

Supporting information for
“Theoretical study of intermolecular interaction in
meso-tetraphenylporphyrin diacid dimer (H₄TPPCL₂)₂”

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Table S1. Calculated vibrational frequencies (cm^{-1}) and infrared intensities (km/mol) of H_4TPPCl_2 monomer, and **D1**, **D2** and **D6** dimers at PBE1PBE/3-21G* level.

Monomer			D1		D2		D6	
NO.	Freq.	Int.	Freq.	Int.	Freq.	Int.	Freq.	Int.
1	13.5562	0.0000	0.8450	0.0065	9.2236	0.0199	17.9528	0.0015
2	25.5731	2.0373	10.3601	0.0000	12.5637	0.0000	32.1485	2.1106
3	35.6923	0.3733	10.4234	0.0582	13.4829	0.3027	42.7871	0.0326
4	35.6923	0.3733	12.5654	0.5977	19.0481	0.0454	44.1965	0.1630
5	36.2706	0.0000	16.8306	0.0000	23.6848	0.0468	46.3812	0.2651
6	44.1864	1.2400	26.4396	0.0000	30.5278	0.0061	48.4896	0.6021
7	53.8633	0.2334	28.5929	0.0000	32.3535	0.9615	50.2250	0.2950
8	53.8633	0.2334	32.5966	0.0247	33.8079	1.8768	54.9505	0.2205
9	55.5165	0.4567	34.1010	2.7879	35.9021	0.0850	58.7200	0.5777
10	55.5165	0.4567	36.2333	0.0000	37.7130	0.4248	66.5829	0.1978
11	57.8954	0.0000	39.8446	0.0000	40.5647	0.2426	67.2536	0.4939
12	77.5761	1.5204	41.9870	0.0862	43.2735	0.1818	76.5696	1.4056
13	77.5761	1.5204	42.9076	3.8543	43.5289	0.6330	80.6745	0.5696
14	78.2942	0.0000	46.3230	0.0000	45.5427	0.6632	80.7868	1.7480
15	84.9679	0.0000	46.5933	0.1799	46.7159	1.0083	88.6996	1.3184
16	101.1351	0.0000	47.5565	0.0000	49.1617	0.7856	98.8490	4.9018
17	105.1275	9.0519	48.7430	0.0000	50.7559	0.1546	103.7128	0.5242
18	110.7404	0.0000	53.3854	0.6788	56.0683	0.2155	105.9327	2.0551
19	128.2583	4.9925	54.3758	0.6267	58.0551	0.2532	109.9216	4.5220
20	128.2583	4.9925	56.2059	0.7710	58.1182	0.0120	119.8001	0.2488
21	146.0754	0.0000	58.1854	0.0000	58.7788	0.1374	129.3546	4.8662
22	160.5277	0.7779	58.6427	0.0000	60.6402	0.0975	129.5947	0.1671
23	160.5278	0.7779	62.5972	0.0213	62.4775	0.2192	143.2886	1.2695
24	198.2409	2.2256	63.5875	0.0000	66.0673	0.1391	151.7941	0.5440
25	202.2045	19.3737	69.7325	0.0000	71.3604	0.0557	157.2345	3.6323
26	203.7723	0.0000	73.6013	0.1116	72.3570	1.1206	174.1280	12.5139
27	218.4022	4.9089	75.1498	2.1700	73.8283	1.1208	191.3160	5.8640
28	218.4022	4.9088	78.1692	0.0000	78.2411	0.2879	196.4527	7.7051
29	228.5773	0.8010	83.5802	0.0000	79.2408	0.2664	206.8101	0.2296
30	228.5773	0.8010	85.5353	0.0000	81.3569	0.2079	216.7777	3.3521
31	232.1633	22.0344	86.1095	0.0180	86.1593	0.1211	219.7062	1.6459
32	257.8080	0.0713	86.3759	2.1893	87.1404	4.4230	225.1570	6.6404
33	257.8080	0.0713	90.6068	0.0252	89.6727	0.5545	230.1703	8.7581
34	257.9795	0.0000	91.7520	0.0000	90.3477	0.9844	241.3739	8.7655
35	268.5845	1.8727	95.0952	0.0000	90.6114	0.0019	256.6454	0.0300
36	281.7340	0.0000	100.6462	6.4463	103.0520	0.0962	258.1496	0.4629
37	320.3633	0.0000	102.9115	0.0000	104.1870	0.1626	267.0294	9.1369

38	330.4587	1.6003	103.0256	0.0337	107.3411	0.7994	277.6631	5.4629
39	330.4587	1.6003	105.2308	0.0000	109.5397	0.2142	280.2625	1.2912
40	344.2574	0.0000	111.1919	22.3091	110.6130	19.0931	311.2650	64.2133
41	354.0207	0.0000	113.7719	0.0496	116.8244	1.3935	317.0747	0.5120
42	389.3803	0.0000	120.3629	0.0000	124.3822	0.3323	326.0553	1.0386
43	393.5198	2.9169	123.2935	10.2813	128.3002	7.2787	332.6794	0.0175
44	393.5198	2.9169	128.0302	0.0000	128.5153	1.4735	346.4166	2.0861
