Table 1: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Planar PH_3 obtained at B97D/aug-cc-pVTZ. The imaginary frequency is indicated with an italicized i.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
PH_3-TS	P	0.000000	0.000000	0.000000	1065.25i	988.65	988.66
	H	-0.000000	1.385978	0.000000	2527.54	2616.26	2616.27
	H	1.200292	-0.692989	-0.000000			
	H	-1.200292	-0.692989	-0.000000			

Table 2: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Pyramidal PH_3 obtained at B97D/aug-cc-pVTZ.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
PH_3	P	0.060000	-0.150000	-0.129700	1026.69	1144.20	1144.29
	H	1.185550	-0.168462	0.648551	2352.39	2352.73	2370.63
	H	-0.738777	-0.942390	0.648551			
	H	-0.446862	1.111073	0.648397			

Table 3: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Planar PH_3 obtained at CCSD(T)/aug-cc-pVTZ. The imaginary frequency is indicated with an italicized i.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
PH_3-TS	P	0.000000	0.000000	0.000000	1092.64i	1011.96	1012.15
	H	0.000000	1.373102	-0.000000	2595.20	2675.15	2675.82
	H	1.189141	-0.686551	-0.000000			
	H	-1.189141	-0.686551	-0.000000			

Table 4: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Pyramidal PH_3 obtained at CCSD(T)/aug-cc-pVTZ.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
PH_3	P	-0.000000	-0.000000	0.079444	1009.70	1140.55	1141.09
	H	-0.000000	1.348217	-0.397222	2416.72	2423.47	2426.88
	H	-1.167590	-0.674108	-0.397222			
	H	1.167590	-0.674108	-0.397222			

Table 5: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Planar $OH_3{}^+$ obtained at B97D/aug-cc-pVTZ. The imaginary frequency is indicated with an italicized i.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
OH_3^+-TS	O	0.000000	0.000000	0.000000	$641.11i$	1585.65	1585.66
	H	0.000000	0.975514	-0.000000	3544.14	3695.62	3695.62
	H	0.844819	-0.487757	-0.000000			
	H	-0.844819	-0.487757	-0.000000			

Table 6: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Pyramidal $OH_3{}^+$ obtained at B97D/aug-cc-pVTZ.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
OH_3^+	O	-0.410000	-0.030000	-0.077405	842.44	1653.74	1654.18
	H	0.467947	0.815843	0.206410	3498.93	3597.65	3597.76
	H	0.472962	-0.812934	0.206439			
	H	-0.940581	-0.002887	0.206391			

Table 7: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Planar OH_3^+ obtained at CCSD(T)/aug-cc-pVTZ. The imaginary frequency is indicated with an italicized i.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
OH_3^+-TS	O	0.000000	0.000000	0.000000	$680.05i$	1632.71	1633.29
	H	-0.000000	0.933469	0.000000	3655.84	3806.95	3807.33
	H	0.808408	-0.466734	0.000000			
	H	-0.808408	-0.466734	0.000000			

Table 8: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of Pyramidal OH_3^+ obtained at CCSD(T)/aug-cc-pVTZ.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
OH_3^+	O	-0.000000	-0.000000	0.130000	896.12	1698.30	1699.17
	H	-0.000000	1.348217	-0.346667	3601.40	3700.12	3700.30
	H	-1.167590	-0.674108	-0.346667			
	H	1.167590	-0.674108	-0.346667			

Table 9: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of C_{60} obtained at B97D/aug-cc-pVTZ.

Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
	C	0.725528	2.598567	-2.304806	257.60	257.60	257.68
	C	-0.725528	2.598567	-2.304806	257.68	257.68	333.93
	C	-1.424539	3.030453	-1.173907	333.93	333.94	346.01
	C	-0.698947	3.478624	-0.280000	346.01	346.01	346.01
	C	0.698947	3.478624	-0.280000	398.55	398.55	398.85
	C	1.424539	3.030453	-1.173907	398.85	398.85	424.08
	C	1.173895	1.424539	-3.030405	424.08	424.59	424.59
	C	-0.000000	0.698945	-3.478603	424.59	474.54	475.47
	C	-1.173895	1.424539	-3.030405	475.47	475.47	481.41
	C	-2.304804	0.725538	-2.598546	525.45	525.46	525.46
	C	-2.598597	2.304840	-0.725558	525.85	525.86	525.86
	C	-1.424547	3.030412	1.173903	526.25	526.25	551.19
	C	-0.725534	2.598509	2.304784	551.19	551.19	559.38
	C	0.725534	2.598509	2.304784	559.38	559.38	564.80
	C	1.424547	3.030412	1.173903	564.80	564.80	565.30
	C	2.598489	2.304767	0.725523	570.84	570.84	570.84
	C	2.598597	2.304840	-0.725558	663.45	663.45	663.87
	C	3.030378	1.173889	-1.424514	663.87	663.87	706.28
	C	2.304804	0.725538	-2.598546	706.28	706.69	706.69
	C	-0.000000	-0.698945	-3.478603	706.69	713.34	713.34
	C	1.173895	-1.424539	-3.030405	713.34	727.92	727.92
	C	2.304804	-0.725538	-2.598546	727.92	728.42	728.42
C_{60}	C	3.030378	-1.173889	-1.424514	745.64	745.64	745.64
	C	3.478693	-0.000000	-0.698941	745.67	750.39	750.60
	C	3.478556	-0.000000	0.698933	750.60	750.60	753.83
	C	3.030478	1.173925	1.424561	753.83	753.83	765.65
	C	2.304806	0.725532	2.598540	765.65	765.66	765.86
	C	1.173911	1.424530	3.030441	765.86	773.97	773.97
	C	-2.598489	2.304767	0.725523	773.97	774.33	788.51
	C	-1.173911	-1.424530	3.030441	788.51	788.51	824.08
	C	-2.304806	-0.725532	2.598540	824.08	824.08	947.12
	C	-3.030478	-1.173925	1.424561	955.58	956.10	956.10
	C	-2.598489	-2.304767	0.725523	956.11	958.51	958.52
	C	-1.424547	-3.030412	1.173903	958.52	1073.04	1073.24
	C	0.725534	-2.598509	2.304784	1073.26	1073.26	1094.32
	C	1.173911	-1.424530	3.030441	1094.33	1094.67	1094.68
	C	0.000000	-0.698943	3.478633	1094.68	1176.72	1176.72
	C	0.000000	0.698943	3.478633	1176.73	1181.07	1181.07
	C	-1.173911	1.424530	3.030441	1181.07	1203.01	1203.02
	C	-2.304806	0.725532	2.598540	1203.02	1203.10	1203.11
	C	-3.478556	0.000000	0.698933	1233.62	1233.63	1233.76
	C	-3.478693	0.000000	-0.698941	1233.77	1233.77	1264.53
	C	-3.030378	-1.173889	-1.424514	1264.54	1264.55	1291.40
	C	-2.598597	-2.304840	-0.725558	1291.51	1291.51	1291.51
	C	-1.424539	-3.030453	-1.173907	1297.19	1297.73	1297.73
	C	-0.698947	-3.478624	-0.280000	1297.73	1318.26	1318.26

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Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	0.698947	-3.478624	-0.280000	1318.27	1326.09	1326.11
	C	1.424547	-3.030412	1.173903	1326.11	1326.57	1326.58
	C	2.304806	-0.725532	2.598540	1406.49	1406.50	1406.58
	C	3.030478	-1.173925	1.424561	1406.58	1406.58	1408.12
	C	2.598489	-2.304767	0.725523	1408.13	1408.13	1408.61
	C	2.598597	-2.304840	-0.725558	1417.99	1418.00	1418.00
C_{60}	C	1.424539	-3.030453	-1.173907	1460.59	1477.83	1477.98
	C	0.725528	-2.598567	-2.304806	1477.98	1477.98	1512.83
	C	-0.725528	-2.598567	-2.304806	1512.84	1512.84	1541.81
	C	-1.173895	-1.424539	-3.030405	1541.81	1541.82	1541.96
	C	-2.304804	-0.725538	-2.598546	1541.97	1554.87	1554.89
	C	-3.030478	1.173925	1.424561	1554.95	1554.96	1554.96
	C	-3.030378	1.173889	-1.424514			
	C	-0.725534	-2.598509	2.304784			

Table 10: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of OH_3^+@C_{60} obtained at B97D/aug-cc-pVTZ.

Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	0.293260	3.444992	-0.802233	80.27	94.98	182.75
	C	1.639712	3.115746	-0.367857	220.70	257.66	257.85
	C	2.453352	2.285884	-1.147011	260.51	260.65	264.43
	C	1.938951	1.747664	-2.392694	291.73	301.50	336.15
	C	0.639734	2.057940	-2.810556	339.99	341.04	344.92
	C	-0.197839	2.925122	-2.002573	348.39	349.30	351.12
	C	-0.560756	3.490151	0.370751	399.16	399.20	399.32
	C	0.254741	3.186988	1.531762	399.49	399.62	426.12
	C	1.613384	2.952482	1.074475	426.17	426.79	428.18
	C	2.403492	1.968723	1.683880	428.36	472.67	479.40
	C	3.274718	1.263964	-0.516417	479.58	479.72	483.33
	C	2.436737	0.389481	-2.528349	525.17	525.61	526.56
OH_3^+-C_{60}	C	1.616168	-0.602252	-3.082287	529.67	529.70	531.14
	C	0.271238	-0.276290	-3.524028	531.92	532.13	553.03
	C	-0.207585	1.029820	-3.387971	553.17	553.25	565.82
	C	-1.566644	1.260660	-2.935471	565.85	565.99	566.28
	C	-1.560537	2.431444	-2.078591	567.03	568.70	568.97
	C	-2.380821	2.472206	-0.948362	572.00	572.03	572.89
	C	-1.871267	3.010457	0.299209	665.64	665.87	665.91
	C	-0.268278	2.421913	2.578170	666.25	666.25	712.13
	C	-1.631377	1.929780	2.506179	712.54	713.24	713.74
	C	-2.415586	2.216629	1.385816	714.02	719.20	720.84
	C	-3.261793	1.188801	0.809235	721.09	741.65	741.75
	C	-3.239908	1.346220	-0.632787	742.10	743.16	743.43
	C	-3.245806	0.219131	-1.458089	747.39	747.64	747.75
	C	-2.391807	0.175012	-2.630312	747.82	763.67	764.04

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Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	-1.892831	-1.180868	-2.770176	764.14	764.36	765.50
	C	-0.586198	-1.404078	-3.212007	765.78	765.87	766.82
	C	3.268111	0.090191	-1.373516	766.94	775.73	776.29
	C	0.521771	-3.483827	-0.373178	776.74	790.49	790.70
	C	1.837550	-3.012069	-0.303494	790.76	791.17	793.91
	C	2.345259	-2.468191	0.944306	794.08	796.74	825.95
	C	1.517568	-2.424063	2.074081	826.08	826.20	949.51
	C	0.155186	-2.922455	2.002378	955.42	956.19	956.27
	C	-1.678727	-3.117190	0.363696	956.97	958.25	958.34
	C	-1.656661	-2.960840	-1.078499	959.33	1037.01	1071.96
	C	-0.297523	-3.188388	-1.533962	1073.72	1073.78	1074.25
	C	0.228112	-2.426483	-2.580515	1093.40	1093.64	1095.01
	C	1.591854	-1.933217	-2.502697	1095.11	1095.21	1174.97
	C	2.387439	-2.220519	-1.388345	1176.85	1177.12	1180.76
	C	3.218712	-1.347966	0.632625	1180.93	1182.30	1201.16
	C	3.223763	-0.219941	1.462536	1201.29	1202.92	1203.67
	C	2.362974	-0.175505	2.634493	1203.87	1232.04	1232.15
	C	1.527225	-1.256183	2.936405	1233.69	1233.89	1234.05
OH_3^+-C_{60}	C	0.167382	-1.029884	3.393120	1264.20	1264.95	1265.06
	C	-0.678881	-2.058987	2.816963	1290.85	1290.90	1291.13
	C	-1.972143	-1.742818	2.393288	1291.63	1295.82	1297.77
	C	-2.480938	-2.281804	1.145301	1298.04	1298.15	1317.11
	C	-2.438280	-1.973821	-1.684263	1317.39	1318.66	1325.72
	C	-3.273939	-1.108299	-0.873260	1326.48	1326.57	1327.52
	C	-3.295278	-1.259487	0.515209	1327.82	1402.25	1404.19
	C	-3.288999	-0.089072	1.372477	1404.59	1405.78	1405.89
	C	-2.472048	-0.387885	2.533938	1407.91	1408.78	1409.03
	C	-1.659633	0.602506	3.091890	1409.62	1416.49	1418.43
	C	-0.314149	0.274983	3.526673	1418.49	1460.45	1477.32
	C	0.547040	1.398840	3.208228	1478.08	1478.30	1478.71
	C	1.859197	1.177990	2.774364	1511.85	1512.00	1512.20
	C	3.240240	-1.192245	-0.812237	1539.72	1539.93	1541.75
	C	3.253299	1.108990	0.875450	1541.89	1542.27	1554.54
	C	-0.333088	-3.440763	0.799746	1554.59	1555.20	1555.29
	H	0.824947	0.006066	-0.930539	1555.60	1606.45	1608.69
	H	0.824925	0.800758	0.466511	3243.13	3244.58	3281.73
	H	0.824932	-0.805939	0.455880			
	O	0.464013	0.000399	-0.002662			

