

Table 1 Calculated normal mode wavenumbers (in cm^{-1}) for C60, isolated LDOPAc (I), and the A, B, C, D adsorption geometries of LDOPAc on C60.

C60	I	A	B	C	D	C60	I	A	B	C	D
		1.0027	3.6697	1.4578	3.5285	438.8003		441.8284	442.282	441.4935	441.7234
		4.8873	7.8372	5.2687	6.2182	438.8004		442.1686	442.4141	442.0369	442.3489
	16.9107	12.0794	12.5303	9.6473	10.9723	438.8005		442.7335	442.9992	442.6216	442.9286
	20.4722	12.8793	12.9715	11.3178	14.2854		444.0977	451.6592	456.5358	457.3361	458.5686
		21.4988	17.7851	20.3369	20.7169		451.4645	459.0164	467.5748	469.8275	469.8275
		24.079	30.4802	24.7349	24.0658		467.8030	479.6696	486.3493	477.4466	486.3794
		37.8164	37.619	34.6217	35.4162			486.4424	490.5914	486.3398	491.8067
		44.3492	54.5677	50.4915	55.9209			492.1475	492.3432	491.5099	492.0522
	64.7697	65.6756	69.4824	64.179	70.1595			492.7759	492.6645	492.0792	492.2179
	85.4656	78.3041	101.1702	94.4499	105.0993			492.9834	493.1676	492.6108	494.1733
		163.3653	162.6624	183.8272	177.5474			493.5913	493.297	493.9331	498.4019
		174.3628	177.2873	187.0496	193.068			512.1211	520.6558	518.2305	521.1753
	232.1961	231.7172	244.6293	235.1209	242.8444			541.791	542.3059	540.9017	541.5498
		249.3333	266.4134	252.2075	267.6385			542.503	542.6313	541.9321	542.2894
		267.7616	267.6465	267.5848	267.5802			543.3096	543.2489	542.3312	542.8525
		268.1284	267.8779	267.6829	268.2193			543.4842	543.6171	543.4436	543.5235
		268.2506	268.1777	267.9431	268.3953			543.9566	544.187	543.8297	544.0013
		268.3916	268.2823	268.2589	268.6875			544.7263	544.5965	544.4814	544.4096
	274.7160	268.7416	268.8384	269.1369	280.8318			545.0869	545.0374	544.7642	544.6623
		292.9431	292.8768	286.3771	295.1134			545.6093	546.3566	545.9781	545.4871
		305.8217	304.9141	301.7254	304.8218		548.9811	546.8416	548.6514	549.5423	554.6315
	340.5463	340.8266	328.1804	321.6668	348.5012			570.289	570.6316	570.7885	570.815
343.7034		348.2594	348.0879	347.8502	348.9396			570.8954	570.795	570.8279	570.9823
343.7035		348.9365	348.8488	348.6574	349.3518			570.9636	571.1733	571.241	571.2186
343.7036		349.3163	349.6344	349.4645	352.9168			574.4962	574.3385	574.2595	574.2893
359.4862		360.1436	359.7626	358.5529	359.5375			574.5817	574.6799	574.5163	574.4235
359.4863		360.5787	360.861	359.456	360.1911			574.8235	574.8222	574.7359	574.9186
359.4867		361.1418	361.0215	360.7034	360.5778			577.7715	578.5844	577.4521	578.4434
		361.1888	361.6997	360.9345	360.9294			579.1167	579.0606	578.2998	578.8702
	360.9987	361.7295	367.5497	362.1198	362.1754			579.6678	579.4537	579.7115	579.2605
		378.4947	384.6674	380.617	411.0764			582.9713	579.8575	583.2235	580.0232
408.6332		410.9986	410.9978	397.1177	411.3662			583.274	582.8699	583.256	583.1745
408.6333		411.1072	411.0722	411.285	411.5075			583.3071	583.208	583.4431	583.2125
408.6334		411.2174	411.3353	411.4469	411.6069			583.5038	583.3163	583.6643	583.6677
408.6336		411.3667	411.5018	411.5071	411.7259			586.1523	583.6423	584.0986	583.8106
408.6339		411.5787	411.5777	411.5879	421.6018		585.6324	622.409	603.5079	598.8848	598.0908
		417.1087	440.576	411.7002	439.7505		625.1851	674.2562	656.5211	655.8082	662.4228
438.8		440.8682	441.5023	439.9274	440.8375			677.4897	677.67	677.2978	677.7397
438.8001		441.3724	441.8677	441.3431	441.4775			677.9287	677.8244	678.0257	677.9258
438.8003		441.8284	442.282	441.4935	441.7234			677.9917	678.022	678.3258	678.0671