45	421.7508	0.9332	129.7785	0.0000	130.6179	6.0761	353.2259	1.3137
46	421.7508	0.9332	131.0785	7.3926	134.6939	2.8343	389.4403	3.2024
47	429.6137	0.0000	148.6368	0.0000	147.2343	0.9785	391.9802	0.6989
48	429.7406	0.0000	150.6318	3.6586	155.7852	4.3509	393.4031	45.8704
49	429.9137	1.2788	160.7997	0.0000	161.5320	0.4242	398.4157	68.6812
50	429.9137	1.2788	162.3763	0.0000	164.0665	0.6947	419.7059	0.2958
51	441.4542	0.0000	163.1129	1.4192	166.3991	2.1197	420.3218	0.4260
52	447.0158	0.0000	164.8177	0.3063	173.1626	0.7972	430.8611	0.5778
53	486.2125	19.3249	195.3157	0.0000	195.3460	12.9676	431.0183	0.4575
54	502.3877	16.2958	196.0983	40.2662	199.2010	23.6763	435.3103	3.6770
55	502.3877	16.2958	201.4916	0.0000	201.8153	12.4755	437.9038	2.0497
56	522.5658	0.0000	202.2065	17.4168	204.2978	0.1009	441.4104	0.1413
57	583.9807	1.7151	205.0787	4.6254	205.7751	0.1099	447.2480	0.3885
58	585.8654	0.4251	205.4031	0.0000	207.4963	0.8929	491.8011	14.3050
59	585.8654	0.4251	215.4327	9.0420	213.7023	3.9358	507.9437	11.2104
60	595.8535	0.0000	216.2403	0.0000	216.2708	3.0896	516.8101	19.8456
61	656.6513	0.0000	220.3598	8.3267	217.9250	11.8443	532.6476	0.0587
62	656.8073	0.1392	221.0745	0.0000	224.2730	8.3185	581.7370	1.0752
63	656.8073	0.1392	227.4719	0.6306	227.4456	1.6810	583.9053	4.4643
64	657.4867	0.1396	227.5904	0.0000	230.2040	0.5434	586.8020	1.9848
65	665.0315	0.0000	229.4800	0.0000	231.8405	0.2903	594.3178	0.6094
66	678.8125	5.9540	229.9951	18.9620	231.9148	29.0600	655.8909	0.0802
67	678.8125	5.9540	234.4449	0.0000	233.2195	14.5145	657.0965	0.1007
68	685.8211	0.0000	234.5746	30.0102	241.4362	1.5713	658.1455	0.0526
69	709.0407	0.0000	258.4080	0.0000	258.9917	2.0924	658.5949	0.1261
70	710.8439	18.4838	258.5152	1.2901	259.7584	0.0884	666.7390	0.3266
71	710.8439	18.4839	259.2154	0.0007	259.9848	0.5028	674.8827	50.4682
72	718.5289	0.0000	259.2686	0.0000	261.9629	2.3706	679.1797	15.5434
73	732.4487	0.0000	260.7370	0.0000	263.6453	0.0626	679.6294	5.3812
74	733.1471	30.1481	261.6482	3.7598	264.8384	2.1968	685.9915	0.1746
75	733.1471	30.1481	270.6057	0.0000	270.1633	1.5340	705.2984	4.9069
76	733.8182	179.8118	270.7726	2.9307	276.1078	0.2634	708.1912	15.8561
77	745.4291	0.0696	283.6156	0.0001	283.5445	0.1147	711.2574	13.0330
78	745.4292	0.0696	283.6409	0.0000	284.9438	0.0471	719.1092	0.3385
79	746.2012	44.9272	320.5783	0.2582	322.4616	0.0591	735.6075	13.1602
80	746.9013	0.0000	321.7532	0.0000	323.0879	0.0001	736.1597	100.4946
81	785.1176	26.6332	328.7841	0.0000	330.9871	1.8139	739.6789	3.9135

82	790.0123	26.8172	328.9684	2.7998	331.5032	1.4483	743.7550	4.5415
83	790.0123	26.8172	332.3148	0.0000	332.9535	1.0736	744.7502	62.9048
84	794.5482	0.0000	332.9927	3.8419	333.1858	1.8181	747.3141	6.5053
85	847.2096	4.0060	344.2877	0.0015	343.8168	0.0127	752.7686	72.7842
86	847.2096	4.0060	344.3163	0.0000	345.1213	0.0146	753.9769	7.0301
87	847.4880	0.0000	353.6187	0.0000	355.0952	0.9212	786.1062	28.7519
88	848.0213	90.3377	353.9226	0.1641	357.0174	0.1979	790.6497	18.0455
89	858.9782	0.5124	391.1104	0.0000	390.2220	0.0041	791.7898	56.4843
90	858.9782	0.5124	391.2434	0.0065	391.1212	0.0347	796.1061	1.0381
91	868.8420	0.0000	394.6131	5.0192	394.4457	2.2208	834.8817	0.8215
92	869.1447	34.5203	394.6337	4.9332	395.0346	2.0551	839.5524	17.5727
93	878.8556	0.0000	394.6351	0.0000	395.3079	1.0424	850.9278	7.9929
