4.23597700	4.85685000	-0.22065700

N(*para*–Cl–phenyl)$_2$(*para*–NMe$_2$–phenyl)

0 1

C	-1.09162900	-0.06622100	0.02134400
C	1.08934100	-1.19501100	0.02752800

C	0.96937600	1.27087200	-0.01437300
C	-1.84155300	0.62378700	0.98156200
C	-1.78058700	-0.82272000	-0.93453500
C	0.64234100	-2.30569400	0.76446700
C	2.28080300	-1.31592400	-0.70991300
C	2.16154800	1.50385700	0.69485300
C	0.40072600	2.33571500	-0.73521300
C	-3.23109500	0.56880900	0.98569900
H	-1.32885200	1.22133500	1.72990200
C	-3.16885600	-0.90235800	-0.92603300
H	-1.21984800	-1.35782700	-1.69554300
C	1.35988500	-3.49922200	0.76467900
H	-0.27477000	-2.23093100	1.33896400
C	3.01035300	-2.50208900	-0.69946100
H	2.63550100	-0.47658100	-1.29871200
C	2.77456600	2.75398200	0.67133100
H	2.60880800	0.70130500	1.27180100
C	1.00124400	3.59208500	-0.74775700
H	-0.51851100	2.17538100	-1.28828400
C	-3.93724200	-0.21068000	0.03963300
H	-3.76548900	1.12916900	1.74328200
H	-3.65441000	-1.49845600	-1.68922700
C	2.54516100	-3.59181300	0.03610400
H	1.00619900	-4.34913900	1.33893500
H	3.92690100	-2.58451400	-1.27426600
C	2.19014300	3.79586600	-0.04824400
H	3.69295700	2.92198100	1.22411500
H	0.55415000	4.40548000	-1.30969300
N	0.33783300	0.00464700	0.01239900
N	-5.32353200	-0.30057600	0.06408200
C	-6.01493800	-0.94002100	-1.04212400
H	-5.84143100	-0.43521200	-2.00638500
H	-5.70427500	-1.98660400	-1.14791400
H	-7.08835400	-0.93569900	-0.84273700
C	-6.07892600	0.58826600	0.93015100
H	-7.14391500	0.37544900	0.81880100
H	-5.81926200	0.42737400	1.98367100

H	-5.91462500	1.65317200	0.69876100
Cl	3.45881400	-5.09593900	0.04156400
Cl	2.95678300	5.37987400	-0.07032900

N(*para*–Cl–phenyl) (*para*–NMe_2–phenyl)$_2$

0 1

C	1.22557800	-0.41782900	-0.00070100
C	0.00019400	1.72168500	-0.00012400
C	-1.22581300	-0.41748800	0.00045600
C	1.43785500	-1.46126600	0.90938500
C	2.24635100	-0.13197100	-0.91694300
C	1.05351400	2.44678800	0.59120000
C	-1.05292200	2.44715900	-0.59136400
C	-2.24676900	-0.13087900	0.91626600
C	-1.43814400	-1.46136700	-0.90912200
C	2.61711400	-2.19849200	0.90176500
H	0.66412200	-1.70014100	1.63308600
C	3.43851900	-0.84927600	-0.91737400
H	2.10969800	0.67279700	-1.63347000
C	1.05819100	3.83890600	0.58594100
H	1.87272000	1.91314100	1.06036800
C	-1.05718400	3.83927300	-0.58598100
H	-1.87229800	1.91379700	-1.06056300
C	-3.43906900	-0.84797000	0.91684300
H	-2.11017300	0.67425600	1.63239100
C	-2.61756000	-2.19834600	-0.90136500
H	-0.66434300	-1.70076600	-1.63257700
C	3.65338800	-1.91796200	-0.01756300
H	2.72898800	-2.99284700	1.63000200
H	4.19950500	-0.57769800	-1.63914600
C	0.00061100	4.53306100	0.00000800
H	1.87562500	4.38216900	1.04891500
H	-1.87445900	4.38282200	-1.04890300
C	-3.65394400	-1.91715800	0.01763100
H	-4.20015100	-0.57583300	1.63830600
H	-2.72957300	-2.99286100	-1.62940500
N	-0.00002900	0.31394400	-0.00019700

N	4.82685700	-2.67088300	-0.04547000
N	-4.82755700	-2.66983400	0.04571700
C	5.95039300	-2.19264300	-0.83243100
H	6.31841000	-1.20531400	-0.50654200
H	6.77202900	-2.90773200	-0.75214200
H	5.68250200	-2.11969300	-1.89296800
C	5.11289200	-3.56735900	1.06141800
H	4.33565300	-4.33493200	1.15473200
H	6.05729700	-4.08120300	0.86926500
H	5.19371200	-3.04677000	2.03029100
C	-5.95140600	-2.19061900	0.83164000
H	-6.31863300	-1.20325800	0.50498100
H	-6.77340000	-2.90526900	0.75106700
H	-5.68430700	-2.11727400	1.89235800
C	-5.11289700	-3.56783300	-1.06003500
H	-4.33516800	-4.33508500	-1.15215800
H	-6.05702400	-4.08204200	-0.86742700
H	-5.19380800	-3.04860700	-2.02964300
Cl	0.00087200	6.29560400	0.00009000

N(*para*–CF_3–phenyl)$_2$(*para*–NO_2–phenyl)

0 1

C	0.00096200	1.72273400	0.00008500
C	-1.22852900	-0.40911100	0.00899200
C	1.22760600	-0.41062700	-0.00897900
C	1.00259100	2.43790000	0.68719400
C	-0.99945700	2.43944000	-0.68719100
C	-2.27569300	-0.02075300	0.85963300
C	-1.40010200	-1.52644800	-0.82326600
C	1.39744600	-1.52882700	0.82247800
C	2.27573800	-0.02276400	-0.85868400
C	1.00810900	3.82571900	0.68372000
H	1.77013800	1.89902200	1.23126000
C	-1.00283400	3.82726500	-0.68375200
H	-1.76775300	1.90176200	-1.23137400
C	-3.47382000	-0.72794600	0.86547600
H	-2.14468100	0.83120200	1.51852300

C	-2.59439700	-2.23987000	-0.80227500
H	-0.59593700	-1.83264500	-1.48407500
C	2.59089200	-2.24367600	0.80149600
H	0.59260200	-1.83461500	1.48264900
C	3.47300100	-0.73138500	-0.86448800
H	2.14610800	0.82991500	-1.51691700
C	0.00315500	4.51121900	0.00000200
H	1.76762800	4.38578800	1.21527100
H	-1.76144300	4.38852800	-1.21533500
C	-3.63839000	-1.84258700	0.03816800
H	-4.27459600	-0.42711300	1.53272900
H	-2.71719300	-3.10525000	-1.44518600
C	3.63578900	-1.84697100	-0.03808300
H	2.71229500	-3.10974200	1.44373900
H	4.27447600	-0.43095500	-1.53109200
N	0.00002700	0.31120800	-0.00002700
N	0.00433100	5.97363100	0.00000000
O	-0.90921100	6.54714300	-0.59616900
O	0.91880900	6.54561800	0.59618100
C	-4.94933400	-2.57897800	0.01230600
C	4.94587000	-2.58487500	-0.01233200
F	-5.78390200	-2.08225300	-0.93061200
F	-5.59704900	-2.49133800	1.19480500
F	-4.78155400	-3.89068100	-0.26628800
F	4.77671000	-3.89625900	0.26690000
F	5.78140300	-2.08862100	0.92998700
F	5.59322100	-2.49847300	-1.19513700

N(*para*–CF_3–phenyl)(*para*–NO_2–phenyl)$_2$

0 1

C	-0.99328200	1.25556200	-0.00379700
C	1.09064400	-0.04458400	-0.01262500
C	-1.07343700	-1.20637800	-0.00197000
C	-2.17660500	1.44529100	-0.74348200
C	-0.46190700	2.33415100	0.72894100
C	1.82037900	0.75636400	-0.90382200
C	1.77500300	-0.89414600	0.86913700

C	-0.62460400	-2.31338300	-0.74726000
C	-2.25514600	-1.32231500	0.75516100
C	-2.81774900	2.67680500	-0.74388600
H	-2.58447500	0.62637800	-1.32573400
C	-1.09412000	3.57036200	0.72210300
H	0.44336400	2.19538000	1.30954900
C	3.21130300	0.71498000	-0.90359000
H	1.29515500	1.40425400	-1.59796200
C	3.16573900	-0.94359600	0.85524000
H	1.21525800	-1.51245300	1.56327200
C	-1.33548900	-3.50611800	-0.73556100
H	0.27912900	-2.23044200	-1.34086200
C	-2.97464000	-2.50981300	0.76094300
H	-2.60020400	-0.48139300	1.34658900
C	-2.26928600	3.73045400	-0.01220300
H	-3.72380500	2.83897800	-1.31464700
H	-0.70134800	4.40630400	1.28773700
C	3.88977800	-0.13689700	-0.02721800
H	3.77013100	1.32958100	-1.60140800
H	3.68929500	-1.60585100	1.53660500
C	-2.50701600	-3.59316000	0.01660600
H	-1.00644000	-4.36288000	-1.31062500
H	-3.88058500	-2.61597700	1.34494100
N	-0.33593200	0.00199100	-0.00554500
C	5.39428300	-0.14181600	0.00682200
F	5.87395400	0.77676600	0.87686700
F	5.92346400	0.14766100	-1.20180600
F	5.88229600	-1.34095200	0.39196300
N	-2.94063300	5.03216700	-0.01633000
N	-3.26149000	-4.84858200	0.02621300
O	-2.41869800	5.94611800	0.62355200
O	-3.98612200	5.13344000	-0.65962000
O	-4.30001900	-4.88558000	0.68741000
O	-2.81136200	-5.79057300	-0.62737600

N(*para*–CF_3–phenyl)$_2$(*para*–OMe–phenyl)

0 1

C	0.05640300	1.84127100	-0.09509800
C	1.19877000	-0.33113100	-0.03163800
C	-1.26870000	-0.22374700	-0.01002500
C	-0.62813100	2.55275900	-1.09430500
C	0.79998800	2.55251300	0.85047100
C	2.31586200	0.11073300	-0.76271100
C	1.31655600	-1.50386600	0.73764800
C	-1.48610700	-1.44716500	-0.67004200
C	-2.34281800	0.37248700	0.67597600
C	-0.57317500	3.93876300	-1.13632500
H	-1.20624600	2.00985600	-1.83593400
C	0.87754900	3.94628400	0.80323500
H	1.32927700	2.01196600	1.62944700
C	3.51034600	-0.60044100	-0.72709800
H	2.24163900	1.01456800	-1.35751900
C	2.50981300	-2.21634700	0.75992400
H	0.47248500	-1.84722900	1.32592200
C	-2.73474700	-2.05790200	-0.63253600
H	-0.67410300	-1.91494000	-1.21613500
C	-3.59153200	-0.23749700	0.69952700
H	-2.18972300	1.31206000	1.19540200
C	0.18441400	4.64866700	-0.19062000
H	-1.09961500	4.49750400	-1.90358400
H	1.46648300	4.46733300	1.54908900
C	3.61684100	-1.76996600	0.03085900
H	4.36379800	-0.24587300	-1.29564700
H	2.58931700	-3.11191500	1.36790600
C	-3.79727200	-1.45906900	0.05055500
H	-2.88555000	-3.00248800	-1.14469500
H	-4.40648200	0.22862500	1.24421500
N	-0.00558800	0.41111500	-0.04905200
O	0.18065800	6.00458700	-0.32623200
C	0.92527900	6.77690200	0.60270200
H	0.78326900	7.81799900	0.30777000
H	0.55889000	6.63751500	1.62841400
H	1.99507500	6.53219500	0.56519100
C	4.88538800	-2.57187100	0.02113000

C	-5.16097400	-2.08556200	0.04120400
F	5.96751600	-1.80345700	-0.23873000
F	4.86343500	-3.54476100	-0.92234000
F	5.10032000	-3.18974300	1.20567600
F	-5.10205800	-3.42428900	-0.13970700
F	-5.94000800	-1.59240300	-0.95261700
F	-5.82555700	-1.86052200	1.19842600