Table 11: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of OH_3^+-TS@C_{60} obtained at B97D/aug-cc-pVTZ. The imaginary frequencies are indicated with an italicized i.

Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	2.933709	-1.849495	0.727097	$661.35i$	$20.86i$	64.21
	C	2.933709	-1.849495	-0.727097	104.22	152.40	249.22

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Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	3.171198	-0.664698	-1.431592	253.73	256.17	259.98
	C	3.410314	0.567742	-0.701083	261.41	271.55	280.50
	C	3.410314	0.567742	0.701083	335.17	336.36	338.23
	C	3.171198	-0.664698	1.431592	345.14	346.25	346.28
	C	1.892108	-2.753975	1.176803	347.09	398.93	399.11
	C	1.248088	-3.309360	-0.000000	399.36	399.55	399.70
	C	1.892108	-2.753975	-1.176803	423.18	424.43	424.89
	C	1.130692	-2.440162	-2.307671	425.29	426.05	473.29
	C	2.384902	-0.337828	-2.607873	476.66	477.08	477.44
	C	2.784947	1.657072	-1.430712	482.40	520.77	524.14
	C	2.176555	2.701166	-0.726606	524.52	527.55	528.33
	C	2.176555	2.701166	0.726606	529.97	530.49	531.56
	C	2.784947	1.657072	1.430712	553.01	553.08	553.30
	C	2.147430	1.094916	2.607465	565.91	566.05	566.17
	C	2.384902	-0.337828	2.607873	566.30	566.93	567.36
	C	1.381566	-1.210885	3.037648	568.18	571.94	572.18
	C	1.130692	-2.440162	2.307671	572.23	665.32	665.51
	C	-0.132713	-3.533243	0.000000	665.66	666.49	666.86
	C	-0.922358	-3.213601	1.175750	711.64	713.02	713.24
	C	-0.301969	-2.675809	2.307508	713.49	713.93	718.93
	C	-0.936473	-1.593291	3.035619	719.49	719.55	741.48
OH_3^+-C_{60}-TS	C	0.104106	-0.686822	3.485581	741.95	742.02	742.03
	C	-0.123857	0.691680	3.484632	742.56	747.30	747.98
	C	0.916479	1.598964	3.035991	748.24	748.25	763.19
	C	0.283123	2.682813	2.306724	763.69	763.83	764.12
	C	0.900726	3.225667	1.175655	765.93	766.76	766.84
	C	2.147430	1.094916	-2.607465	767.06	767.50	775.43
	C	-1.907035	2.755772	-1.174599	777.50	778.36	788.86
	C	-1.148491	2.445034	-2.306794	790.11	791.43	791.72
	C	-1.400618	1.215002	-3.034183	792.19	793.12	794.45
	C	-2.402359	0.341676	-2.601315	825.68	826.42	826.56
	C	-3.190607	0.664777	-1.425980	949.65	955.76	956.95
	C	-2.947707	1.849309	0.725819	957.12	957.61	958.74
	C	-1.907035	2.755772	1.174599	959.26	959.51	1073.06
	C	-1.264758	3.316669	0.000000	1073.72	1074.24	1074.70
	C	0.112949	3.548587	-0.000000	1094.13	1094.72	1095.17
	C	0.900726	3.225667	-1.175655	1095.20	1095.50	1175.68
	C	0.283123	2.682813	-2.306724	1177.24	1178.19	1181.47
	C	-0.123857	0.691680	-3.484632	1181.79	1182.98	1200.85
	C	0.104106	-0.686822	-3.485581	1202.97	1203.33	1204.25
	C	-0.936473	-1.593291	-3.035619	1204.66	1233.02	1233.45
	C	-2.165971	-1.089905	-2.601487	1233.83	1234.68	1235.35
	C	-2.809868	-1.650062	-1.426521	1264.65	1265.69	1266.05
	C	-3.443169	-0.565790	-0.699334	1291.74	1291.82	1291.96
	C	-3.443169	-0.565790	0.699334	1292.28	1297.01	1297.94
	C	-3.190607	0.664777	1.425980	1298.17	1298.64	1318.90
	C	-1.148491	2.445034	2.306794	1319.02	1320.03	1326.10
	C	-1.400618	1.215002	3.034183	1326.56	1327.07	1327.43
	C	-2.402359	0.341676	2.601315	1328.59	1406.22	1406.41
	C	-2.165971	-1.089905	2.601487	1406.86	1407.25	1407.41