94	880.3533	8.5469	394.7401	0.0000	397.2000	3.5651	851.7337	21.8784
95	880.3533	8.5469	423.4079	1.4883	423.0517	1.5620	854.5273	8.0367
96	882.3344	0.0000	423.4215	0.0000	423.4079	0.2871	863.8209	2.1242
97	911.6643	3.7111	423.7589	2.6295	425.6086	3.0336	865.9702	74.2024
98	911.6643	3.7111	423.8146	0.0000	425.8007	1.8630	869.3384	0.0779
99	915.8799	0.0000	430.4316	0.0000	429.9624	0.7360	883.6107	2.5715
100	917.8860	0.0000	430.4832	0.4033	430.0087	0.2144	884.9997	4.8653
101	959.7593	5.0386	430.6152	0.8113	430.7507	0.1100	908.0546	3.8114
102	959.7593	5.0385	430.6162	0.0000	431.1270	0.2913	908.3635	1.3159
103	963.8206	0.0000	435.1392	0.0000	432.4829	0.0407	912.0488	3.5635
104	964.8173	32.4651	436.0411	3.1336	432.6971	0.6022	913.3588	3.8585
105	970.4515	9.5035	436.3944	1.5169	436.2124	1.5059	916.9824	1.8024
106	970.4515	9.5035	436.4718	0.0000	436.8981	0.6856	918.2159	0.0111
107	974.0553	0.0000	443.6578	0.2471	442.7648	0.1402	929.4558	15.0800
108	975.0736	0.0000	443.9225	0.0000	444.0305	0.3178	950.3479	217.6395
109	981.2222	9.6516	448.7899	0.0000	448.4582	0.0029	963.7381	1.2713
110	981.2222	9.6516	448.8901	0.1533	453.0565	0.2362	967.0413	0.0158
111	982.4092	0.0000	486.9399	0.0000	480.1467	14.9790	969.1281	2.6443
112	999.6642	251.0061	487.1174	42.2834	488.3063	21.8654	971.5629	3.7201
113	1019.5324	0.0000	502.9365	0.0000	492.4186	5.0164	978.3691	0.2427
114	1019.5947	7.7869	502.9534	16.1188	496.5491	17.9996	978.4139	2.7546
115	1019.5947	7.7869	503.1129	0.0000	504.8151	15.8015	983.8135	17.6482
116	1020.0865	0.0000	503.7846	29.7824	504.9872	16.1042	988.9558	51.8824
117	1020.9433	0.0032	522.4217	1.3244	514.2986	1.6736	994.9965	14.1815
118	1020.9433	0.0032	523.3672	0.0000	524.7193	0.1168	995.7243	1.7879
119	1021.4500	0.0000	582.3878	0.0000	582.9642	4.1775	1012.5633	22.2716
120	1024.2153	1.1078	582.7374	2.1983	583.1429	0.2133	1020.4443	0.2243
121	1027.2788	7.6964	585.5569	0.3089	585.7915	0.5499	1022.5295	3.1451
122	1027.2788	7.6964	586.0595	0.0000	588.1405	1.3239	1022.7040	3.0375
123	1033.5225	0.0000	587.7755	1.5430	588.2922	0.1018	1024.8229	1.2606
124	1046.1825	0.0000	588.9556	0.0000	589.4613	0.4035	1027.2929	5.4311
125	1048.2971	0.0000	596.4531	0.0000	596.9250	0.0058	1028.3442	6.9932

126	1048.4363	0.0476	597.8245	0.0345	602.5671	0.1285	1028.4159	8.5495
127	1048.4363	0.0476	655.7954	0.0426	654.5903	0.0064	1033.9784	0.8036
128	1048.6362	0.0632	655.8128	0.0000	655.1966	0.4771	1042.6658	1.8656
129	1049.4293	15.9840	656.3052	0.0000	656.8371	0.0648	1042.7356	1.6759
130	1049.4293	15.9839	656.5521	0.8389	657.0310	1.0360	1044.0786	3.0622
131	1057.2933	0.0000	656.8186	0.0000	657.2967	0.2252	1047.9578	12.0819
132	1068.7265	0.0000	656.8213	0.1601	657.8426	0.8029	1048.7070	15.6266
133	1069.0767	16.3500	657.2486	0.0000	658.0846	0.0570	1050.1404	0.0123
134	1069.0767	16.3500	657.3932	0.8289	658.4859	0.2506	1050.3407	0.1885
135	1070.3602	0.0000	664.9967	0.0000	664.3098	0.0215	1057.3834	0.2446
136	1122.0237	0.0000	665.3035	0.0236	665.7311	0.1097	1071.0299	6.1153
137	1123.8681	5.0899	677.4117	0.0000	674.8434	1.9991	1071.6506	12.1603
138	1123.8681	5.0899	677.4888	6.1731	676.4313	7.4275	1073.6269	7.2249
139	1124.4856	0.3629	678.2102	0.0000	679.3623	3.6046	1074.8976	4.9271
140	1124.7833	0.0000	678.7327	13.6081	679.9320	8.4733	1117.2359	4.9042