N(*para*–CF_3–phenyl)(*para*–OMe–phenyl)$_2$

0 1

C	1.11174800	1.25766600	0.14205300
C	-0.94080400	-0.10647400	0.08148400
C	1.27543900	-1.18756400	0.10792900
C	2.11289400	1.52640900	1.09091800
C	0.78705200	2.25040900	-0.78817200
C	-1.74779400	0.90262400	0.64662100
C	-1.57846100	-1.21119000	-0.51870100
C	1.04022400	-2.23818300	1.01235600
C	2.34464000	-1.30141000	-0.78559200
C	2.76863700	2.74943200	1.10165900
H	2.37540400	0.76397900	1.81786100
C	1.42700400	3.49226300	-0.77034700
H	0.02088500	2.05442900	-1.53219000
C	-3.13305400	0.81079900	0.60261200
H	-1.28068600	1.75428100	1.12823300
C	-2.96494800	-1.29919300	-0.54980900
H	-0.98043400	-1.99826900	-0.96404700
C	1.84226800	-3.37074800	1.00606500
H	0.22007300	-2.16075300	1.71961800
C	3.16988200	-2.42853900	-0.78381100
H	2.54036000	-0.49587300	-1.48667000
C	2.42846300	3.74657700	0.17425500
H	3.54384400	2.96274500	1.83096500
H	1.14683700	4.23970100	-1.50384800
C	-3.75708400	-0.29063800	0.00742300
H	-3.73547400	1.59244400	1.05470200
H	-3.43548400	-2.15883400	-1.01640100

C	2.91812700	-3.47552900	0.11027800
H	1.66450100	-4.18575800	1.70069700
H	3.99235200	-2.47942300	-1.48808700
N	0.46125300	-0.01406700	0.12083400
O	3.12635000	4.91540400	0.27624200
O	3.65158600	-4.62384300	0.19354300
C	2.82529200	5.95804100	-0.63609200
H	3.48665100	6.78609300	-0.37442400
H	3.01772100	5.65547800	-1.67424900
H	1.78104700	6.28608800	-0.54527600
C	4.74756400	-4.78421400	-0.69146300
H	5.18501600	-5.75580400	-0.45441600
H	4.42394300	-4.77936800	-1.74102400
H	5.50376600	-4.00120200	-0.54506500
C	-5.25075700	-0.35717700	-0.08750500
F	-5.71990000	0.23655900	-1.21447200
F	-5.85420400	0.26632000	0.95197700
F	-5.70151400	-1.63333800	-0.11122300

N(*para*–CF_3–phenyl)$_2$(*para*–Me–phenyl)

0 1

C	-0.00199000	2.13989100	-0.00159500
C	-1.23188500	0.01200900	-0.00178300
C	1.23326800	0.01461300	0.00151400
C	0.78199700	2.85378300	0.91498100
C	-0.78439300	2.84986200	-0.92201800
C	-2.33090000	0.50599700	0.72241700
C	-1.38805200	-1.17364500	-0.74314500
C	1.39260600	-1.16887700	0.74562600
C	2.33047400	0.50910500	-0.72506300
C	0.78479600	4.24684400	0.90002000
H	1.39133200	2.31377600	1.63331700
C	-0.78685800	4.24337700	-0.91286600
H	-1.38667600	2.30695300	-1.64409800
C	-3.54788800	-0.16717500	0.70529900
H	-2.22552600	1.41940600	1.29766400
C	-2.60316100	-1.84852600	-0.74621200

H	-0.55593100	-1.55661600	-1.32408100
C	2.60915400	-1.84116300	0.74925300
H	0.56181200	-1.55214600	1.32827400
C	3.54892200	-0.16143300	-0.70739500
H	2.22258400	1.42081800	-1.30255100
C	-0.00361000	4.97014600	-0.00594300
H	1.40412000	4.78170500	1.61651400
H	-1.39955800	4.77576700	-1.63677800
C	-3.69308000	-1.34978700	-0.02516700
H	-4.38799300	0.22665500	1.26770800
H	-2.71283900	-2.75525800	-1.33258300
C	3.69732300	-1.34186800	0.02595700
H	2.72133800	-2.74618700	1.33777400
H	4.38766300	0.23278500	-1.27157300
N	-0.00007100	0.70986200	-0.00030100
C	-0.02688200	6.48062200	0.01234300
H	-0.29591900	6.88904300	-0.96748000
H	-0.76181200	6.85933100	0.73552400
H	0.94720600	6.89414800	0.29516400
C	-4.98585400	-2.11220300	0.00504200
C	4.99178200	-2.10146900	-0.00362000
F	-6.04060400	-1.30988400	0.27321800
F	-5.23357600	-2.72993700	-1.17303100
F	-4.98066700	-3.07995500	0.95387700
F	4.98874200	-3.06998800	-0.95167200
F	5.24093800	-2.71763300	1.17496600
F	6.04472900	-1.29702900	-0.27253100

N(*para*–CF_3–phenyl)(*para*–Me–phenyl)$_2$

0 1

C	-1.52756900	-1.23294100	0.01041100
C	0.59784400	0.01288800	0.01533800
C	-1.54850000	1.22255200	-0.00404200
C	-2.61927200	-1.41870300	0.87016100
C	-1.16289800	-2.27844200	-0.85108300
C	1.32320700	-0.99762100	0.67635300
C	1.31491100	1.03706500	-0.63329100

C	-1.21404000	2.27126200	0.86517700
C	-2.63746500	1.38869400	-0.87187600
C	-3.32678700	-2.61921600	0.85986100
H	-2.90866800	-0.62013100	1.54623000
C	-1.86764600	-3.47980900	-0.83697000
H	-0.32285900	-2.14717300	-1.52617400
C	2.71284500	-0.98657500	0.67763200
H	0.79006900	-1.78649600	1.19518800
C	2.70451400	1.04799000	-0.61733400
H	0.77591300	1.82242700	-1.15134100
C	-1.94326000	3.45840200	0.84888700
H	-0.38347900	2.15119400	1.55395500
C	-3.36923200	2.57407900	-0.86373600
H	-2.91049300	0.58324900	-1.54658500
C	-2.96693400	-3.67430900	0.01112400
H	-4.16882900	-2.74203800	1.53747200
H	-1.56355700	-4.27807200	-1.51053400
C	3.41683300	0.03668000	0.03493800
H	3.25481000	-1.76720700	1.20187200
H	3.23998100	1.84623000	-1.12138500
C	-3.03446400	3.63597000	-0.01235600
H	-1.66687000	4.25742900	1.53332100
H	-4.21254200	2.67862500	-1.54293300
N	-0.81191000	0.00103000	0.00614300
C	4.91532600	0.01634900	-0.00801800
F	5.38609000	-0.66139900	-1.08493800
F	5.44633200	-0.58150500	1.08399700
F	5.43660400	1.26318200	-0.08121700
C	-3.75092200	-4.96583600	-0.00985700
H	-4.51669000	-4.95696900	-0.79749300
H	-3.10157800	-5.82723700	-0.20141700
H	-4.26605600	-5.13684900	0.94139200
C	-3.80768800	4.93382200	-0.03900600
H	-3.40586600	5.62402800	-0.79338700
H	-4.86272500	4.76775100	-0.28281400
H	-3.76125100	5.44772600	0.92718300

N(*para*–CF_3–phenyl)$_2$(*para*–NMe_2–phenyl)

0 1

C	0.04926900	1.56061900	0.01290000
C	-1.26795200	-0.50933500	0.02707100
C	1.20094900	-0.60548700	-0.02451400
C	0.75328000	2.24541100	1.01006100
C	-0.59293800	2.31053700	-0.97921100
C	-2.34168600	0.06803200	0.73049900
C	-1.48968200	-1.71228400	-0.66945400
C	1.33123600	-1.82328400	0.66898900
C	2.31405000	-0.11044400	-0.72936400
C	0.82073000	3.63418500	1.01709300
H	1.26343600	1.68165900	1.78592500
C	-0.54857800	3.70009200	-0.97099200
H	-1.13582600	1.79753500	-1.76799600
C	-3.59105900	-0.54062800	0.73778800
H	-2.18652900	0.99268100	1.27527800
C	-2.73936800	-2.32124100	-0.64928900
H	-0.67999300	-2.16499700	-1.23133300
C	2.53105300	-2.52563800	0.64580700
H	0.49000600	-2.21396800	1.23107000
C	3.51325100	-0.81259900	-0.74034400
H	2.22840000	0.82459600	-1.27181800
C	0.15605800	4.40512500	0.03377200
H	1.38712700	4.11827500	1.80331400
H	-1.05846200	4.23613400	-1.76209800
C	-3.80040300	-1.74202100	0.05305200
H	-4.40449500	-0.08921400	1.29697300
H	-2.89233400	-3.24942600	-1.19020400
C	3.63176600	-2.02748200	-0.05757400
H	2.61411200	-3.46370000	1.18493700
H	4.35777300	-0.42382900	-1.30053400
N	-0.00693000	0.12777000	0.00376100
N	0.18639900	5.79198800	0.05888100
C	-0.33804900	6.53971000	-1.07124700
H	0.19737500	6.32693100	-2.01045400
H	-1.40095100	6.32029500	-1.23005600

H	-0.25108300	7.60790000	-0.86367900
C	1.07239300	6.47037100	0.98965600
H	0.94922700	7.54930900	0.87823900
H	0.82429400	6.21555800	2.02726500
H	2.13392900	6.22616400	0.82394100
C	-5.16434400	-2.36584300	0.02443900
C	4.94521200	-2.75175300	-0.03302300
F	-5.83862100	-2.15682200	1.17924400
F	-5.93616100	-1.85865700	-0.96876200
F	-5.10623700	-3.70231500	-0.17534700
F	5.75934700	-2.29666000	0.95157900
F	5.62535500	-2.60079300	-1.19346600
F	4.78927400	-4.07880500	0.17631000

N(*para*–CF_3–phenyl)(*para*–NMe_2–phenyl)$_2$

0 1

C	-0.81404900	1.26072500	0.01707700
C	1.24044600	-0.10125500	0.00883900
C	-0.97235400	-1.18440200	0.05710500
C	-1.82523300	1.53361700	-0.91209900
C	-0.48335000	2.26147300	0.93970100
C	2.02777000	0.93073800	-0.54586200
C	1.90329500	-1.23025000	0.53578600
C	-0.80294300	-2.20600800	-0.88636100
C	-1.99188600	-1.33045900	1.00522900
C	-2.48807500	2.75624500	-0.91964600
H	-2.09722500	0.77403000	-1.63912800
C	-1.12534200	3.49552300	0.92645000
H	0.29743400	2.07511500	1.67144500
C	3.41308500	0.83574200	-0.56466000
H	1.54345400	1.80228300	-0.97118600
C	3.28911400	-1.31887700	0.50608000
H	1.32313700	-2.03557400	0.97175600
C	-1.60418400	-3.34265200	-0.87102600
H	-0.03027100	-2.10993300	-1.64377700
C	-2.81250100	-2.45364200	1.01580500
H	-2.15272200	-0.54470300	1.73755000

C	-2.15995200	3.77483300	0.00416400
H	-3.26036600	2.91695600	-1.66221800
H	-0.82284300	4.23926700	1.65374200
C	4.06066000	-0.28929800	-0.04282600
H	3.99723600	1.63560500	-1.00920200
H	3.77677100	-2.19719700	0.91724800
C	-2.63107400	-3.50428800	0.08748200
H	-1.43141100	-4.10128900	-1.62502900
H	-3.59388800	-2.51052200	1.76418700
N	-0.15843800	-0.00946900	0.03212900
C	5.55554800	-0.35996000	-0.01628100
F	6.07985500	0.20515800	1.10206100
F	6.11472100	0.28832900	-1.06642000
F	6.00546100	-1.63704100	-0.04460000
N	-2.83465600	4.99341100	0.01389700
N	-3.42033200	-4.65136900	0.12107800
C	-2.30556500	6.08624000	0.81187000
H	-2.95972300	6.95428300	0.70630300
H	-2.28275500	5.82058000	1.87540600
H	-1.28640000	6.38355100	0.51421300
C	-3.70565000	5.32593900	-1.10034000
H	-4.52377800	4.60117000	-1.18882500
H	-4.15493600	6.30520700	-0.92207100
H	-3.17634200	5.35990500	-2.06700700
C	-4.60449300	-4.66889900	0.96232600
H	-5.33927100	-3.89307000	0.68998600
H	-5.08871100	-5.64394400	0.87604700
H	-4.33843300	-4.52675800	2.01643000
C	-3.36939000	-5.57571400	-0.99853400
H	-2.35917100	-5.98262200	-1.12558200
H	-4.03721500	-6.41610900	-0.79786400
H	-3.67217700	-5.11449100	-1.95319400

N(*para*–NO_2–phenyl)$_2$(*para*–OMe–phenyl)