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Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	-2.809868	-1.650062	1.426521	1408.53	1409.00	1409.67
	C	-2.200781	-2.694291	0.726067	1409.83	1417.25	1418.81
	C	-2.200781	-2.694291	-0.726067	1419.52	1460.95	1478.78
OH_3^+-C_{60}-TS	C	-0.922358	-3.213601	-1.175750	1478.88	1479.16	1480.27
	C	-0.301969	-2.675809	-2.307508	1511.76	1513.22	1513.57
	C	0.916479	1.598964	-3.035991	1524.78	1533.14	1541.18
	C	1.381566	-1.210885	-3.037648	1542.73	1543.20	1543.32
	C	-2.947707	1.849309	-0.725819	1543.65	1554.97	1555.57
	H	1.273875	0.211455	-0.000000	1555.89	1556.38	1556.47
	H	0.127391	-1.045495	-0.000000	3225.06	3429.19	3594.06
	H	-0.391185	0.579155	0.000000			
	O	0.326174	-0.082598	-0.000000			

Table 12: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of $PH_3@C_{60}$ obtained at B97D/aug-cc-pVTZ.

Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	-1.599577	1.729554	-2.642695	65.56	141.71	185.36
	C	-2.537471	1.925779	-1.553034	223.51	244.14	268.62
	C	-2.192558	2.748120	-0.475200	269.17	269.50	269.91
	C	-0.900699	3.411788	-0.446204	270.02	274.61	348.53
	C	0.003499	3.215494	-1.496327	355.88	360.06	361.63
	C	-0.352734	2.362092	-2.616102	364.02	368.86	371.13
	C	-1.707276	0.352416	-3.086803	398.50	398.84	398.98
	C	-2.716336	-0.303351	-2.272460	399.07	399.09	436.17
	C	-3.232098	0.670722	-1.324460	436.94	439.33	440.15
	C	-3.555680	0.278912	-0.019409	442.21	484.67	490.71
PH_3-C_{60}	C	-2.522208	2.342218	0.877370	491.72	492.57	494.16
	C	-0.429494	3.420026	0.929428	527.00	527.90	531.56
	C	0.932963	3.227061	1.200458	538.46	538.79	539.41
	C	1.868474	3.021875	0.106089	539.61	540.69	551.57
	C	1.413847	3.018988	-1.216791	551.68	551.75	560.76
	C	1.929265	2.045914	-2.166224	561.87	564.32	564.51
	C	0.837015	1.641259	-3.032747	564.61	564.87	565.45
	C	0.736334	0.312951	-3.461542	572.46	572.57	573.28
	C	-0.560473	-0.342199	-3.486524	663.49	663.80	663.99
	C	-2.539415	-1.634740	-1.881189	664.08	664.15	707.07
	C	-1.343523	-2.352441	-2.288795	708.53	709.09	709.78
	C	-0.374707	-1.722310	-3.078651	710.30	712.85	713.78
	C	1.037102	-1.921664	-2.800649	714.16	732.67	733.73
	C	1.724976	-0.664123	-3.038796	733.88	734.49	734.75
	C	2.777379	-0.275465	-2.202331	744.51	744.63	744.81
	C	2.879589	1.104279	-1.758385	744.97	753.21	753.59
	C	3.345005	1.100467	-0.382934	754.08	754.66	760.36