141	1126.8520	2.3763	685.3064	0.7093	682.7427	0.9261	1124.9585	3.9740
142	1126.8520	2.3763	685.5347	0.0000	686.5614	0.0431	1125.1615	5.1054
143	1132.0542	21.1290	707.5307	0.0000	709.3963	5.7706	1125.9101	0.2954
144	1143.8812	0.0000	708.0489	1.5062	710.3800	3.9959	1126.9767	0.1270
145	1220.5446	0.0000	709.8932	35.9903	710.4117	9.7887	1129.9998	5.4636
146	1233.2116	0.0000	710.0796	0.0000	712.3679	21.4654	1131.4365	3.8881
147	1233.2141	0.0704	710.6171	36.9460	713.5014	14.1157	1133.9447	10.9936
148	1233.2141	0.0704	711.0205	0.0000	713.6491	23.5110	1137.9894	2.6759
149	1233.3378	0.0211	718.7553	0.0000	718.9835	0.2774	1145.6001	2.7145
150	1242.6655	0.0000	718.9600	0.7745	721.1165	0.1708	1148.4493	5.1341
151	1242.6699	26.2349	734.6832	16.1810	733.9860	17.8556	1222.3470	0.0940
152	1242.6699	26.2349	734.7353	0.0000	734.3435	5.8792	1233.1819	3.2527
153	1243.3541	0.0000	735.3969	0.0000	734.9188	120.7710	1233.2247	3.0103
154	1258.8613	25.9062	735.4874	257.5297	735.0406	58.1550	1234.5086	0.1156
155	1258.8613	25.9062	739.2840	0.0000	737.1438	28.1230	1234.5633	0.0231
156	1273.0710	0.0000	740.5474	289.4882	738.2444	51.0069	1243.1858	13.5694
157	1273.1504	68.7457	741.5797	4.1636	738.8149	4.7068	1243.4264	11.5094
158	1273.1504	68.7458	741.9238	0.0000	740.3043	35.1523	1256.1663	16.1904
159	1281.3121	0.0000	743.1930	0.0000	741.6853	199.9371	1258.5900	8.5435
160	1301.3663	0.0000	743.4729	15.6681	742.8188	2.9925	1261.6871	10.6482
161	1327.7338	3.6203	744.0151	0.0000	743.0961	0.0724	1262.9509	22.0347
162	1330.1015	1.5128	744.2536	2.7519	744.2536	1.6491	1273.0259	24.9768
163	1330.1015	1.5128	744.3892	13.1981	745.1904	0.1361	1274.7455	55.1886
164	1342.4285	0.0000	744.6688	0.0000	745.8304	26.3033	1276.4518	45.2895
165	1345.2437	0.0081	745.6549	0.6146	747.3266	0.0095	1283.9623	1.8777
166	1345.2437	0.0081	745.7796	0.0000	755.1643	36.3506	1302.2550	0.7472
167	1350.5635	0.1055	786.0058	0.0000	786.4044	23.0275	1328.0612	5.5164
168	1366.5061	0.2358	786.8343	52.3013	787.8927	52.1951	1328.8089	1.5159
169	1366.5061	0.2358	790.6994	30.0291	790.9144	24.0099	1334.3876	1.2343

170	1379.5880	0.0000	791.7426	60.8973	791.8312	17.6916	1341.3063	1.8077
171	1385.4391	0.0000	791.8090	0.0000	792.9463	16.3416	1345.5841	0.2220
172	1388.7933	0.0000	791.8165	0.0000	794.0034	42.0623	1348.9107	5.0939
173	1389.2848	3.6969	796.0433	0.5351	795.9480	4.2092	1350.8432	4.9833
174	1389.3652	6.3132	796.0915	0.0000	796.6849	5.2191	1368.6492	2.9758
175	1389.3652	6.3132	840.6048	0.0000	841.6916	19.7871	1372.0272	3.4358
176	1393.2507	0.0000	840.9497	40.1386	845.0485	29.3166	1383.7491	1.3837
177	1430.5998	0.0000	843.0039	17.8908	845.4012	0.5129	1389.7507	1.9370
178	1431.6190	1.0199	843.3795	82.5719	846.2634	29.6760	1389.9223	1.9289
179	1431.6190	1.0199	843.4462	0.0000	848.0480	25.8145	1389.9995	5.5066
180	1462.2209	0.0000	843.5494	0.0000	850.9724	11.1769	1396.8875	1.0172
181	1487.0567	0.0000	843.7675	0.0000	851.9452	51.2812	1420.4751	0.2880
182	1501.5366	16.4067	844.7315	49.5447	859.9892	0.0097	1420.7486	5.8689
183	1501.5366	16.4067	859.5837	1.0086	860.1140	0.0118	1427.0477	1.0107
184	1502.1397	18.8020	860.4140	0.0000	862.7656	0.1310	1432.6757	0.0837
185	1505.1402	0.0000	861.2234	0.0000	864.3403	4.5155	1437.0113	0.8203
186	1524.6965	0.1490	861.2494	16.5631	867.1081	86.2073	1462.5303	0.0110