0 1

C	0.15123400	1.54474700	-0.10452000
C	1.13121300	-0.70215900	-0.04065100

C	-1.32111000	-0.41440600	-0.02388400
C	-0.42226700	2.29449400	-1.14371800
C	0.88656400	2.20286800	0.88403200
C	2.29264700	-0.30946900	-0.73636000
C	1.15286800	-1.90409600	0.69683600
C	-1.62511400	-1.63575500	-0.66076000
C	-2.35513200	0.28982300	0.62568900
C	-0.26662600	3.67253800	-1.18336000
H	-0.99214300	1.78922300	-1.91769600
C	1.06250700	3.58744400	0.84237600
H	1.32945000	1.62936200	1.69286800
C	3.43678700	-1.09379600	-0.70241900
H	2.28727600	0.61139700	-1.30833600
C	2.29328300	-2.69408300	0.72697700
H	0.27614300	-2.20820300	1.25757700
C	-2.91564700	-2.14450400	-0.63442700
H	-0.84733900	-2.17666300	-1.18806500
C	-3.64847000	-0.21262500	0.64685000
H	-2.13428400	1.22917000	1.11944700
C	0.48044300	4.33179200	-0.19247700
H	-0.70566100	4.26386900	-1.98038000
H	1.64037300	4.07006900	1.62173700
C	3.42893200	-2.28332900	0.02734700
H	4.33104100	-0.80616400	-1.24153400
H	2.32403500	-3.61392200	1.29807800
C	-3.91999100	-1.42918400	0.01970600
H	-3.16157500	-3.07693000	-1.12762700
H	-4.44786900	0.31572900	1.15170600
N	-0.01589700	0.11889100	-0.06006100
O	0.57769700	5.68131400	-0.32747200
C	1.31803200	6.40813700	0.64307600
H	1.26256300	7.45425400	0.33808800
H	0.88344100	6.29828900	1.64508400
H	2.36900800	6.09200800	0.66660600
N	-5.28090600	-1.96147400	0.04391200
N	4.63290800	-3.11118200	0.06404700
O	4.58612200	-4.16303800	0.70497100

O	5.62447900	-2.70840800	-0.54763800
O	-5.48185000	-3.04649900	-0.50546300
O	-6.14746200	-1.29408700	0.61251300

N(*para*–NO_2–phenyl)(*para*–OMe–phenyl)$_2$

0 1

C	-1.25884600	-0.18105900	0.04603800
C	0.72407100	1.28001500	0.12423600
C	1.00373700	-1.15334600	0.09765100
C	-1.83641800	-1.36149000	-0.47824200
C	-2.12304000	0.83232500	0.52426300
C	0.40181700	2.24362600	-0.83611800
C	1.67114700	1.59865300	1.11128800
C	2.05074200	-1.24268200	-0.82321600
C	0.85148200	-2.17494600	1.05063000
C	-3.21213100	-1.52069800	-0.52209500
H	-1.19541600	-2.14633300	-0.86210800
C	-3.49835700	0.67408000	0.47675000
H	-1.70368200	1.73906500	0.94395900
C	0.99143500	3.50977900	-0.81010400
H	-0.32167100	2.00591300	-1.61019500
C	2.27606400	2.84718800	1.13255900
H	1.93157800	0.85628100	1.85937100
C	2.93599000	-2.32282300	-0.80368600
H	2.18092000	-0.45550200	-1.55955900
C	1.71536200	-3.26081700	1.06518500
H	0.04868900	-2.11240700	1.77910100
C	-4.04174000	-0.50226900	-0.04627300
H	-3.65757700	-2.41857700	-0.93296300
H	-4.16261500	1.44335100	0.85135100
C	1.93797700	3.81699800	0.17518800
H	0.71600200	4.23518200	-1.56696900
H	3.00908300	3.10183500	1.89144500
C	2.76851500	-3.34358900	0.13996400
H	3.73926900	-2.35869300	-1.53053600
H	1.60432100	-4.05495500	1.79669000
N	0.12778900	-0.02097500	0.09171300

N	-5.48569500	-0.66703100	-0.09679100
O	-6.18809800	0.26279400	0.31251500
O	-5.93134900	-1.72732300	-0.54670700
O	2.58228000	5.01289900	0.29028100
O	3.56547800	-4.44437900	0.24615200
C	2.27708700	6.03455900	-0.64557100
H	2.89124300	6.89171100	-0.36403800
H	2.52719200	5.73098200	-1.67087400
H	1.21709600	6.31804600	-0.60204100
C	4.64309800	-4.58512900	-0.66585300
H	5.13756800	-5.52179800	-0.40261000
H	4.28868400	-4.64171600	-1.70363000
H	5.36022600	-3.75851100	-0.57434100

N(*para*–NO_2–phenyl)$_2$(*para*–Me–phenyl)

0 1

C	-0.00198900	1.84084700	-0.00151700
C	-1.23297200	-0.28144500	0.00395400
C	1.23451500	-0.27853500	-0.00369000
C	0.70526400	2.55003200	0.97759800
C	-0.70728500	2.54597500	-0.98355300
C	-2.34030900	0.25731900	0.68937400
C	-1.38882400	-1.49543800	-0.69585000
C	1.39364300	-1.49115300	0.69780400
C	2.34013700	0.26187800	-0.69054000
C	0.70805000	3.94290500	0.96405400
H	1.25295400	2.00769700	1.74250800
C	-0.70904600	3.93994100	-0.97543600
H	-1.24874100	2.00125700	-1.75118400
C	-3.56381900	-0.39749300	0.68037500
H	-2.23129500	1.18829400	1.23399900
C	-2.60870700	-2.15706300	-0.69973000
H	-0.55249800	-1.90983100	-1.24763300
C	2.61508600	-2.14983500	0.70198700
H	0.55859200	-1.90669900	1.25065700
C	3.56524800	-0.39000300	-0.68122100
H	2.22861100	1.19173300	-1.23658200

C	-0.00290100	4.66481300	-0.00590600
H	1.26523900	4.47881400	1.72878400
H	-1.25971600	4.47353800	-1.74625700
C	-3.68899800	-1.60260400	-0.01178700
H	-4.41892600	0.00216500	1.21150800
H	-2.74214500	-3.08544100	-1.24138800
C	3.69368900	-1.59376500	0.01264700
H	2.75105800	-3.07709400	1.24492600
H	4.41909300	0.01093700	-1.21341800
N	-0.00003400	0.40554400	0.00014500
C	-0.02399700	6.17513100	0.01031800
H	-0.28527500	6.58259400	-0.97154300
H	-0.76313100	6.55357100	0.72892700
H	0.94862800	6.58713900	0.30048000
N	-4.97655800	-2.29554400	-0.01940300
N	4.98293300	-2.28358400	0.02067000
O	-5.04721900	-3.36648600	-0.62526700
O	-5.91494800	-1.76748500	0.58041100
O	5.91979300	-1.75410700	-0.58028000
O	5.05643100	-3.35350000	0.62801700

N(*para*−NO_2−phenyl)(*para*−Me−phenyl)$_2$

0 1

C	0.93747900	-0.00170500	-0.00010200
C	-1.20097100	-1.22462800	0.00468300
C	-1.19745000	1.22676900	-0.00344400
C	1.66295400	1.08237700	-0.54541600
C	1.66031600	-1.08760100	0.54508300
C	-0.91456900	-2.23901300	-0.91999100
C	-2.24028500	-1.41811300	0.92333100
C	-2.24223500	1.42092900	-0.91578900
C	-0.90814400	2.23907000	0.92266700
C	3.04879800	1.08192700	-0.54347800
H	1.12896400	1.91897500	-0.98060300
C	3.04617300	-1.09087300	0.54234900
H	1.12436000	-1.92276400	0.98061600
C	-1.64605000	-3.42430900	-0.90898400

H	-0.11572200	-2.09656300	-1.64148200
C	-2.97499700	-2.60244500	0.91198400
H	-2.46785500	-0.63940600	1.64482600
C	-2.97736300	2.60486500	-0.89876000
H	-2.47874600	0.63987600	-1.63182500
C	-1.64037600	3.42398100	0.91747300
H	-0.11170900	2.09203600	1.64590100
C	3.73755100	-0.00544300	-0.00082900
H	3.60893400	1.90531700	-0.96960000
H	3.60431300	-1.91578400	0.96815000
C	-2.69365900	-3.62870400	0.00060100
H	-1.40486200	-4.20084700	-1.63139500
H	-3.77609900	-2.73495800	1.63553600
C	-2.68825000	3.63210500	0.00920800
H	-3.78684100	2.73514500	-1.61332000
H	-1.40172100	4.19598600	1.64559100
N	-0.46221400	0.00007200	-0.00026600
N	5.19337100	-0.00749100	-0.00146300
O	5.76937000	-0.99343000	0.46783500
O	5.77172600	0.97679300	-0.47135300
C	-3.50642300	-4.90211500	-0.02118000
H	-4.29395800	-4.85970200	-0.78564700
H	-2.88235400	-5.77322000	-0.24927900
H	-3.99650600	-5.08057900	0.94156600
C	-3.46314900	4.92898900	-0.00211700
H	-3.58600900	5.33215900	1.00919400
H	-2.94766600	5.69637500	-0.59527600
H	-4.45949400	4.79660600	-0.43642700

N(*para*–NO_2–phenyl)$_2$(*para*–NMe_2–phenyl)

0 1

C	1.21200900	0.39644000	0.00970700
C	-1.18078600	0.92642200	0.01895100
C	-0.42830600	-1.42449200	-0.01366000
C	2.08268500	0.01122200	1.03531000
C	1.70498900	1.21370400	-1.01368000
C	-0.98354000	2.15342200	0.68550800

C	-2.39885200	0.71005700	-0.65970500
C	-1.54609700	-1.95792400	0.66229200
C	0.44527600	-2.30674800	-0.68233300
C	3.40960500	0.42394200	1.04019300
H	1.71751500	-0.62488100	1.83663700
C	3.02566300	1.64578700	-1.01076800
H	1.04528300	1.51481000	-1.82250500
C	-1.97199300	3.12677700	0.68369000
H	-0.05126400	2.33206200	1.20877600
C	-3.39143800	1.67920200	-0.65794000
H	-2.55622500	-0.21575200	-1.20150500
C	-1.79135600	-3.32334200	0.65599000
H	-2.21272700	-1.29729800	1.20519000
C	0.20535100	-3.67310300	-0.68595000
H	1.30862000	-1.90926600	-1.20347100
C	3.91876200	1.26595500	0.02117900
H	4.04902900	0.09512300	1.85015500
H	3.36440800	2.27484300	-1.82466400
C	-3.17231700	2.88289700	0.01430100
H	-1.83399200	4.06781300	1.20183400
H	-4.32579200	1.52615500	-1.18396400
C	-0.91376700	-4.17378700	-0.01877400
H	-2.64129100	-3.74304900	1.18001200
H	0.86397200	-4.35742900	-1.20653000
N	-0.15666700	-0.04160400	0.00499700
N	5.23015300	1.70291500	0.03568500
C	5.75311200	2.45833300	-1.09042000
H	5.72412100	1.88721700	-2.03111000
H	5.19163000	3.38932700	-1.24114700
H	6.79117100	2.72780400	-0.88901200
C	6.15150700	1.19087800	1.03637400
H	7.12812200	1.65679100	0.89534900
H	5.81186700	1.43231100	2.05178900
H	6.28013700	0.09958800	0.97087200
N	-4.21428800	3.90615800	0.01210100
N	-1.16824400	-5.61189200	-0.02203400
O	-3.97904800	4.96644400	0.59617000

O	-5.26879200	3.65064300	-0.57372400
O	-0.36301800	-6.33610200	-0.61178200
O	-2.17343200	-6.01836900	0.56514300

N(*para*–NO_2–phenyl)(*para*–NMe_2–phenyl)$_2$

0 1

C	0.58848300	-1.44204000	0.00997000
C	0.89472900	1.00083800	0.00669900
C	-1.36494100	0.05582600	0.03946200
C	-0.16642600	-2.54981700	0.46811100
C	1.90506000	-1.67899800	-0.45633900
C	1.88755600	1.18490200	0.97673700
C	0.72766900	1.99576800	-0.96319100
C	-1.94902000	0.87423500	1.01275500
C	-2.19826100	-0.51206200	-0.93218400
C	0.36706400	-3.82741100	0.45839500
H	-1.17105900	-2.39291500	0.84222500
C	2.43746100	-2.95713000	-0.46432300
H	2.49916900	-0.85013100	-0.82237300
C	2.69905400	2.31436100	0.97054700
H	2.03469800	0.42739600	1.74131400
C	1.52156800	3.13705200	-0.96796700
H	-0.03712000	1.87349100	-1.72461200
C	-3.31858400	1.11387000	1.02415900
H	-1.31876600	1.33902100	1.76526500
C	-3.57153400	-0.29386800	-0.91906000
H	-1.76485700	-1.13565600	-1.70893100
C	1.66908900	-4.03223400	-0.00787400
H	-0.20505700	-4.67383300	0.81851800
H	3.43988500	-3.14190600	-0.83109600
C	2.53123700	3.33287900	0.00337500
H	3.46010300	2.40348200	1.73635400
H	1.35486900	3.87514200	-1.74330500
C	-4.17540100	0.52025300	0.06785900
H	-3.72028800	1.76344700	1.79240900
H	-4.17219600	-0.75346000	-1.69467000
N	0.05143900	-0.15697200	0.01760400