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Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	2.848768	2.037915	0.529502	762.67	762.78	762.98
	C	-1.433571	2.754397	1.747133	763.35	763.55	763.91
	C	1.707769	-0.358594	3.102740	764.17	774.68	776.61
	C	0.559918	0.341751	3.489718	777.62	778.23	787.82
	C	-0.734654	-0.312925	3.456977	788.05	788.19	823.26
	C	-0.837835	-1.643775	3.040610	823.47	823.75	946.42
	C	0.353477	-2.374555	2.638346	951.91	952.22	952.53
	C	2.542276	-1.935823	1.571327	953.09	954.03	954.11
	C	3.218810	-0.673019	1.331182	954.36	1057.87	1067.12
	C	2.703373	0.299847	2.276254	1067.72	1068.16	1068.58
	C	2.521407	1.630379	1.882322	1089.94	1090.02	1090.51
	C	1.338240	2.362180	2.297887	1090.69	1090.82	1169.72
	C	0.372560	1.724278	3.083267	1170.46	1170.80	1174.23
	C	-1.720479	0.662265	3.028673	1175.31	1175.65	1185.65
	C	-2.774234	0.273521	2.196171	1192.50	1197.75	1198.07
PH_3-C_{60}	C	-2.885652	-1.106299	1.759630	1198.74	1199.31	1200.67
	C	-1.929858	-2.042744	2.169674	1226.10	1226.80	1227.24
	C	-1.415891	-3.014065	1.224324	1228.15	1228.79	1258.79
	C	-0.005840	-3.218156	1.510138	1259.00	1259.20	1284.78
	C	0.896817	-3.400018	0.457110	1285.42	1285.53	1285.98
	C	2.193800	-2.748766	0.486809	1292.49	1292.64	1292.92
	C	3.532379	-0.279462	0.024918	1293.08	1313.26	1313.54
	C	3.181141	-1.129905	-1.098191	1314.38	1320.91	1321.30
	C	2.521035	-2.341120	-0.869625	1321.50	1321.90	1322.27
	C	1.427425	-2.742164	-1.736494	1395.67	1396.04	1398.82
	C	0.423221	-3.394059	-0.915598	1399.74	1400.21	1401.38
	C	-0.935425	-3.202988	-1.186731	1401.97	1402.48	1402.62
	C	-1.875098	-3.011564	-0.097222	1409.84	1410.08	1411.50
	C	-2.871809	-2.044387	-0.525228	1450.79	1470.20	1471.41
	C	-3.371397	-1.106635	0.389270	1472.46	1472.80	1504.65
	C	-1.037820	1.922894	2.801026	1505.14	1506.10	1533.80
	C	-3.185192	1.129342	1.099505	1534.54	1535.36	1536.02
	C	1.606372	-1.744176	2.669125	1536.15	1547.32	1547.80
	P	0.117098	-0.021052	-0.180355	1548.42	1548.99	1549.43
	H	0.398883	-0.717938	0.996327	2604.08	2618.03	2635.46
	H	-1.243785	-0.318572	-0.103755			
	H	-0.042950	1.189136	0.494900			

Table 13: Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) for the optimized geometry of PH_3-C_{60}-TS obtained at B97D/aug-cc-pVTZ. The imaginary frequency is indicated with an italicized i.

Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	-0.200849	2.687651	2.305936	1030.50i	78.38	201.00
	C	1.220862	2.402232	2.304647	217.30	221.02	222.22

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Species	Atom	Coordinates			Frequencies (cm^{-1})		
		x	y	z			
	C	1.990899	2.690367	1.171267	240.53	267.53	270.75
	C	1.373394	3.281854	-0.002613	270.82	276.48	286.00
	C	-0.000000	3.550983	-0.001561	348.16	349.62	357.19
	C	-0.798944	3.248652	1.172794	362.13	369.56	372.31
	C	-0.873393	1.630587	3.041944	372.44	398.71	398.88
	C	0.137282	0.688250	3.498738	399.02	399.16	399.38
	C	1.432782	1.167896	3.039848	422.67	422.88	423.10
	C	2.402379	0.258547	2.601694	440.01	440.23	484.42
	C	2.999611	1.749936	0.722881	489.44	491.32	491.44
	C	2.003584	2.706133	-1.181868	493.30	516.56	516.62
	C	1.229082	2.419443	-2.317045	532.42	535.15	537.80
	C	-0.198825	2.699478	-2.311520	537.95	539.00	539.19
	C	-0.799866	3.254974	-1.176387	545.19	545.31	551.31
	C	-2.091857	2.768763	-0.726296	552.03	552.45	564.27
	C	-2.091245	2.767332	0.724473	564.70	564.73	565.06
	C	-2.737224	1.745174	1.424885	565.67	571.91	572.69
	C	-2.118086	1.165184	2.603124	572.76	662.41	662.73
	C	-0.137282	-0.688250	3.498738	663.74	663.82	664.23
	C	-1.432782	-1.167896	3.039848	701.06	701.72	706.91
PH_3-C_{60}-TS	C	-2.402379	-0.258547	2.601694	706.96	707.51	707.82
	C	-3.198491	-0.555969	1.424107	707.99	712.76	730.39
	C	-3.406317	0.682223	0.698718	731.02	731.08	731.81
	C	-3.408712	0.681055	-0.698683	732.05	744.50	744.98
	C	-2.736641	1.743248	-1.422979	745.03	745.22	746.60
	C	-2.114763	1.161767	-2.596573	750.63	750.79	751.62
	C	-0.868824	1.628033	-3.028408	759.21	762.28	762.52
	C	3.010258	1.756927	-0.730064	763.27	763.49	764.82
	C	0.868824	-1.628033	-3.028408	764.95	765.24	768.52
	C	2.114763	-1.161767	-2.596573	775.92	776.02	778.76
	C	2.736641	-1.743248	-1.422979	788.00	788.06	788.09
	C	2.091857	-2.768763	-0.726296	823.48	823.67	823.97
	C	0.799866	-3.254974	-1.176387	946.72	951.03	952.38
	C	-1.229082	-2.419443	-2.317045	953.24	953.30	955.19
	C	-1.435322	-1.171608	-3.037446	955.50	955.62	991.47
	C	-0.138706	-0.686125	-3.476030	994.48	1067.16	1067.72
	C	0.138706	0.686125	-3.476030	1068.07	1070.98	1090.19
	C	1.435322	1.171608	-3.037446	1090.88	1090.91	1091.29
	C	2.404539	0.261217	-2.600643	1091.39	1169.12	1169.38
	C	3.408712	-0.681055	-0.698683	1173.39	1175.51	1177.57
	C	3.406317	-0.682223	0.698718	1177.70	1196.20	1198.20
	C	2.737224	-1.745174	1.424885	1198.28	1201.14	1201.26
	C	2.091245	-2.767332	0.724473	1226.53	1226.64	1227.50
	C	0.798944	-3.248652	1.172794	1229.50	1229.52	1258.63
	C	0.000000	-3.550983	-0.001561	1258.92	1259.82	1285.17
	C	-1.373394	-3.281854	-0.002613	1286.20	1286.25	1287.02
	C	-2.003584	-2.706133	-1.181868	1292.85	1292.93	1293.21
	C	-2.404539	-0.261217	-2.600643	1294.10	1313.53	1315.69
	C	-3.206021	-0.558677	-1.426902	1315.70	1321.65	1321.94
	C	-3.010258	-1.756927	-0.730064	1322.76	1322.82	1322.94
	C	-2.999611	-1.749936	0.722881	1395.16	1395.16	1397.82