187	1527.6473	7.6023	867.2150	130.9092	868.7650	0.3617	1488.0922	0.3717
188	1527.6473	7.6023	868.7956	0.0000	869.4177	0.0026	1502.1321	12.5206
189	1544.9703	61.5710	869.6934	0.0000	870.4201	25.9634	1502.2418	15.6130
190	1544.9703	61.5710	870.2076	0.0323	881.2684	3.3869	1503.5220	18.8436
191	1545.3698	0.0000	881.8081	5.4853	881.7572	2.4686	1505.5703	1.1515
192	1545.5245	0.0000	881.8476	0.0000	881.9516	3.8689	1523.6829	0.2350
193	1554.4102	145.2295	883.4468	0.0000	883.0596	8.0685	1528.5076	9.0735
194	1554.4102	145.2296	883.4872	4.7878	883.9667	3.0503	1529.6259	15.9894
195	1583.5503	0.0000	896.5925	0.0000	888.3630	0.0866	1547.8952	30.6059
196	1598.7928	22.6940	898.0200	5.6233	892.5513	16.6548	1547.8990	30.5042
197	1598.7928	22.6941	898.2846	0.1959	896.3183	0.2563	1555.7205	140.8769
198	1601.5995	0.0000	899.6154	0.0000	898.3709	17.3624	1555.9632	186.8833
199	1608.1451	0.0000	911.9586	0.0000	910.9950	1.8834	1560.7621	10.1911
200	1613.2755	5.2424	912.0915	5.2191	911.8492	2.6576	1560.9084	4.4125
201	1623.2827	5.5148	913.5553	0.0000	913.0493	2.3295	1587.0367	3.6059
202	1623.2827	5.5148	913.9670	3.2926	913.9205	4.5856	1599.5551	15.6510
203	1623.8706	0.0000	917.3072	2.9382	915.9396	1.4716	1602.1111	21.5439
204	1625.7892	8.7025	917.5717	0.0000	916.6568	0.5508	1606.0315	0.0633
205	1648.3308	0.0000	917.8459	0.1416	917.6509	1.2003	1614.2659	9.3889
206	1648.4057	0.0386	918.2758	0.0000	918.6679	0.1718	1621.2259	3.3756
207	1648.4057	0.0386	951.2580	0.0000	951.6035	12.9668	1625.3167	5.7512
208	1648.5265	0.0000	951.6131	39.9339	961.6310	2.7831	1625.5602	3.3412
209	2644.6629	236.3702	961.8114	0.0000	962.1387	26.5952	1625.8800	0.1568
210	2644.6629	236.3701	962.1032	3.3898	964.3299	0.0533	1628.5299	10.8552
211	2789.8916	0.0000	963.4691	292.4467	965.8746	1.8377	1650.1307	0.0044
212	2804.6838	2165.5266	964.4052	0.0000	966.0536	196.5303	1650.1902	0.0154
213	3215.1427	0.0000	965.5595	179.9958	969.6397	0.0018	1652.8658	0.3219

214	3215.1616	4.1911	965.8924	10.5187	970.6501	46.0137	1652.9682	0.0716
215	3215.1617	4.1911	966.2349	0.0000	971.5882	36.5452	1719.4392	29.9535
216	3215.2024	0.0000	968.5663	0.0000	972.9435	1.2127	2632.7599	232.0395
217	3222.5337	0.0000	968.8393	0.0000	973.5951	2.8849	2782.8308	1132.4156
218	3222.5701	3.2425	969.0387	3.6529	975.0839	0.3312	2962.5767	315.3647
219	3222.5701	3.2425	971.8366	0.0000	976.4721	52.2539	3106.8054	542.4485
220	3222.6062	2.7953	971.9997	3.1764	976.8010	1.2123	3120.4634	64.0576
221	3231.2203	0.0000	972.9975	143.4468	977.8586	55.9032	3129.2370	167.2329
222	3231.2526	22.1392	974.1524	0.0000	978.4576	0.0472	3211.6881	1.1665
223	3231.2526	22.1392	977.0219	0.0000	981.8503	107.2618	3211.7031	0.7476
224	3231.3419	0.0000	978.2845	17.1889	982.9176	3.4305	3214.7195	2.0385
225	3238.1283	0.0000	984.5713	49.5433	983.2598	12.7313	3214.7482	1.8929
226	3238.1756	3.8392	986.1404	0.0000	985.5668	22.6123	3220.3441	4.6048
227	3238.1756	3.8392	987.5590	1.4101	987.0778	89.0586	3220.3599	0.5449
228	3238.2255	10.6298	988.0887	55.8719	993.3590	10.3690	3222.1440	1.3552
229	3246.7050	0.0000	988.1082	0.0000	996.9826	112.5029	3222.1783	3.0550
230	3246.7150	32.0627	988.1349	0.0000	1009.4512	1.9834	3230.0253	0.0441
231	3246.7150	32.0629	1011.9014	10.7574	1012.1809	9.2429	3230.0637	24.3294
232	3246.8069	0.0000	1012.2300	0.0000	1014.4300	3.1294	3230.4082	11.6112