N	2.22751000	-5.37178800	-0.01822500
O	3.38814700	-5.51350500	-0.41927200
O	1.51314600	-6.30101300	0.37432200
N	3.31471600	4.48052100	0.01456200
N	-5.54978800	0.72143500	0.10076600
C	3.26336700	5.38662800	-1.12010400
H	3.93127800	6.22992800	-0.93376500
H	3.56753900	4.90830000	-2.06526700
H	2.25285700	5.79088800	-1.25560500
C	4.47139400	4.54235000	0.89185700
H	5.21491500	3.75758000	0.67739500
H	4.95641200	5.51351100	0.77512200
H	4.17354700	4.44773200	1.94309800
C	-6.36126800	0.27902200	-1.02022500
H	-7.40982600	0.49958000	-0.81067600
H	-6.08845500	0.77061300	-1.96822500
H	-6.27546400	-0.80475000	-1.16426800
C	-6.10095400	1.72255800	0.99766200
H	-7.18865100	1.72682100	0.90288000
H	-5.86277700	1.48837800	2.04224600
H	-5.73229500	2.73923500	0.78469200

N(*para*−OMe−phenyl)$_2$(*para*−Me−phenyl)

0 1

C	-0.22099100	1.71889300	-0.02546400
C	-1.10934800	-0.57957700	-0.10686000
C	1.31824800	-0.20455200	-0.08810100
C	0.62630000	2.55087400	0.72565500
C	-1.28421000	2.31389300	-0.72616100
C	-2.20605100	-0.40270900	0.74505200
C	-1.12067800	-1.67566600	-0.98893800
C	1.66748400	-1.28625100	0.72840100
C	2.30538700	0.34371100	-0.92767800
C	0.41507000	3.92730100	0.76378500
H	1.45377900	2.11442900	1.27582900
C	-1.49198200	3.68933100	-0.66256800
H	-1.94342500	1.69296500	-1.32423200

C	-3.29561500	-1.27668200	0.71335900
H	-2.21356700	0.43306000	1.43775600
C	-2.18889700	-2.56149100	-1.00896900
H	-0.27985800	-1.82856500	-1.65820400
C	2.95782800	-1.82196100	0.70794900
H	0.91959500	-1.72083200	1.38438600
C	3.59522100	-0.16828900	-0.93613300
H	2.05206500	1.17925200	-1.57276800
C	-0.65005300	4.52813000	0.08008700
H	1.09032100	4.54617300	1.35130800
H	-2.32108800	4.12196300	-1.21902400
C	-3.29102000	-2.36773100	-0.16269900
H	-4.12847700	-1.10208400	1.38515400
H	-2.19939700	-3.40797500	-1.68873800
C	3.93388600	-1.25996200	-0.12210400
H	3.18750000	-2.66363200	1.35169300
H	4.35916800	0.25357800	-1.58198000
N	-0.00565400	0.31894100	-0.08194600
O	-4.29623000	-3.28891400	-0.27115400
O	5.22722700	-1.69440300	-0.21490600
C	-5.43457000	-3.13428500	0.55742500
H	-6.10397200	-3.95961900	0.30681100
H	-5.17244800	-3.19254000	1.62280100
H	-5.94803300	-2.18173700	0.36734400
C	5.62115200	-2.79203300	0.58924300
H	6.67362400	-2.97074400	0.36031100
H	5.51706400	-2.56852200	1.65984200
H	5.04168100	-3.69547800	0.35469300
C	-0.89684800	6.01679400	0.16052100
H	-1.39216900	6.39015000	-0.74277400
H	-1.54149500	6.27450000	1.01243000
H	0.03885700	6.57317000	0.28465800

N(*para*–OMe–phenyl)(*para*–Me–phenyl)$_2$

0 1

C	-1.08217500	0.19540100	0.08170200
C	0.85000600	-1.32596900	0.02141500

C	1.19487800	1.11736700	0.00101900
C	-1.64840800	1.11088000	0.98691000
C	-1.93633800	-0.51269100	-0.77092300
C	0.27004700	-2.33761000	0.80313700
C	1.94939700	-1.65805500	-0.78855200
C	2.40006700	1.12459800	0.72252500
C	0.86451900	2.25417900	-0.75475400
C	-3.02088100	1.31364800	1.02628800
H	-1.00001600	1.66551700	1.65805400
C	-3.32066600	-0.33102200	-0.72135500
H	-1.51491800	-1.22043100	-1.47808700
C	0.77488000	-3.63595700	0.76778200
H	-0.58082200	-2.10287800	1.43479500
C	2.45303200	-2.95599700	-0.79903900
H	2.40380600	-0.89406400	-1.41137900
C	3.24522900	2.23068400	0.67523100
H	2.67272700	0.25801400	1.31643100
C	1.71180300	3.35954400	-0.77679500
H	-0.05771700	2.26491800	-1.32700000
C	-3.87160800	0.59053100	0.17631400
H	-3.46194600	2.02020000	1.72260400
H	-3.95043600	-0.90139100	-1.39466500
C	1.87906700	-3.97417500	-0.02472700
H	0.30401400	-4.40058600	1.38217500
H	3.30316200	-3.18540100	-1.43850900
C	2.91961300	3.37421200	-0.06664700
H	4.17429900	2.20743800	1.24116400
H	1.43224100	4.22531700	-1.37371900
N	0.32792600	-0.00592500	0.03856000
O	-5.20668500	0.85555900	0.30372100
C	-6.10984300	0.15346000	-0.53193300
H	-7.10669600	0.50826300	-0.26286900
H	-5.92620900	0.36347600	-1.59450800
H	-6.05530800	-0.93130500	-0.36683400
C	2.44605200	-5.37486900	-0.02983600
H	2.78872700	-5.66635200	-1.02944000
H	3.30915200	-5.46364900	0.64434500

H	1.70212900	-6.10914500	0.29739800
C	3.82182100	4.58644200	-0.07843000
H	3.73893500	5.13848500	-1.02126500
H	3.56749200	5.28657200	0.72942700
H	4.87243200	4.30640200	0.05620500

N(*para*–OMe–phenyl)$_2$(*para*–NMe$_2$–phenyl)

0 1

C	-1.11830700	0.13680300	-0.03822600
C	0.87783900	-1.30057100	-0.09753100
C	1.12194500	1.15157700	-0.11758700
C	-1.71927800	1.04407100	0.84475500
C	-1.95963200	-0.62320300	-0.86302300
C	0.36442700	-2.31808600	0.71665400
C	1.97999600	-1.60230600	-0.92057000
C	2.30224900	1.21090600	0.63455500
C	0.77061100	2.27529300	-0.88990900
C	-3.10171800	1.19340500	0.89896800
H	-1.09314000	1.65186900	1.49113600
C	-3.34320900	-0.49779500	-0.79753500
H	-1.52129900	-1.32485400	-1.56649000
C	0.91722100	-3.60147500	0.70940900
H	-0.48363400	-2.10734100	1.36043900
C	2.54761300	-2.86869100	-0.91508100
H	2.39019300	-0.83121300	-1.56501600
C	3.12065100	2.34323900	0.61162700
H	2.59012500	0.35929900	1.24281600
C	1.56748400	3.41149200	-0.89841700
H	-0.13846100	2.24976500	-1.48237700
C	-3.95827400	0.41159000	0.09237900
H	-3.51100800	1.91928900	1.59128600
H	-3.94446900	-1.10751400	-1.46135400
C	2.01929100	-3.88414800	-0.10408700
H	0.48623200	-4.36127700	1.35182500
H	3.39753600	-3.10105500	-1.54960600
C	2.75437700	3.45630500	-0.15211000
H	4.02845000	2.34562600	1.20460600

H	1.29592500	4.27814400	-1.49351600
N	0.29749200	-0.00437500	-0.10482000
N	-5.34801200	0.52065100	0.18144300
C	-6.16493700	-0.09186500	-0.85192200
H	-5.96669800	0.31165300	-1.85935500
H	-6.00411300	-1.17564400	-0.88519600
H	-7.21901200	0.07403100	-0.61807200
C	-5.91607200	1.64721300	0.90141300
H	-7.00546600	1.56912100	0.88309500
H	-5.60512000	1.63622700	1.95245200
H	-5.63203600	2.62369200	0.47379500
O	2.64462100	-5.09980300	-0.18364700
O	3.47316200	4.61852300	-0.23946800
C	2.14330200	-6.15755900	0.61246100
H	2.77282300	-7.02314800	0.39604900
H	2.20595500	-5.92458000	1.68448000
H	1.10085300	-6.39667500	0.36021800
C	4.67537100	4.71330400	0.50205600
H	5.08212100	5.70473400	0.29230500
H	4.49543600	4.61791000	1.58182600
H	5.40448300	3.95125800	0.19352700

N(*para*−OMe−phenyl)(*para*−NMe$_2$−phenyl)$_2$

0 1

C	-0.12238200	1.69977000	0.06562500
C	1.28243500	-0.32095400	-0.00416300
C	-1.16839300	-0.52888900	-0.02152600
C	-1.10409200	2.36962000	-0.67693900
C	0.74375700	2.47113900	0.86473500
C	2.30719300	0.17318400	-0.82341000
C	1.57148400	-1.43652300	0.79470500
C	-1.25521600	-1.62807300	-0.88733100
C	-2.26585600	-0.27326100	0.81342100
C	-1.23410500	3.75966000	-0.62107800
H	-1.78055500	1.79672300	-1.30316500
C	0.63370000	3.85407700	0.90624100
H	1.50852200	1.97403200	1.45296200

C	3.56931200	-0.41266400	-0.83796000
H	2.11671700	1.03889000	-1.45073100
C	2.82334100	-2.04238600	0.76755300
H	0.80115900	-1.83588000	1.44764800
C	-2.38465100	-2.44057500	-0.91626700
H	-0.41847200	-1.85868200	-1.53979100
C	-3.40750700	-1.06684500	0.77330000
H	-2.22440900	0.56184700	1.50629500
C	-0.35941200	4.51387600	0.16780500
H	-2.01070600	4.23694000	-1.20847600
H	1.30267800	4.44770000	1.52203700
C	3.86139700	-1.55163300	-0.05553200
H	4.32616400	0.02125200	-1.48060700
H	2.99031400	-2.89963400	1.40897300
C	-3.50522600	-2.17353100	-0.09929100
H	-2.38910500	-3.28337900	-1.59742300
H	-4.22233200	-0.82283200	1.44476600
N	-0.00371900	0.28698000	0.02032100
N	5.11302100	-2.17321900	-0.10441400
N	-4.66179700	-2.95738800	-0.16021100
C	5.45374600	-3.13415700	0.93044400
H	6.45490400	-3.52621900	0.73695900
H	5.44122900	-2.70285600	1.94591600
H	4.76212900	-3.98442000	0.91694400
C	6.21191600	-1.47390500	-0.74754500
H	6.44724900	-0.50515000	-0.27459000
H	7.10557900	-2.10100600	-0.70750000
H	5.99035000	-1.28783100	-1.80469300
C	-5.64444100	-2.83014600	0.90209500
H	-6.47943500	-3.50432800	0.69793200
H	-5.24023500	-3.07222300	1.89980000
H	-6.04852600	-1.81190400	0.94055800
C	-4.60440200	-4.22814500	-0.86138600
H	-5.58729000	-4.70309900	-0.81896200
H	-4.35869700	-4.07942600	-1.91916400
H	-3.86368200	-4.92681100	-0.43617100
O	-0.38857000	5.87848600	0.28806600

C	-1.36806200	6.58816200	-0.44660100
H	-1.21799200	7.64357600	-0.20962100
H	-1.25026700	6.44108000	-1.52926700
H	-2.38649400	6.29434300	-0.15641000