Table 2 Calculated normal mode wavenumbers (in cm^{-1}) for C60, isolated LDOPAc (I), and the A, B, C, D adsorption geometries of LDOPAc on C60.

C60	I	A	B	C	D	C60	I	A	B	C	D
679.8754	676.1770	678.2636	678.1949	678.6038	678.3103	805.2174	808.2043	808.2039	808.4228	808.6771	808.6771
	707.3510	678.3575	678.2631	678.7589	678.7068	805.2177	808.6788	808.406	808.7051	808.8103	808.8103
		709.3435	716.4505	710.199	713.8431		818.0997	808.5512	809.0547	823.9648	823.9648
		716.744	717.6598	716.8548	716.4187	814.66	823.4462	823.9218	819.9511	824.3465	824.3465
721.0946		717.6522	718.5033	717.7508	716.9791	840.7505	823.6044	824.164	823.4631	824.4301	824.4301
721.0947		718.7584	719.0792	718.6101	717.9832	840.7508	824.1359	824.2434	824.1006	824.4959	824.4959
721.0948		719.0509	719.4086	719.6379	718.6538	840.7511	842.2088	856.78	824.4166	856.728	856.728
721.095		719.5371	719.7116	719.9572	719.3012		873.8337	897.5765	904.929	874.9041	874.9041
721.095		722.0035	721.6599	721.7757	721.1819		912.4022	912.4022	912.5989	913.295	913.295
724.708		723.8063	723.2015	721.8288	723.2277		928.2552	933.0214	944.565	921.9112	921.9112
724.7081		723.785	723.752	723.5605	723.4148		956.8207	940.4557	962.2057	942.2686	942.2686
724.7081		724.281	724.895	724.0494	729.948		967.0287	967.1075	967.1127	967.0336	967.0336
738.7585		734.1121	735.1402	736.3578	733.5391	966.2475	967.1305	967.1075	967.2734	967.1302	967.1302
738.7587		737.9935	735.1739	737.1649	735.7458	977.9638	967.2763	967.4332	967.5645	967.587	967.587
738.7588		738.496	736.3064	738.2125	736.7303	977.9640	967.3394	967.7666	967.7108	967.7063	967.7063
744.1928		738.7037	737.0141	738.4487	736.9762	977.9642	967.4528	968.0135	967.744	968.1043	968.1043
744.193		739.5183	737.9076	739.5331	737.614	983.2239	967.9151	968.1876	968.2224	968.3174	968.3174
744.1933		739.839	738.0928	739.7578	738.0118	983.2240	968.1078	968.3886	968.3919	968.7615	968.7615
744.1936		740.4162	738.9182	740.0393	738.2811	983.2243	968.3518	988.4353	977.935	998.299	998.299
744.1937		740.6513	739.4104	740.4508	739.0488	983.2244	981.9853	1024.974	1004.835	1005.531	1005.531
753.2669		741.4756	742.2198	741.55	740.7089	1094.8665	1053.636	1047.257	1051.475	1045.377	1045.377
753.2669		741.5623	742.0085	740.5295	740.9044	1094.8666	1095.272	1095.527	1095.362	1095.514	1095.514
753.2671		742.8477	742.2198	742.0085	741.9675	1094.8667	1095.506	1095.756	1095.744	1095.664	1095.664
757.1575		742.4629	741.4222	742.2176	741.9675	1094.8668	1095.569	1095.962	1096.014	1096.195	1096.195
757.1575		743.0971	742.6912	743.4833	742.5569		1098.892	1099.538	1099.558	1099.768	1099.768
757.1576	743.9756	743.5612	748.4798	744.0751	744.6465		1098.892	1099.538	1099.558	1099.768	1099.768
757.1577		744.2414	749.2393	751.3266	747.1019		1099.576	1099.754	1099.7	1100.085	1100.085
757.1575		744.5612	748.4798	744.0751	744.6465		1099.505	1099.754	1099.7	1100.056	1100.056
757.1575		746.7031	761.3892	761.419	767.1734		1099.636	1100.454	1100.489	1100.596	1100.596
757.1576		767.5211	767.6953	768.0593	768.0604		1100.138	1100.701	1100.878	1101.01	1101.01
767.1193		767.6648	768.0313	768.2394	768.1414		1100.468	1100.784	1104.009	1104.142	1104.142
767.1194	766.4463	768.0841	768.038	768.3133	768.2182	1127.2449	1125.765	1134.705	1121.011	1142.933	1142.933
767.1196		768.4029	768.1312	768.6182	768.4215	1127.2452	1157.599	1176.119	1169.074	1161.329	1161.329
788.1376		773.1576	773.2534	773.3266	772.9919	1127.2460	1172.59	1183.495	1181.835	1176.906	1176.906
788.1378		773.2874	773.3695	773.3695	773.1421	1127.2467	1180.378	1190.973	1188.094	1192.111	1192.111
788.1381		773.589	773.6642	773.5079	773.3474	1127.2471	1192.01	1192.354	1192.141	1192.546	1192.546
788.1383		773.7738	773.6881	773.6335	773.9946		1192.329	1192.692	1192.712	1192.876	1192.876
788.1384		773.8555	773.8553	773.9913	774.4689		1192.628	1192.793	1193.18	1193.1	1193.1
	784.9099	784.9471	785.0784	783.4884	778.6416	1201.3567	1202.827	1202.71	1202.77	1202.845	1202.845
805.2172		808.0931	802.1282	803.3857	808.4234	1201.3569	1203.053	1203.361	1203.37	1203.37	1203.37