233	3311.8710	0.0000	1020.8815	0.0000	1020.5606	3.1406	3230.4623	9.2175
234	3311.9186	0.0595	1020.8950	5.8798	1020.6680	3.8916	3237.5690	1.5072
235	3311.9186	0.0595	1021.1872	0.0000	1021.0743	3.1242	3237.6084	8.0884
236	3311.9523	0.0000	1021.1888	6.6139	1021.3944	4.7256	3241.2576	28.1748
237	3331.3341	0.1943	1021.5068	0.0000	1021.8703	3.8357	3241.3159	26.7330
238	3331.4027	0.0722	1021.8836	0.5376	1022.0949	1.3909	3246.1871	15.9743
239	3331.4027	0.0722	1023.1737	0.0000	1024.5838	2.0485	3246.2379	15.5356
240	3331.4967	0.0000	1023.3264	1.9869	1025.0947	2.5183	3287.2834	173.3540
241			1026.4983	0.0000	1025.3700	1.5304	3312.0154	0.0186
242			1026.9118	0.3749	1025.8041	3.7531	3312.0214	0.2078
243			1026.9694	9.6042	1027.8696	0.9960	3312.8188	0.0736
244			1027.0248	0.0000	1028.3467	17.7812	3315.2779	0.0164
245			1027.0828	11.8559	1028.3742	1.3981	3331.3860	0.0393
246			1027.7710	0.0000	1028.7116	1.8514	3331.3917	0.3195
247			1031.8500	0.0000	1029.3041	16.8326	3332.0780	0.0361
248			1031.9596	4.8303	1029.6664	4.0837	3334.6835	0.0353
249			1035.8568	0.0000	1033.1935	1.1935	3604.7430	12.9101
250			1036.0716	10.0258	1033.8441	0.0591		
251			1036.3707	0.0000	1034.9166	7.1844		
252			1036.4134	3.6674	1035.3003	3.4413		
253			1044.9102	0.0000	1044.7208	3.8265		
254			1044.9487	5.2336	1046.1312	1.9001		
255			1048.2747	0.0000	1048.2052	0.0000		
256			1048.3146	22.3194	1048.2895	14.5072		
257			1048.6147	0.0666	1048.4414	0.0475		

258	1048.6206	0.0000	1048.4535	3.0881
259	1048.6405	0.0000	1048.8432	9.2767
260	1048.7255	16.5638	1048.9265	0.0194
261	1048.9183	20.2695	1049.0384	11.6562
262	1048.9673	0.0000	1049.1376	7.5397
263	1056.7391	0.0000	1051.2789	1.9059
264	1056.7601	1.9207	1051.8972	0.6989
265	1068.5035	0.0000	1054.8032	4.2444
266	1068.6236	6.5093	1056.7898	1.2069
267	1068.8165	0.0000	1058.0346	2.7973
268	1068.9561	27.7644	1060.4779	0.0375
269	1069.7144	0.0000	1068.3398	11.7584
270	1069.7443	25.2116	1068.7243	3.8974
271	1070.3035	1.0889	1068.9693	3.3960
272	1070.3957	0.0000	1069.2281	20.0053
273	1071.4230	0.0000	1069.8534	12.3311
274	1071.4276	0.0000	1070.4464	10.3235
275	1071.4333	5.7294	1070.9947	1.1477
276	1071.4939	2.2783	1071.5625	2.7053
277	1116.1197	5.6020	1112.1603	17.2054
278	1116.4793	0.0000	1119.6152	1.6720
279	1121.5282	4.3551	1124.6453	1.9267
280	1122.4775	0.0000	1124.6626	4.0737
281	1123.9717	0.0000	1125.0896	1.5818
282	1123.9758	7.0139	1125.9871	1.4360
283	1124.5855	2.5716	1126.0940	5.7842
284	1124.9742	0.0000	1126.1896	1.0645
285	1129.1268	0.0000	1127.6303	3.2844
286	1129.5312	5.5138	1127.8297	0.0004
287	1130.4345	0.0000	1128.6367	0.0553
288	1130.6703	4.3466	1130.5581	1.3413
289	1130.8202	0.0000	1131.9151	8.1409
290	1131.2869	12.0802	1132.2282	12.3094
291	1133.6726	40.1204	1132.8001	10.2998
292	1134.5435	0.0000	1135.9902	15.3856
293	1137.8983	0.0000	1137.8710	6.7592
294	1137.9834	0.2440	1140.4629	0.1939
295	1222.6541	0.0000	1219.2020	0.0215
296	1222.8976	1.6497	1224.7812	0.5256
297	1232.1135	1.0115	1230.4172	0.0113
298	1232.1404	0.0000	1230.4652	0.0066
299	1232.1431	0.0000	1231.4406	0.2003
300	1232.2099	1.3503	1231.5074	0.1273
301	1232.8494	0.0000	1234.0124	0.0000

302	1232.8502	0.0068	1234.0711	0.1149
303	1232.9079	0.0000	1234.1392	0.0005
304	1232.9150	0.1931	1234.2083	0.0986
305	1243.0558	0.0000	1243.0226	6.7498
306	1243.0850	19.7360	1243.0630	11.9012