N(*para*–Me–phenyl)$_2$(*para*–NMe$_2$–phenyl)

0 1

C	-0.79489500	-0.03559100	0.01767900
C	1.36139900	-1.21404500	0.02559600
C	1.29800500	1.25356700	-0.02932000
C	-1.53043300	0.75347500	0.91135800
C	-1.50658600	-0.85911200	-0.86433900
C	0.92085900	-2.29979100	0.80069500
C	2.53487600	-1.37106900	-0.73116500
C	2.47635000	1.46670900	0.70579300
C	0.78747600	2.31971000	-0.78881200
C	-2.92131200	0.72833300	0.92191200
H	-1.00466400	1.40662500	1.60156900
C	-2.89649100	-0.90909200	-0.84464100
H	-0.96158900	-1.47196200	-1.57628200
C	1.63028700	-3.49838500	0.80787600
H	0.02107600	-2.19699400	1.39880300
C	3.24223400	-2.57047400	-0.69932600
H	2.89152900	-0.54726200	-1.34117700
C	3.12052400	2.70112400	0.66808400
H	2.88653200	0.65923400	1.30383000
C	1.43407200	3.55314300	-0.80178400
H	-0.11705400	2.17397200	-1.37062300
C	-3.64765900	-0.12013600	0.05598000
H	-3.43929300	1.36877400	1.62587500
H	-3.39528700	-1.56148700	-1.55148300
C	2.80528200	-3.66263500	0.06237000
H	1.26741900	-4.32103900	1.42095800
H	4.14960100	-2.66176600	-1.29309100
C	2.61347800	3.77358600	-0.07774200
H	4.03318900	2.83561400	1.24523500
H	1.01738800	4.35936700	-1.40236700

N	0.63148600	0.00203000	0.00089800
N	-5.04038800	-0.18670600	0.09781900
C	-5.74344800	-0.86638800	-0.97652000
H	-5.56709300	-0.41220300	-1.96604800
H	-5.44741500	-1.92049600	-1.03179000
H	-6.81632700	-0.83915000	-0.77364700
C	-5.76956300	0.82374400	0.84456400
H	-6.83905700	0.61120400	0.78161300
H	-5.49343200	0.80179900	1.90520200
H	-5.59783000	1.84692800	0.47017700
C	3.55574100	-4.97420100	0.05854400
H	3.20189600	-5.64033800	-0.74070000
H	4.62922500	-4.82251200	-0.10016600
H	3.42881500	-5.51133200	1.00519100
C	3.29508800	5.12221100	-0.07892700
H	3.13971800	5.64958000	-1.02689700
H	2.90816700	5.77156900	0.71879200
H	4.37509100	5.02650800	0.07876800

N(*para*–Me–phenyl)(*para*–NMe$_2$–phenyl)$_2$

0 1

C	-0.05012500	2.00767700	0.01163700
C	-1.20333300	-0.17124500	0.02605200
C	1.24884600	-0.08738500	0.05738800
C	0.91938800	2.77743500	0.67949800
C	-1.06627300	2.68626600	-0.68476900
C	-2.27252000	0.13819400	0.87787100
C	-1.35277500	-1.26878100	-0.83256300
C	1.47203400	-1.15750000	0.93407700
C	2.28933900	0.26926700	-0.81187000
C	0.87017100	4.16853400	0.64140500
H	1.71373300	2.27882200	1.22529300
C	-1.10925700	4.07818200	-0.69846800
H	-1.81875200	2.11602400	-1.21955800
C	-3.44690400	-0.60793800	0.86606900
H	-2.18778900	0.98529000	1.55206300
C	-2.51452900	-2.03381900	-0.83467200

H	-0.54357800	-1.52789300	-1.50883600
C	2.68075400	-1.84646900	0.94277900
H	0.68027400	-1.46346100	1.61139200
C	3.50917300	-0.39927000	-0.79346000
H	2.14050000	1.08514200	-1.51290300
C	-0.14569400	4.85282900	-0.03951600
H	1.63690100	4.73515100	1.16643900
H	-1.90624200	4.57345900	-1.24996400
C	-3.59731200	-1.72966300	0.02038400
H	-4.24550200	-0.31503800	1.53724000
H	-2.57539600	-2.86875600	-1.52268200
C	3.74496100	-1.47551000	0.09116800
H	2.79259500	-2.67435600	1.63269400
H	4.27655600	-0.08308100	-1.49002100
N	-0.00188900	0.59450400	0.03540500
N	-4.75504900	-2.51154200	0.04048700
N	4.97718200	-2.13306300	0.13098000
C	-4.97712800	-3.45768200	-1.03921200
H	-5.91600400	-3.98717600	-0.86198900
H	-5.03176600	-2.97900700	-2.03162800
H	-4.17914800	-4.20857700	-1.07083000
C	-5.92542500	-2.00897600	0.73859300
H	-6.29715100	-1.05293700	0.33223900
H	-6.72779800	-2.74676700	0.66652800
H	-5.71127500	-1.86186600	1.80350000
C	5.92060800	-1.91518500	-0.95205100
H	6.82701500	-2.49284100	-0.75686100
H	5.52609200	-2.21317200	-1.93828500
H	6.21175300	-0.86001600	-1.01029300
C	5.07703600	-3.38524400	0.86027800
H	6.10448800	-3.75146800	0.80082600
H	4.84295000	-3.23886600	1.92103200
H	4.40689200	-4.17020500	0.47028300
C	-0.21409200	6.36247100	-0.04053000
H	-0.76634400	6.74479900	0.82950300
H	0.78555000	6.81059500	-0.00851800
H	-0.72191400	6.73978700	-0.93531800

O(*para*–H–phenyl)$_2$

0 1

O	-0.00010700	1.18036000	-0.00083100
C	1.20152700	0.49943700	-0.03789100
C	1.39044300	-0.65887700	-0.79860000
C	2.26638700	1.07169500	0.66198900
C	2.65564000	-1.24624700	-0.84300100
H	0.55947400	-1.08820800	-1.34850600
C	3.52749300	0.47871600	0.60168600
H	2.08978700	1.97406200	1.23880700
C	3.72773600	-0.68390500	-0.14624700
H	2.80256700	-2.14600000	-1.43465500
H	4.35428700	0.92643200	1.14660800
H	4.70977700	-1.14607600	-0.18785700
C	-1.20159500	0.49926800	0.03719300
C	-2.26725300	1.07200800	-0.66111000
C	-1.38964300	-0.65968100	0.79714600
C	-3.52823800	0.47888300	-0.59998800
H	-2.09132300	1.97485600	-1.23738200
C	-2.65476500	-1.24716900	0.84238100
H	-0.55810700	-1.08943400	1.34585400
C	-3.72763200	-0.68436600	0.14720500
H	-4.35561900	0.92698600	-1.14370100
H	-2.80099400	-2.14741800	1.43345300
H	-4.70959000	-1.14665400	0.18945100

O(*para*–H–phenyl)(*para*–Cl–phenyl)

0 1

O	0.95693200	1.30073800	-0.00982600
C	-0.30957700	0.75896500	0.00465300
C	-0.62573600	-0.43033700	0.66930400
C	-1.31279100	1.50347400	-0.62194400
C	-1.94662800	-0.87766900	0.69497000
H	0.15140900	-1.00145600	1.16548900
C	-2.63377400	1.06162200	-0.58983800
H	-1.04506900	2.42611800	-1.12655200

C	-2.94184200	-0.13066900	0.06576500
H	-2.20115300	-1.79845200	1.20899400
H	-3.41656700	1.63503900	-1.07465500
C	2.07716300	0.48751900	-0.03413500
C	3.15389100	0.87584800	0.76492000
C	2.17677500	-0.62260600	-0.87811700
C	4.34100400	0.14412600	0.71990300
H	3.04656500	1.74664100	1.40387200
C	3.36701000	-1.35071800	-0.90643700
H	1.33709700	-0.90566100	-1.50464600
C	4.45149800	-0.97312300	-0.11098700
H	5.17931600	0.44761700	1.34102400
H	3.44679400	-2.21340000	-1.56243400
H	5.37544000	-1.54327700	-0.14099500
Cl	-4.60654300	-0.69868600	0.10001000

O(*para*−H−phenyl)(*para*−CF_3−phenyl)

0 1

O	1.64565500	-1.35541800	0.08942100
C	2.74314700	-0.50641600	0.05522900
C	2.94561600	0.45648700	1.04726700
C	3.68563900	-0.70821800	-0.95251300
C	4.10589400	1.23082800	1.01590400
H	2.20582800	0.58834100	1.83071200
C	4.84657700	0.06719500	-0.96798600
H	3.50118200	-1.47045200	-1.70285100
C	5.05828300	1.03995300	0.01118300
H	4.26836100	1.98016600	1.78578500
H	5.58397600	-0.08945700	-1.75040100
C	0.36832100	-0.85238100	0.06569800
C	-0.63844100	-1.72057200	0.50516800
C	0.04378800	0.42415500	-0.40711600
C	-1.96649900	-1.31218900	0.47204900
H	-0.35957100	-2.70419400	0.86849000
C	-1.29047500	0.82458700	-0.43172100
H	0.82247300	1.09479500	-0.75200200
C	-2.30036300	-0.03533900	0.00685800

H	-2.74619100	-1.98149600	0.82040100
H	-1.54509700	1.81582300	-0.79265700
H	5.96130200	1.64327000	-0.00530700
C	-3.73877800	0.38576100	-0.07934000
F	-3.88307500	1.72242800	0.07105800
F	-4.49857400	-0.21383300	0.86570200
F	-4.28876800	0.06956400	-1.27693800

O(*para*–H–phenyl)(*para*–NO_2–phenyl)

0 1

O	-1.21459300	-1.36888000	0.03609300
C	0.03759900	-0.82304900	0.01881200
C	1.09763800	-1.73853200	0.12118500
C	0.29235100	0.55030000	-0.10382000
C	2.40764600	-1.28574700	0.10333500
H	0.86806500	-2.79476100	0.21326800
C	1.60771000	1.00297700	-0.12065500
H	-0.52742800	1.25386100	-0.18715900
C	2.65176100	0.08523100	-0.01646900
H	3.24297400	-1.97054900	0.18121700
H	1.83538600	2.05763700	-0.21516300
C	-2.33925500	-0.54577100	0.02352300
C	-2.81312300	-0.00527100	1.21891800
C	-3.01531000	-0.34947600	-1.17943600
C	-3.98660900	0.75069500	1.20293000
H	-2.27045300	-0.18711600	2.14140500
C	-4.18957300	0.40631900	-1.18253200
H	-2.62440300	-0.79374900	-2.08938700
C	-4.67529500	0.95818700	0.00505800
H	-4.36445600	1.17281300	2.12986300
H	-4.72452200	0.56128700	-2.11524000
N	4.03245000	0.56735000	-0.03398300
O	4.21582600	1.78163800	-0.13843800
O	4.93302800	-0.26905900	0.05680900
H	-5.58964400	1.54435500	-0.00172400

O(*para*–H–phenyl) (*para*–Me–phenyl)

0 1

O	-0.54084500	1.25738300	-0.08609200
C	-1.68086000	0.48350200	-0.00281300
C	-1.75059200	-0.69529500	0.74667400
C	-2.81455400	0.97891200	-0.65318200
C	-2.96491100	-1.37880200	0.83064800
H	-0.86912900	-1.06728200	1.25796500
C	-4.02230400	0.28939400	-0.55411900
H	-2.73044300	1.89907600	-1.22281500
C	-4.10368900	-0.89412000	0.18402400
H	-3.01827200	-2.29429500	1.41407100
H	-4.90158100	0.67803400	-1.06096400
C	0.71388300	0.67549300	-0.06296100
C	1.69467500	1.30510400	0.70379800
C	1.03662300	-0.44528500	-0.83292600
C	2.99835200	0.80998300	0.69795700
H	1.42355100	2.17481200	1.29410800
C	2.34358400	-0.93109600	-0.81864500
H	0.27281500	-0.92963900	-1.43288500
C	3.34869700	-0.31520800	-0.05989800
H	3.75568000	1.30653500	1.30041500
H	2.58684700	-1.80548000	-1.41828100
C	4.76939400	-0.83123900	-0.08242400
H	4.80033900	-1.91616400	-0.23114800
H	5.34876800	-0.37603000	-0.89720900
H	5.29315000	-0.60504100	0.85266000
H	-5.04476600	-1.43164800	0.25601300

O(*para*–H–phenyl) (*para*–OMe–phenyl)