Table 3 Calculated normal mode wavenumbers (in cm^{-1}) for C60, isolated LDOPAc (I), and the A, B, C, D adsorption geometries of LDOPAc on C60.

C60	I	A	B	C	D	C60	I	A	B	C	D
1201.358		1203.71	1203.514	1203.832	1204.112	1372.232	1434.8401	1420.448	1434.718	1421.19	1462.384
		1206.828	1207.7	1207.37	1204.653	1454.832		1464.171	1466.242	1464.572	1465.114
		1207.868	1208.268	1208.668	1207.902	1454.832		1466.359	1466.677	1467.122	1466.607
		1208.105	1208.825	1208.779	1208.63	1454.832		1466.974	1467.081	1467.185	1466.874
		1208.39	1209.482	1209.923	1208.898	1454.832		1467.209	1467.088	1467.401	1467.278
		1208.767	1209.776	1209.213	1209.758	1454.832		1467.404	1467.307	1467.677	1467.477
1214.643	1208.7662	1212.007	1212.007	1209.499	1210.051	1460.389		1467.555	1467.427	1467.789	1467.783
1214.643	1218.1778	1217.511	1217.511	1215.519	1214.126	1460.389		1467.687	1467.667	1467.972	1467.972
1214.644	1255.3085	1220.87	1228.026	1224.652	1241.399	1460.389		1467.931	1467.703	1468.314	1468.271
1245.416		1260.723	1262.181	1261.417	1261.612	1464.222		1468.256	1468.133	1468.369	1468.914
1245.416		1261.409	1262.464	1261.688	1262.206	1464.222		1482.678	1482.696	1482.361	1481.423
1245.416		1262.557	1262.946	1263.138	1263.769	1464.223		1484.484	1484.171	1484.822	1483.884
1245.416		1272.538	1272.17	1270.816	1272.855	1464.223		1484.697	1484.774	1485.533	1486.97
1245.417		1272.705	1272.77	1273.058	1273.29	1503.413	1498.2918	1498.895	1505.535	1496.648	1500.219
1276.967		1273.033	1273.384	1273.632	1273.653		1518.1120	1519.904	1508.794	1510.278	1516.543
1276.967		1273.547	1273.535	1273.853	1274.323			1528.832	1529.467	1529.602	1529.535
1276.967		1273.669	1273.815	1274.183	1275.416	1537.995		1530.933	1531.357	1531.207	1531.007
1276.968	1274.0191	1274.304	1274.333	1274.849	1275.711	1537.996		1531.409	1531.506	1531.648	1531.821
1276.968	1286.7517	1282.957	1303.862	1300.613	1303.882	1537.996		1531.932	1531.872	1532.011	1532.226
1302.816		1303.152	1304.162	1303.465	1304.253	1537.996		1532.323	1532.084	1532.397	1532.377
1302.817		1303.437	1304.487	1304.161	1305.048		1544.3372	1543.753	1544.659	1543.92	1545.543
1302.817		1304.019	1304.643	1304.655	1305.245	1566.623		1557.779	1558.223	1558.307	1557.883
		1304.273	1304.93	1304.904	1305.399	1566.623		1558.528	1558.441	1558.538	1558.761