307	1243.3376	25.0424	1243.1897	27.2535
308	1243.4360	0.0000	1243.3385	8.2689
309	1250.5196	10.6651	1245.1948	5.0005
310	1250.6612	0.0000	1245.6505	9.6965
311	1250.8624	0.0000	1248.2107	0.8412
312	1251.7190	16.7378	1250.5887	29.8055
313	1259.6155	40.3519	1250.9852	21.7117
314	1259.8675	0.0000	1260.4261	15.3189
315	1261.2333	0.0000	1261.1029	10.3261
316	1261.4320	22.8077	1262.1841	5.0574
317	1272.3520	0.0000	1266.3879	16.7556
318	1272.4445	70.5908	1271.8585	88.0906
319	1274.1102	53.7416	1272.7099	19.2893
320	1274.1637	0.0000	1274.3113	26.2810
321	1274.6260	0.0000	1274.3942	91.2356
322	1274.6298	158.8605	1274.8443	55.3428
323	1281.6913	0.3544	1279.3730	3.9013
324	1281.7683	0.0000	1280.7623	9.6334
325	1301.9626	0.0000	1298.7221	0.9394
326	1302.1384	0.0119	1302.4645	2.5163
327	1326.9518	11.9380	1325.3162	5.0999
328	1327.2636	0.0000	1326.0568	3.7742
329	1329.3684	0.0000	1327.4979	0.9540
330	1329.9938	2.1062	1329.9657	4.5840
331	1332.3132	3.5461	1330.2413	1.3018
332	1332.8160	0.0000	1330.7255	4.3674
333	1341.6474	0.2462	1342.3918	0.2094
334	1341.6669	0.0000	1342.9102	0.4674
335	1344.7149	0.0470	1344.7597	0.0070
336	1345.0662	0.0000	1344.8280	0.4544
337	1346.5490	3.0594	1345.7594	0.2869
338	1346.8555	0.0000	1346.5811	0.6082
339	1350.4133	2.0037	1349.1604	0.2350
340	1350.5570	0.0000	1351.1857	0.4989
341	1366.7471	0.0000	1363.5091	0.4931
342	1366.9812	2.2712	1366.8089	0.0035
343	1370.8699	0.7621	1369.2546	2.5980
344	1371.1719	0.0000	1369.7393	1.1779
345	1382.4563	0.0000	1379.7493	0.0027

346	1382.6066	0.4924	1381.3788	0.1899
347	1388.8022	3.7840	1386.3451	0.8106
348	1389.0558	0.0000	1387.5563	0.3022
349	1389.9152	9.6284	1389.1010	0.4829
350	1389.9326	0.0000	1389.2933	3.0676
351	1390.0308	0.0000	1389.5429	3.3427
352	1390.0601	5.1116	1389.5669	2.7963
353	1394.8625	0.0000	1392.1391	3.0291
354	1394.8838	6.2499	1393.3999	0.0008
355	1398.4975	7.6481	1393.6815	0.2965
356	1398.7310	0.0000	1393.7607	3.9980
357	1399.6246	0.0000	1394.6034	7.6671
358	1399.9393	13.5425	1396.1887	14.8723
359	1429.0717	0.0000	1425.3613	0.0017
360	1429.2922	1.3246	1430.8402	1.5430
361	1431.2875	3.9437	1431.1769	2.0540
362	1431.3214	0.0000	1433.1415	0.2035
363	1435.8551	1.7992	1434.9204	2.5784
364	1436.0420	0.0000	1436.5356	2.4079
365	1462.1368	0.0000	1459.3904	0.4491
366	1462.2736	0.1136	1466.3367	0.0076
367	1486.8145	1.2002	1484.0381	0.1941
368	1486.9407	0.0000	1484.3872	0.1030
369	1499.7857	39.4355	1497.2179	26.4585
370	1500.0553	0.0000	1498.0497	32.7639
371	1500.3600	0.0000	1499.8462	16.2826
372	1500.5145	42.6260	1500.3527	3.8467
373	1501.2014	0.0000	1502.4107	18.9310
374	1501.2298	35.4111	1503.0178	13.7195
375	1503.9038	0.0000	1504.5781	1.7774
376	1504.1173	0.0220	1505.7763	0.8368
377	1524.4032	15.7260	1521.7625	4.8335
378	1524.5740	0.0000	1523.8606	1.9091
379	1525.3338	0.0000	1525.1772	2.3829
380	1525.6334	9.6254	1525.6015	26.4531
381	1530.2287	12.2773	1525.8515	3.3934
382	1530.2862	0.0000	1529.0240	5.5804
383	1545.4162	0.0000	1543.6878	162.4410
384	1545.5881	172.8382	1544.5656	41.1855
385	1546.1521	70.5446	1545.1456	8.9700
386	1546.1660	0.0000	1545.6822	96.6929
387	1547.4971	0.0000	1546.1178	64.7124
388	1547.6442	47.4766	1546.2567	1.1679
389	1548.0998	14.1630	1546.5056	0.2048

390	1548.1799	0.0000	1547.4131	42.2075
391	1549.8180	0.0000	1548.1362	1.9077