0 1

O	0.98786900	1.27298000	0.16370100
C	-0.28184900	0.71531100	0.16805100
C	-0.66490700	-0.22188800	1.13570100
C	-1.20956700	1.17986300	-0.75786500
C	-1.97136900	-0.69196500	1.16118500
H	0.06118300	-0.57254900	1.86252200
C	-2.52953600	0.71690200	-0.72894200

H	-0.89737200	1.91218700	-1.49577200
C	-2.91427500	-0.22590500	0.23066400
H	-2.29080400	-1.41700700	1.90315200
H	-3.23747200	1.09580000	-1.45690000
C	2.09845500	0.46980600	0.00864300
C	3.31343400	1.01946100	0.43181500
C	2.06164100	-0.79925600	-0.57741700
C	4.49235600	0.29517200	0.26881200
H	3.31100500	2.00811300	0.88014000
C	3.25156300	-1.51500900	-0.72900500
H	1.11917400	-1.21831000	-0.91245000
C	4.46904100	-0.97736600	-0.30943400
H	5.43321800	0.72706100	0.59971000
H	3.22038200	-2.50115300	-1.18518200
O	-4.17065900	-0.74995600	0.34930400
H	5.38902600	-1.54165000	-0.43149700
C	-5.16788000	-0.30829900	-0.55564200
H	-6.07984900	-0.84216200	-0.28175600
H	-5.34193700	0.77289200	-0.47005100
H	-4.90687400	-0.54838000	-1.59536400

O(*para*−H−phenyl) (*para*−NMe$_2$−phenyl)

0 1

O	-1.40485100	-1.13364100	0.66858900
C	-0.10796700	-0.70591100	0.40990300
C	0.42780500	0.40864200	1.05494700
C	0.70083400	-1.46527400	-0.43133300
C	1.75688800	0.76821100	0.85042200
H	-0.19623100	0.99019900	1.72708900
C	2.03431400	-1.11586300	-0.63307900
H	0.28389800	-2.34260700	-0.91664100
C	2.59570500	0.02135300	-0.00957200
H	2.14094700	1.63430200	1.37560100
H	2.63551800	-1.73848600	-1.28435800
C	-2.47616100	-0.39782500	0.21194700
C	-2.37536200	0.62028700	-0.74145100
C	-3.72390100	-0.74952000	0.74067000

C	-3.53283200	1.28445100	-1.15549200
H	-1.40878500	0.88647000	-1.15439600
C	-4.86843100	-0.07988900	0.31508800
H	-3.77182700	-1.54527700	1.47759400
C	-4.78110600	0.94308600	-0.63422800
H	-3.45070600	2.07494400	-1.89725000
H	-5.83372600	-0.35783100	0.73036000
C	4.51853700	1.41284000	0.60904000
H	5.54525100	1.58992400	0.28164900
H	3.97902200	2.36345800	0.52308700
H	4.53975900	1.12919300	1.67448100
N	3.91841900	0.39781900	-0.23963000
C	4.80782700	-0.53449800	-0.91090000
H	5.79378700	-0.07609800	-1.01283400
H	4.92430000	-1.48745700	-0.36840900
H	4.44675200	-0.76262300	-1.92074400
H	-5.67498300	1.46573800	-0.96230100

O(*para*−Cl−phenyl)$_2$

0 1

O	0.00000700	-1.56138800	-0.00005500
C	-1.20056400	-0.88003600	-0.00873500
C	-1.40894700	0.27799600	-0.76400700
C	-2.24992200	-1.44994900	0.71546100
C	-2.67047300	0.87233000	-0.78243800
H	-0.59531200	0.71011300	-1.33680500
C	-3.51332300	-0.86195700	0.69052700
H	-2.06564900	-2.35262900	1.28876600
C	-3.71410500	0.29962400	-0.05547400
H	-2.84282400	1.77038300	-1.36596600
H	-4.33341600	-1.29862900	1.25025800
C	1.20056700	-0.88002300	0.00867300
C	2.25001400	-1.45005300	-0.71531400
C	1.40886200	0.27813000	0.76377600
C	3.51340600	-0.86205800	-0.69033400
H	2.06580000	-2.35282600	-1.28849100
C	2.67039000	0.87247000	0.78225100

H	0.59516700	0.71034900	1.33641300
C	3.71410300	0.29964900	0.05550500
H	4.33356600	-1.29881300	-1.24990200
H	2.84266300	1.77062200	1.36564900
Cl	-5.30332800	1.05103800	-0.08116900
Cl	5.30332300	1.05106900	0.08123700

O(*para*–Cl–phenyl) (*para*–CF_3–phenyl)

0 1

O	-0.72144200	-1.66016300	-0.05996000
C	-1.89665800	-0.93075700	-0.03939400
C	-2.14098800	0.10475000	-0.94588700
C	-2.88131300	-1.33005700	0.86467100
C	-3.37589700	0.75182400	-0.93685000
H	-1.37430300	0.39860300	-1.65534200
C	-4.12068300	-0.69051600	0.86902200
H	-2.67018400	-2.14247600	1.55227000
C	-4.35712000	0.34961100	-0.02953900
H	-3.57845000	1.55619600	-1.63578100
H	-4.89352500	-0.99395600	1.56688900
C	0.50286600	-1.03257400	-0.04580000
C	1.56975500	-1.75768400	-0.58662100
C	0.71716500	0.22806800	0.52250200
C	2.85245500	-1.22098400	-0.56060900
H	1.37479400	-2.73267600	-1.02085100
C	2.00484600	0.75881000	0.53761900
H	-0.10973000	0.78486900	0.94882200
C	3.07594100	0.04202200	-0.00284300
H	3.68023700	-1.77819100	-0.98620000
H	2.17559900	1.73854100	0.97198400
C	4.46679200	0.60422700	0.07299100
F	4.46966900	1.95252600	-0.03616600
F	5.26399800	0.11511700	-0.90329200
F	5.06687500	0.31012800	1.25130700
Cl	-5.91416100	1.16411800	-0.02260700

O(*para*–Cl–phenyl) (*para*–NO_2–phenyl)

0 1

O	-0.27368800	-1.61601100	0.04724200
C	0.92211000	-0.94999900	0.02131400
C	2.04942800	-1.71845300	0.34892100
C	1.05769800	0.39656400	-0.34390800
C	3.31134300	-1.14373200	0.31733200
H	1.91126500	-2.75867300	0.62379500
C	2.32379500	0.97234600	-0.37313800
H	0.18646200	0.98434000	-0.60809900
C	3.43626900	0.20062300	-0.04140300
H	4.19767000	-1.71326700	0.56795000
H	2.46120100	2.00916700	-0.65451900
C	-1.47593100	-0.92210600	0.03452000
C	-1.83987500	-0.09568600	1.09972400
C	-2.35128400	-1.14951500	-1.02601300
C	-3.09120000	0.51906300	1.09657800
H	-1.15310400	0.05822400	1.92596800
C	-3.60725600	-0.54199600	-1.02763200
H	-2.04754600	-1.80471800	-1.83586200
C	-3.96558300	0.29088800	0.03240400
H	-3.38934800	1.16245900	1.91719700
H	-4.29954600	-0.71209600	-1.84495000
N	4.76583600	0.81248700	-0.07201000
O	4.84305600	2.00054100	-0.38902800
O	5.72923200	0.10281800	0.22121600
Cl	-5.54316400	1.06119900	0.03205700

O(*para*–Cl–phenyl) (*para*–Me–phenyl)

0 1

O	-0.42769700	1.47918900	-0.07212200
C	0.79130700	0.84122500	-0.03169500
C	1.86958000	1.53240900	-0.59311600
C	0.99487300	-0.39670400	0.58656700
C	3.15097000	0.98908200	-0.54214100
H	1.68952700	2.49393800	-1.06290700
C	2.27721900	-0.94462500	0.63149600
H	0.16141300	-0.92828500	1.03233100

C	3.34647400	-0.25084200	0.06731700
H	3.99050300	1.52121700	-0.97660400
H	2.44345800	-1.90404500	1.10981900
C	-1.60693100	0.75052400	-0.04966400
C	-1.84563400	-0.29956800	-0.94103600
C	-2.59850200	1.15722700	0.84052600
C	-3.08201900	-0.94184300	-0.92322700
H	-1.07187400	-0.60510400	-1.63841400
C	-3.83429800	0.50805900	0.83691700
H	-2.39363800	1.97741200	1.52136900
C	-4.09940400	-0.55112900	-0.03934800
H	-3.26197500	-1.75967400	-1.61754600
H	-4.60371600	0.83051800	1.53444600
C	-5.44375400	-1.24202300	-0.05252900
H	-6.02953500	-0.99337000	0.83827600
H	-6.03685200	-0.94767200	-0.92852400
H	-5.33556600	-2.33230900	-0.08940800
Cl	4.96179600	-0.94687700	0.12433700

O(*para*–Cl–phenyl) (*para*–OMe–phenyl)

0 1

O	0.03314200	1.56628700	-0.03657300
C	-1.17229700	0.87807800	-0.09854200
C	-2.07196900	1.01677300	0.95211900
C	-1.52184200	0.13493200	-1.23221300
C	-3.33321900	0.41527300	0.88376500
H	-1.78722100	1.60489100	1.81890600
C	-2.76916500	-0.47185700	-1.29993600
H	-0.81780100	0.04212000	-2.05342400
C	-3.68490200	-0.33592400	-0.24349800
H	-4.02232500	0.54000100	1.71091100
H	-3.06359200	-1.05131300	-2.16917200
C	1.22131500	0.87395000	-0.00173200
C	2.37259700	1.62338600	-0.26974900
C	1.32634000	-0.48347000	0.31667500
C	3.62630700	1.02079800	-0.22274100
H	2.26804800	2.67611100	-0.51184500

C	2.58385100	-1.08847900	0.35940500
H	0.43793200	-1.06590600	0.53292100
C	3.72466800	-0.33620800	0.08954300
H	4.52073700	1.59823500	-0.43077200
H	2.67269100	-2.14112100	0.60645400
O	-4.88235000	-0.96834800	-0.41527800
C	-5.85114100	-0.86052200	0.61442000
H	-6.71711300	-1.43012000	0.27227000
H	-5.48705300	-1.28749500	1.55862900
H	-6.14776700	0.18352700	0.78251400
Cl	5.30787500	-1.10428300	0.14190100

O(*para*–Cl–phenyl) (*para*–NMe$_2$–phenyl)

0 1

O	0.46150500	1.66690800	0.00180600
C	-0.77616100	1.02743700	0.00111400
C	-1.41773600	0.74586700	1.20515600
C	-1.41831300	0.74976900	-1.20352500
C	-2.69005900	0.18016900	1.20814600
H	-0.92262900	0.98389500	2.14194100
C	-2.69065200	0.18413400	-1.20773900
H	-0.92361500	0.99081300	-2.13975600
C	-3.35692300	-0.13000700	-0.00014300
H	-3.16390000	-0.01475900	2.16237100
H	-3.16494800	-0.00770400	-2.16236300
C	1.61210200	0.91578500	0.00098200
C	1.63864400	-0.48212900	-0.00056700
C	2.81118300	1.63956400	0.00177500
C	2.86459600	-1.15120300	-0.00131100
H	0.71338100	-1.04665000	-0.00116000
C	4.03197800	0.97223900	0.00103100
H	2.76781000	2.72401600	0.00298000
C	4.05179200	-0.42383600	-0.00050800
H	2.89164100	-2.23581700	-0.00251200
H	4.96226300	1.53029600	0.00165400
C	-5.35585200	-0.81804500	1.24500500
H	-6.30365300	-1.32737300	1.05945500

H	-4.80571100	-1.40870900	1.98731700
H	-5.57460000	0.16709500	1.68885100
N	-4.61385900	-0.72770600	-0.00083600
C	-5.35669800	-0.81333800	-1.24651000
H	-6.30455300	-1.32301100	-1.06218000
H	-5.57539500	0.17348000	-1.68662400
H	-4.80724100	-1.40148800	-1.99132600
Cl	5.59580600	-1.27199100	-0.00145100