	1305.5465	1304.882	1320.423	1319.871	1311.729	1566.623		1558.922	1558.825	1559.099	1559.142
1334.492		1329.412	1329.996	1329.842	1330.406	1608.096		1600.952	1601.727	1601.409	1601.258
1334.492		1330.112	1330.489	1330.52	1330.519	1608.096		1602.227	1602.18	1601.706	1601.933
1334.493		1330.622	1330.653	1330.914	1330.982	1608.096		1602.464	1602.592	1603.02	1602.697
1334.494		1331.332	1331.114	1331.721	1331.692	1608.096		1602.642	1602.76	1603.191	1602.991
1335.3		1343.383	1344.596	1343.738	1344.185	1608.097		1603.062	1603.04	1603.233	1603.649
1335.301		1343.575	1344.837	1344.484	1344.531	1617.343		1609.216	1609.624	1609.73	1609.443
1335.301		1344.37	1345.052	1345.168	1345.923	1617.343		1609.981	1609.941	1609.922	1609.821
1335.302		1344.637	1345.74	1345.792	1346.032	1617.343		1610.222	1610.057	1610.477	1610.247
		1345.158	1346.122	1346.443	1346.707	1617.343		1610.499	1610.199	1610.863	1610.655
1371.054	1343.4133	1345.864	1356.244	1352.73	1349.872	1617.343		1610.799	1610.958	1610.991	1611.298
1371.054		1356.457	1361.786	1361.916	1361.665		1643.6669	1644.238	1649.698	1644.013	1648.09
1371.055		1361.507	1362.721	1362.335	1362.424	1659.5986		1660.279	1661.73	1660.007	1656.082
1371.055		1362.033	1363.214	1363.469	1362.916	1669.9486		1670.591	1671.811	1669.86	1669.338
1371.055	1360.6090	1363.549	1365.644	1364.104	1363.511	1693.1233		1692.343	1692.204	1684.719	1687.118
1372.232	1385.7158	1383.653	1383.907	1389.019	1387.445	1719.6897		1713.332	1710.584	1710.304	1693.05
1372.232	1416.8690	1413.571	1410.438	1405.079	1405.623	2957.9094		2776.556	2934.998	2690.331	2978.485

Table 4 Calculated normal mode wavenumbers (in cm^{-1}) for C60, isolated LDOPAc (I), and the A, B, C, D adsorption geometries of LDOPAc on C60.

C60	I	A	B	C	D
3073.3663	3069.949	3041.958	3042.715	3066.595	
3132.3986	3130.928	3098.437	3098.022	3120.262	
3149.0499	3146	3126.6	3124.527	3129.83	
3185.4488	3182.902	3188.898	3180.935	3195.169	
3207.0810	3204.918	3210.75	3204.802	3205.184	
3218.3035	3217.797	3214.076	3207.011	3209.263	
3231.1384	3359.522	3226.892	3375.53	3229.555	
3300.7728	3437.278	3305.611	3468.227	3297.559	
3663.2523	3663.722	3663.74	3665.342	3663.569	
3740.1307	3740.524	3740.659	3740.809	3740.379	