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Species	**Atom**	**Coordinates**			**Frequencies (cm^{-1})**		
		x	y	z			
	C	-1.990899	-2.690367	1.171267	1400.85	1401.17	1402.15
PH_3-C_{60}-TS	C	-1.220862	-2.402232	2.304647	1402.66	1402.71	1403.72
	C	0.200849	-2.687651	2.305936	1408.59	1409.04	1417.48
	C	0.873393	-1.630587	3.041944	1451.11	1471.38	1471.78
	C	2.118086	-1.165184	2.603124	1471.83	1473.36	1504.98
	C	3.206021	0.558677	-1.426902	1505.00	1506.18	1533.14
	C	3.198491	0.555969	1.424107	1533.95	1534.20	1538.81
	C	0.198825	-2.699478	-2.311520	1538.81	1544.31	1547.65
	H	0.654466	0.982152	-0.679202	1548.09	1551.77	1551.82
	H	-0.000000	0.000000	1.361135	2712.14	2798.07	2802.16
	H	-0.654466	-0.982152	-0.679202			
	P	0.000000	-0.000000	-0.000212			

Table 14: Total electronic energies (in Hartree) for PH_3, OH_3^+, and their confined analogues.

Method / Basis Set	**TS (E_{TS})**	**Equilibrium (E_{eq})**	**System**
	PH_3		
B3LYP/aug-cc-pVTZ	-343.1275902	-343.1805498	PH_3
PBE1PBE/aug-cc-pVTZ	-342.9683255	-343.0201966	PH_3
M06-2X/aug-cc-pVTZ	-343.0742908	-343.1271391	PH_3
MN15/aug-cc-pVTZ	-342.9787100	-343.0282507	PH_3
B97D/aug-cc-pVTZ	-343.1115823	-343.1644499	PH_3
MP2/aug-cc-pVTZ	-342.6094529	-342.6612881	PH_3
CCSD(T)/aug-cc-pVQZ	-342.6565165	-342.7093456	PH_3
B3LYP/6-311G**	-343.1191838	-343.1728485	PH_3
PBE1PBE/6-311G**	-342.9589191	-343.0113483	PH_3
M06-2X/6-311G**	-343.0631508	-343.1162936	PH_3
MN15/6-311G**	-342.9874996	-343.0368370	PH_3
B97D/6-311G**	-343.1041727	-343.1576756	PH_3
MP2/6-311G**	-342.5559510	-342.6122934	PH_3
	OH_3^+		
B3LYP/aug-cc-pVTZ	-76.7361794	-76.7385189	OH_3^+
PBE1PBE/aug-cc-pVTZ	-76.6527759	-76.6553427	OH_3^+
M06-2X/aug-cc-pVTZ	-76.7001245	-76.7022348	OH_3^+
MN15/aug-cc-pVTZ	-76.6588163	-76.6599761	OH_3^+
B97D/aug-cc-pVTZ	-76.6986023	-76.7013961	OH_3^+
MP2/aug-cc-pVTZ	-76.5967268	-76.6002077	OH_3^+
CCSD(T)/aug-cc-pVQZ	-76.6338007	-76.6370190	OH_3^+
B3LYP/6-311G**	-76.7280682	-76.7298934	OH_3^+
PBE1PBE/6-311G**	-76.6445407	-76.6465394	OH_3^+
M06-2X/6-311G**	-76.6915271	-76.6931300	OH_3^+
MN15/6-311G**	-76.6509044	-76.6516594	OH_3^+
B97D/6-311G**	-76.6901889	-76.6923557	OH_3^+
MP2/6-311G**	-76.5453648	-76.5484709	OH_3^+
Confined Systems (B97D/aug-cc-pVTZ)			
C_{60} (optimized)	-2284.851824	–	
Pyramidal OH_3^+@C_{60} (optimized)	-2361.835650	–	
Planar OH_3^+@C_{60} (optimized)	-2361.825577	–	
Pyramidal PH_3@C_{60} (optimized)	-2628.254540	–	
Planar PH_3@C_{60} (optimized)	-2628.202573	–	
DLPNO-CCSD(T)/def2-TZVP Energies			
OH_3^+@C_{60}	$E_{\text{complex}} = -2358.59220$	$E_{C_{60}} = -2281.94043$	$E_{OH_3^+} = -76.60273$
PH_3@C_{60}	$E_{\text{complex}} = -2624.63953$	$E_{C_{60}} = -2281.94009$	$E_{PH_3} = -342.67815$