O(*para*–CF_3–phenyl)$_2$

0 1

O	-0.00022600	-1.77751900	0.00268800
C	-1.20179300	-1.10184400	0.00812600
C	-1.41552300	0.06920900	-0.72606800
C	-2.24423600	-1.69045000	0.72925700
C	-2.67989000	0.65362400	-0.72475000
H	-0.60496100	0.51464900	-1.29251400
C	-3.50529700	-1.10263200	0.71916000
H	-2.04970400	-2.59969800	1.28824200
C	-3.72725500	0.07424500	-0.00322500
H	-2.85118200	1.56495000	-1.28787700
H	-4.31507800	-1.55090800	1.28530300
C	1.20175800	-1.10235700	-0.00479800
C	2.23975600	-1.68451300	-0.73721000
C	1.41989400	0.06186300	0.73901000
C	3.50111900	-1.09699300	-0.72893700
H	2.04187900	-2.58860500	-1.30333400
C	2.68422600	0.64613600	0.73575900
H	0.61247500	0.50199300	1.31409100
C	3.72732800	0.07312300	0.00282900
H	4.30759800	-1.54017300	-1.30368300
H	2.85900600	1.55229400	1.30614600
C	5.10254100	0.67837700	0.04695000
F	5.05843800	2.01190500	0.26425300
F	5.77702100	0.47556900	-1.10720300
F	5.85633700	0.14589700	1.03772000
C	-5.10238800	0.67942400	-0.04913000

F	-5.85460600	0.14757700	-1.04147700
F	-5.77872100	0.47503300	1.10375200
F	-5.05843300	2.01317200	-0.26479300

(*para*–CF_3–phenyl) (*para*–NO_2–phenyl)

0 1

O	0.44708200	-1.70061800	0.00772100
C	1.62213400	-0.99451200	-0.00061900
C	2.74776700	-1.68093000	0.47585500
C	1.73878900	0.30788700	-0.50572700
C	3.99187700	-1.06609000	0.45516500
H	2.62481800	-2.68975300	0.85499600
C	2.98524300	0.92474200	-0.52261000
H	0.86803700	0.82822600	-0.88759700
C	4.09709800	0.23475300	-0.04114000
H	4.87795300	-1.57126300	0.81899400
H	3.10907900	1.92852400	-0.90995100
C	-0.77996700	-1.06103600	0.00255700
C	-1.09944600	-0.07486100	0.94001300
C	-1.72511100	-1.50466300	-0.92317700
C	-2.37814600	0.47707200	0.93731300
H	-0.35780500	0.25050500	1.66201500
C	-3.00354400	-0.95227000	-0.91399500
H	-1.44794100	-2.27456600	-1.63546700
C	-3.33170300	0.04217800	0.01187600
H	-2.63513800	1.24727900	1.65670700
H	-3.74255700	-1.28487900	-1.63517600
N	5.40768400	0.88928900	-0.06044200
O	5.46701600	2.03878300	-0.49893600
O	6.37181400	0.25054100	0.36303700
C	-4.72837800	0.60044400	0.04927800
F	-4.75108800	1.86299400	0.53007400
F	-5.29205100	0.61954600	-1.17879600
F	-5.54099600	-0.13643100	0.84153000

O(*para*–CF_3–phenyl) (*para*–Me–phenyl)

0 1

O	1.14077000	-1.57688600	0.09527900
C	-0.09701200	-0.98544700	0.06944300
C	-0.31638600	0.35360200	-0.27203700
C	-1.17736300	-1.82128300	0.38113400
C	-1.61935100	0.84774600	-0.29670100
H	0.51836800	1.00049900	-0.51551800
C	-2.47190200	-1.31844400	0.35049900
H	-0.97940000	-2.85488200	0.64542300
C	-2.70110800	0.02115900	0.01416500
H	-1.79241700	1.88709900	-0.55609100
H	-3.30780600	-1.96393700	0.59975200
C	2.29174100	-0.79833300	0.05595500
C	3.12382000	-0.89816200	-1.05653400
C	2.65145700	0.00154200	1.14208500
C	4.32610700	-0.18931900	-1.07824200
H	2.82578700	-1.52915200	-1.88802200
C	3.85222100	0.70833800	1.10025600
H	1.99660700	0.06356800	2.00593800
C	4.71179300	0.62436800	-0.00527600
H	4.97321700	-0.26987600	-1.94841500
H	4.12911800	1.33228400	1.94690700
C	6.02771200	1.36779600	-0.02311700
H	5.94889300	2.33609400	0.48320600
H	6.81463800	0.79783700	0.48881200
H	6.37126200	1.54947400	-1.04681400
C	-4.10416600	0.54697300	-0.07140800
F	-4.16203000	1.87649800	0.17187500
F	-4.92729200	-0.06366400	0.81203100
F	-4.64510200	0.35415100	-1.29932100

O(*para*–CF_3–phenyl)(*para*–OMe–phenyl)

0 1

O	0.69020400	-1.71899800	0.07329400
C	1.87125900	-0.99004900	-0.03896200
C	2.61270100	-0.71214700	1.10370800
C	2.34761000	-0.61680700	-1.29958900
C	3.84204900	-0.05296100	1.00015900

H	2.23251100	-1.01963900	2.07293200
C	3.56627500	0.04113300	-1.40719200
H	1.76386800	-0.85181500	-2.18426000
C	4.32186900	0.32884600	-0.25870100
H	4.40890300	0.15206200	1.90081000
H	3.95963700	0.33888700	-2.37386700
C	-0.51717200	-1.06807500	0.06112500
C	-1.65078700	-1.89222700	0.09059900
C	-0.65789400	0.32338000	0.03801100
C	-2.91795900	-1.32483200	0.09400800
H	-1.51383000	-2.96838700	0.11471300
C	-1.93562800	0.88159500	0.03964400
H	0.21752800	0.96196100	0.02394300
C	-3.06901900	0.06750900	0.06826100
H	-3.79522500	-1.96311700	0.12486700
H	-2.04797200	1.96066900	0.02825900
O	5.50258500	0.97609900	-0.47701700
C	6.31381600	1.29133500	0.64294300
H	7.19447400	1.79633700	0.24212900
H	5.79648800	1.96423800	1.33988900
H	6.62834300	0.38730400	1.18127500
C	-4.44225400	0.67002300	0.01661100
F	-4.45870200	1.93792000	0.48760900
F	-5.33269900	-0.04453800	0.74377100
F	-4.93040400	0.71821200	-1.24745300

O(*para*–CF_3–phenyl) (*para*–NMe_2–phenyl)

0 1

O	0.27751700	1.80857000	0.01143900
C	1.48300700	1.10681400	0.00614300
C	2.12306400	0.83256500	-1.19988100
C	2.09504800	0.75929700	1.20816200
C	3.36498000	0.20288300	-1.20803900
H	1.65186100	1.12566600	-2.13332500
C	3.33632000	0.12859500	1.20695300
H	1.60263800	0.99540500	2.14685700
C	4.00001200	-0.18083200	-0.00360800

H	3.83961400	0.01447300	-2.16315000
H	3.78872200	-0.11825000	2.15956400
C	-0.90752500	1.12101400	0.01544900
C	-1.00575300	-0.27468500	-0.00891700
C	-2.06712300	1.90863200	0.04846900
C	-2.26518700	-0.87219200	-0.00148700
H	-0.11019200	-0.88447000	-0.02943100
C	-3.31612300	1.30220900	0.05578800
H	-1.96376700	2.98858800	0.07237000
C	-3.42393100	-0.09406500	0.03218800
H	-2.34375600	-1.95443100	-0.01331300
H	-4.21278300	1.91263400	0.08999200
C	5.97260800	-0.93901000	-1.25038400
H	6.89080800	-1.50142600	-1.06972000
H	5.40061400	-1.48032700	-2.01363800
H	6.24675600	0.04487600	-1.66491100
N	5.22324900	-0.84280800	-0.00936800
C	5.94166500	-1.01765000	1.24131700
H	6.86375900	-1.56959900	1.04867100
H	6.20586500	-0.06212100	1.72313700
H	5.35066100	-1.60433000	1.95496700
C	-4.77585800	-0.74234800	-0.01351400
F	-5.24342400	-0.86157500	-1.28112100
F	-4.75852900	-1.98990300	0.50997900
F	-5.70081400	-0.02884900	0.67049200

O(*para*–NO_2–phenyl)$_2$

0 1

O	-0.00001300	-1.62453600	-0.00015500
C	-1.20327700	-0.95773500	0.00877800
C	-2.25558200	-1.57515600	-0.67697300
C	-1.40887500	0.22647600	0.72853500
C	-3.52192900	-1.00378100	-0.65319800
H	-2.06364700	-2.49570900	-1.21752500
C	-2.67506800	0.80161900	0.74775100
H	-0.59160600	0.68527100	1.27380300
C	-3.71532800	0.18215300	0.05574300

H	-4.35601400	-1.45520800	-1.17586800
H	-2.86978700	1.71448200	1.29695100
C	1.20326700	-0.95776500	-0.00894400
C	1.40903400	0.22624400	-0.72899700
C	2.25542100	-1.57498900	0.67719600
C	2.67522400	0.80137100	-0.74811400
H	0.59188600	0.68489700	-1.27456800
C	3.52177500	-1.00361800	0.65352200
H	2.06340000	-2.49538300	1.21798700
C	3.71535900	0.18211600	-0.05570500
H	2.87004000	1.71407900	-1.29754100
H	4.35572100	-1.45492300	1.17652000
N	-5.04998700	0.79202800	0.07785700
N	5.04998000	0.79196800	-0.07771700
O	-5.18660800	1.84278800	0.70442500
O	-5.95048400	0.21534600	-0.53175200
O	5.95035400	0.21546500	0.53222800
O	5.18674200	1.84255000	-0.70453400

O(*para*–NO_2–phenyl) (*para*–Me–phenyl)

0 1

O	0.69805500	1.55452000	0.02725300
C	-0.51217800	0.92233800	0.01458900
C	-1.63503500	1.76248600	0.09400600
C	-0.66963400	-0.46788700	-0.07996700
C	-2.90986000	1.21840900	0.07995000
H	-1.48089500	2.83392300	0.16545000
C	-1.94973700	-1.01223400	-0.09339600
H	0.19810400	-1.11356300	-0.14313300
C	-3.05654600	-0.16847800	-0.01325500
H	-3.79157200	1.84427700	0.14031000
H	-2.10227100	-2.08209200	-0.16604600
C	1.87688900	0.80930000	0.01793100
C	2.55097000	0.61873000	-1.18584000
C	2.41041800	0.34106400	1.21767100
C	3.77341800	-0.05450800	-1.18236500
H	2.12431400	1.00681900	-2.10552000

C	3.63216400	-0.33153200	1.20215200
H	1.87765100	0.51643100	2.14727400
C	4.33214000	-0.54471700	0.00576300
H	4.30274700	-0.19717200	-2.12134700
H	4.05129800	-0.69107000	2.13887100
C	5.64170300	-1.29911700	-0.00286500
H	6.21130000	-1.12405500	0.91608300
H	5.47642100	-2.38201000	-0.08101000
H	6.26858800	-1.00401900	-0.85068700
N	-4.39948500	-0.74681100	-0.02692100
O	-5.35746500	0.02560400	0.04271400
O	-4.49653600	-1.97298800	-0.10722200

O(*para*–NO_2–phenyl) (*para*–OMe–phenyl)

0 1

O	0.24258600	1.66005000	-0.12132800
C	1.45245100	0.97617900	0.00730600
C	2.14380300	0.58401900	-1.13295200
C	1.99758500	0.76637400	1.27683000
C	3.39379000	-0.03200000	-1.01574600
H	1.71004100	0.76707900	-2.11114400
C	3.23854200	0.15392000	1.39765900
H	1.45026900	1.09123800	2.15626700
C	3.94511700	-0.25109600	0.25316100
H	3.92188500	-0.32936300	-1.91406300
H	3.68625200	-0.01875500	2.37099900
C	-0.93672100	0.97342300	-0.07915400
C	-2.09787800	1.75754600	-0.18058200
C	-1.02934900	-0.41988600	0.05083400
C	-3.34589000	1.15518500	-0.15191900
H	-1.99378600	2.83277700	-0.28032900
C	-2.28263300	-1.02282000	0.07968800
H	-0.13223500	-1.02253800	0.12674900
C	-3.42774700	-0.23413100	-0.02121000
H	-4.25586900	1.73736000	-0.22795300
H	-2.38487500	-2.09657600	0.17847900
O	5.15141300	-0.84138300	0.48431200

C	5.91468200	-1.27537600	-0.63052600
H	6.82388600	-1.71519600	-0.21717900
H	5.37841600	-2.03434000	-1.21552300
H	6.18363300	-0.43688900	-1.28656300
N	-4.74213600	-0.87372000	0.00905100
O	-4.78226500	-2.10046800	0.12319400
O	-5.73513000	-0.14904500	-0.08160600

O(*para*–NO_2–phenyl) (*para*–NMe_2–phenyl)

0 1

O	-0.17129600	1.72763300	-0.00002300
C	1.05979400	1.06501600	0.00002200
C	1.69365000	0.77588100	-1.20548400
C	1.69396400	0.77660100	1.20548000
C	2.95465900	0.18615900	-1.20872700
H	1.20343800	1.02478600	-2.14195900
C	2.95501400	0.18686800	1.20871300
H	1.20409400	1.02604500	2.14199000
C	3.61541200	-0.13824800	0.00001300
H	3.42501300	-0.01688700	-2.16286400
H	3.42561900	-0.01553900	2.16285900
C	-1.32937100	1.00802000	0.00001400
C	-1.38303200	-0.39390300	0.00037600
C	-2.51401500	1.76405700	-0.00032800
C	-2.61857900	-1.03237100	0.00038900
H	-0.46788000	-0.97373800	0.00067800
C	-3.74444000	1.12639400	-0.00032100
H	-2.44082000	2.84647100	-0.00059300
C	-3.78682300	-0.27102600	0.00003600
H	-2.68981100	-2.11317300	0.00067500
H	-4.67106700	1.68691400	-0.00057300
C	5.59037000	-0.88756900	-1.24857800
H	6.52904400	-1.41153100	-1.05886400
H	5.02364200	-1.48067500	-1.97675500
H	5.82593500	0.08448700	-1.71114000
N	4.85879700	-0.75681100	-0.00004600
C	5.59050600	-0.88759400	1.24841100

H	6.52881200	-1.41221600	1.05870500
H	5.82674400	0.08445700	1.71065000
H	5.02351000	-1.48013200	1.97682800
N	-5.08210400	-0.94727600	0.00004200
O	-5.08809300	-2.18027200	0.00019700
O	-6.09633400	-0.24615800	-0.00013500

O(*para*–Me–phenyl)$_2$

0 1

O	-0.00006500	-1.39899300	0.00054800
C	1.20158500	-0.71652400	0.01510600
C	1.40949900	0.44199200	0.76803500
C	2.25607100	-1.28140000	-0.70498500
C	2.67474600	1.02969600	0.78388500
H	0.59174600	0.87797700	1.33251600
C	3.51486100	-0.68441500	-0.66915200
H	2.07420300	-2.18166300	-1.28366800
C	3.75020600	0.48138900	0.07287300
H	2.82713700	1.93334700	1.37001800
H	4.32853100	-1.13161100	-1.23597600
C	-1.20161200	-0.71638200	-0.01457900
C	-2.25682500	-1.28203700	0.70394500
C	-1.40879800	0.44294400	-0.76637300
C	-3.51551500	-0.68500300	0.66763000
H	-2.07548100	-2.18295400	1.28177700
C	-2.67406800	1.03071300	-0.78271100
H	-0.59056800	0.87956200	-1.32966100
C	-3.75015900	0.48168600	-0.07333100
H	-4.32971900	-1.13280700	1.23321300
H	-2.82587800	1.93501200	-1.36798800
C	5.12463300	1.10852700	0.12565300
H	5.74378400	0.65434500	0.91126600
H	5.66068000	0.98102800	-0.82143500
H	5.06789600	2.18159500	0.33773800
C	-5.12456400	1.10885300	-0.12638900
H	-5.06807000	2.18050800	-0.34547000
H	-5.74600600	0.64977600	-0.90732600

H	-5.65811000	0.98758900	0.82296100

O(*para*−Me−phenyl) (*para*−OMe−phenyl)

0 1

O	-0.48543800	1.49578400	-0.25273100
C	0.76715800	0.92328900	-0.10242100
C	1.16464900	-0.19655900	-0.83084100
C	1.67629100	1.56497700	0.74386200
C	2.46807300	-0.68731300	-0.70928400
H	0.45966500	-0.68639100	-1.49515700
C	2.97606500	1.08660900	0.85845400
H	1.35269600	2.44050000	1.29786000
C	3.38145900	-0.04531700	0.13588700
H	2.75644800	-1.55998400	-1.28393300
H	3.69684600	1.57361900	1.50761000
C	-1.62569400	0.72952200	-0.11772500
C	-2.76706400	1.19879300	-0.77518100
C	-1.69980000	-0.41799900	0.67480600
C	-3.97310400	0.51714100	-0.63921900
H	-2.69102900	2.09772300	-1.37913300
C	-2.91804800	-1.09069400	0.79235700
H	-0.82088300	-0.77776400	1.19888800
C	-4.07361400	-0.64447900	0.14127700
H	-4.85418900	0.89474500	-1.15379200
H	-2.96668900	-1.98183400	1.41440800
O	4.67756300	-0.43750600	0.32384100
C	5.14675000	-1.56390700	-0.39641900
H	6.19113400	-1.69284200	-0.10580800
H	4.58553100	-2.47273900	-0.13933900
H	5.09050400	-1.40299000	-1.48162900
C	-5.38140700	-1.39373400	0.25716100
H	-5.36484900	-2.09811100	1.09546500
H	-6.22484400	-0.71038100	0.41090600
H	-5.59762900	-1.97174800	-0.65151100

O(*para*−Me−phenyl) (*para*−NMe_2−phenyl)

0 1

O	-0.88399100	-1.44958600	0.45601400
C	0.37102700	-0.88547500	0.26930100
C	0.80336000	0.20813500	1.02033700
C	1.25318100	-1.49732300	-0.61735000
C	2.09960200	0.69355700	0.87373100
H	0.12559700	0.67605100	1.72808100
C	2.55527300	-1.02235000	-0.76002300
H	0.91786500	-2.35988200	-1.18531000
C	3.01020100	0.09850100	-0.03010000
H	2.40102800	1.53942600	1.47959500
H	3.21507700	-1.53356600	-1.45031900
C	-2.01866200	-0.70816000	0.20368500
C	-2.04504600	0.43445300	-0.59817400
C	-3.20513200	-1.19025000	0.76872300
C	-3.26043500	1.08802100	-0.81924000
H	-1.13137500	0.80808300	-1.04726200
C	-4.40466500	-0.52727600	0.53160600
H	-3.16499000	-2.08266900	1.38578600
C	-4.45862600	0.62830300	-0.26395500
H	-3.26987200	1.97703500	-1.44621600
H	-5.31882600	-0.91387300	0.97761800
C	4.80729400	1.57035700	0.75847500
H	5.81718900	1.86597200	0.46587600
H	4.19071400	2.47676100	0.76541900
H	4.84662500	1.17814600	1.78855000
N	4.29950900	0.60481500	-0.20121800
C	5.27211700	-0.18837000	-0.93294400
H	6.21513700	0.36042400	-0.98195200
H	5.46717300	-1.17027600	-0.46998700
H	4.94006400	-0.36063100	-1.96339500
C	-5.76730800	1.34651100	-0.50276500
H	-6.18425200	1.74866500	0.42985200
H	-5.64034600	2.18529500	-1.19504800
H	-6.52453600	0.67622400	-0.92872000

O(*para*–OMe–phenyl)$_2$

0 1

O	-0.00025900	-1.70079600	0.00241200
C	-1.19893900	-1.01100400	0.04760400
C	-1.44951900	0.12877500	-0.71484300
C	-2.21399900	-1.55436800	0.84257000
C	-2.70940200	0.73533900	-0.67878800
H	-0.66605900	0.54605500	-1.33903800
C	-3.46901400	-0.95963400	0.87185500
H	-2.00428200	-2.44552800	1.42572400
C	-3.72657600	0.19290900	0.11463900
H	-2.88143700	1.62105600	-1.27978500
H	-4.26803400	-1.36933700	1.48172900
C	1.19853200	-1.01125100	-0.04518000
C	2.20899500	-1.54870300	-0.84980800
C	1.45355500	0.12262500	0.72464300
C	3.46404500	-0.95400500	-0.88138100
H	1.99600900	-2.43535800	-1.43861300
C	2.71325700	0.72924000	0.68636100
H	0.67347700	0.53513500	1.35624500
C	3.72598700	0.19261300	-0.11680700
H	4.25961900	-1.35922800	-1.49871100
H	2.88883100	1.61038500	1.29303200
O	-4.99116500	0.70443100	0.22087700
C	-5.30814400	1.86050600	-0.53318200
H	-6.35002000	2.09313900	-0.30426600
H	-4.67714000	2.71472400	-0.25132800
H	-5.20665600	1.68169200	-1.61245500
O	4.99007400	0.70460800	-0.22592100
C	5.31126100	1.85545200	0.53436600
H	6.35201400	2.08940300	0.30173100
H	4.67896500	2.71166500	0.26160800
H	5.21528200	1.66928800	1.61289300

O(*para*–OMe–phenyl) (*para*–NMe_2–phenyl)

0 1

O	-0.42351100	1.55969700	-0.34207700
C	0.80875300	0.94097000	-0.19554700
C	1.09832900	-0.30752600	-0.74836400

C	1.81893300	1.65032600	0.45076200
C	2.37868200	-0.84440400	-0.64039800
H	0.32389700	-0.86073700	-1.27066000
C	3.10387600	1.12193700	0.54984700
H	1.59329100	2.62852200	0.86457100
C	3.41651200	-0.15018900	0.02155400
H	2.56477300	-1.81333200	-1.08780800
H	3.86257200	1.71085700	1.05079200
C	-1.58401800	0.84121700	-0.12485900
C	-1.70626500	-0.13025200	0.87759800
C	-2.68976400	1.17227900	-0.90463300
C	-2.92668000	-0.76353800	1.08080200
H	-0.84952600	-0.38515000	1.49254900
C	-3.92076600	0.54375600	-0.69469000
H	-2.58062900	1.93040500	-1.67389600
C	-4.04346700	-0.43367900	0.29891700
H	-3.03967700	-1.51848700	1.85279200
H	-4.76575400	0.82187700	-1.31424000
C	5.03510300	-1.87160000	-0.63472900
H	6.05703300	-2.17590400	-0.39777600
H	4.37863500	-2.71546900	-0.39244200
H	4.97067400	-1.69250700	-1.72140700
N	4.69211000	-0.70445300	0.15940500
C	5.78262900	0.15438900	0.58803400
H	6.69963500	-0.43621200	0.64617300
H	5.96031100	1.00321100	-0.09378000
H	5.59098500	0.55936000	1.58852700
O	-5.19436400	-1.11807900	0.58513000
C	-6.35065800	-0.82115600	-0.17598500
H	-6.19939300	-1.03242000	-1.24369000
H	-7.14037400	-1.46909300	0.20970000
H	-6.65541500	0.22812100	-0.05950500

O(*para*–NMe$_2$–phenyl)$_2$

0 1

O	-0.01315200	-1.71740500	-0.21925000
C	-1.20857900	-1.02592100	-0.16668800

C	-2.30646000	-1.62829400	-0.79056300
C	-1.38358900	0.18128700	0.50665600
C	-3.55741500	-1.02757300	-0.74309500
H	-2.15884600	-2.56408900	-1.32106100
C	-2.64722500	0.77730800	0.55853400
H	-0.54321400	0.65485400	1.00318800
C	-3.76220600	0.19183100	-0.06438300
H	-4.38302800	-1.49695800	-1.26888900
H	-2.75160400	1.70539100	1.10913100
C	1.18814100	-1.03273600	-0.11642800
C	1.51997700	0.02426700	-0.96572000
C	2.13016400	-1.49008700	0.80202200
C	2.77347700	0.62451600	-0.88509600
H	0.79802200	0.37460900	-1.69712200
C	3.39020400	-0.90037100	0.87798500
H	1.87410100	-2.32410000	1.44846700
C	3.74176500	0.18642200	0.04737400
H	2.99605600	1.43716000	-1.56607800
H	4.09809700	-1.29471900	1.59688400
C	-6.17517300	-0.02992600	0.31795500
H	-7.10508300	0.45353000	-0.00145600
H	-6.12545800	-1.00783600	-0.16272700
H	-6.22736900	-0.18949800	1.41041100
N	-5.04086700	0.80167300	-0.07341800
C	-5.13931700	2.15061100	0.45394600
H	-6.12863600	2.55181500	0.20994400
H	-5.01326800	2.21066000	1.55139600
H	-4.38843200	2.79363700	-0.01463100
N	4.98776300	0.81048500	0.15009300
C	6.03327100	0.15715100	0.91863900
H	6.92942800	0.78150700	0.90426400
H	5.73274200	0.04091100	1.96640500
H	6.29987100	-0.83995600	0.52917200
C	5.40389100	1.71657900	-0.90673700
H	4.71854800	2.56873400	-0.98346200
H	6.39216600	2.11458600	-0.66597400
H	5.45727800	1**.23352400**	**-1.89698300**