392	1549.8647	112.6956	1548.4556	39.1410
393	1557.4836	0.0000	1552.8715	159.7241
394	1557.8035	329.4656	1556.1586	226.2483
395	1583.5713	10.9144	1580.7375	0.7518
396	1583.5956	0.0000	1580.9389	1.1066
397	1598.1336	0.0000	1594.2571	7.3092
398	1598.4858	19.6227	1601.1888	40.7079
399	1601.0397	0.0000	1601.7285	14.8163
400	1601.0642	34.5283	1601.7368	8.7629
401	1602.9472	0.0000	1602.0066	4.2589
402	1602.9505	3.1258	1605.3165	0.5103
403	1612.2325	13.7150	1609.5258	1.0675
404	1612.3884	0.0000	1609.5634	7.4922
405	1615.6657	18.9871	1612.2930	13.6615
406	1615.8624	0.0000	1612.6944	7.2048
407	1621.5834	0.0000	1619.3604	3.7570
408	1621.7300	5.7437	1620.9513	4.5184
409	1622.3928	9.1683	1622.3676	1.3059
410	1622.4115	0.0000	1623.0773	9.3955
411	1623.6005	0.0000	1624.3447	4.8023
412	1623.6580	6.1129	1624.5323	1.5833
413	1625.7088	0.0000	1625.0753	5.8476
414	1625.7424	18.4834	1625.6323	5.5153
415	1647.8711	0.0000	1645.8005	0.6981
416	1648.0197	4.2299	1645.9711	0.4404
417	1648.0218	0.0000	1647.7549	0.0131
418	1648.0398	5.2059	1647.8622	2.8438
419	1648.8270	0.8667	1649.1297	0.0112
420	1648.8407	0.0000	1649.1953	0.0349
421	1648.9208	0.0000	1650.2591	0.3418
422	1648.9382	0.9041	1650.4312	0.0223
423	2640.6288	0.0000	2629.2971	305.5738
424	2641.2647	337.5425	2649.0074	148.5090
425	2793.3197	2290.6125	2792.2949	1084.2732
426	2794.1140	0.0000	2812.3651	1313.7726
427	2886.2365	571.4907	2823.7410	340.0526
428	2887.9911	0.0000	2883.5867	144.5665
429	2987.6848	0.0000	2967.3579	488.6281
430	3000.5447	2740.9294	2989.3596	1626.6255
431	3167.3688	0.0000	3190.0179	7.9818
432	3167.4923	43.1398	3193.3320	21.2422
433	3171.7592	52.5488	3210.4678	1.9064

434	3171.8049	0.0000	3210.4935	0.5804
435	3211.5094	1.3373	3211.7730	0.5024
436	3211.5158	0.0000	3211.8009	5.4246
437	3211.5168	0.0000	3213.8923	1.9792
438	3211.5279	0.3404	3213.9240	3.3419
439	3214.3604	0.0000	3214.9999	2.2295
440	3214.3611	3.7239	3215.0269	2.2909
441	3214.3902	5.3258	3221.5905	1.3228
442	3214.3924	0.0000	3221.6174	3.3498
443	3221.9842	1.0066	3221.6812	3.5653
444	3221.9883	0.0000	3221.7056	1.3128
445	3222.0152	0.0000	3222.3282	8.6968
446	3222.0199	7.4816	3222.3493	2.5026
447	3222.2874	0.0000	3223.4938	1.3686
448	3222.2959	5.7510	3223.5446	8.3339
449	3222.3232	22.8080	3230.3457	4.1878
450	3222.3419	0.0000	3230.3952	11.0211
451	3230.9996	0.0000	3230.7395	12.4047
452	3231.0001	27.2921	3230.7880	14.8541
453	3231.0504	24.5800	3231.7750	9.0226
454	3231.0609	0.0000	3231.8891	15.9414
455	3232.9325	1.4575	3233.0003	0.6542
456	3232.9479	0.0000	3233.0283	13.7931
457	3232.9761	0.0000	3237.5076	5.4193
458	3233.0210	27.2363	3237.5249	2.9205
459	3237.8858	0.9708	3237.5531	5.2824
460	3237.8866	0.0000	3237.5678	8.6903
461	3237.9258	0.0000	3239.0973	1.2459
462	3237.9287	17.8561	3239.1331	6.3106
463	3241.9143	0.0000	3241.0628	21.8656
464	3241.9563	44.0423	3241.1236	17.1909
465	3241.9897	36.3641	3245.8166	16.0782
466	3242.0181	0.0000	3245.8645	17.9774
467	3246.2525	0.0000	3246.5111	8.5413
468	3246.2553	28.5285	3246.5511	17.9058
469	3246.2966	30.4996	3246.6272	15.0260
470	3246.3043	0.0000	3246.6854	13.1706
471	3312.0101	0.0000	3304.3755	0.0607
472	3312.0101	0.0877	3304.4154	16.2418
473	3313.5726	0.0000	3309.8299	0.0316
474	3313.5793	0.2811	3310.0285	0.0000
475	3313.7380	0.0186	3311.1317	0.0287
476	3313.7428	0.0000	3313.4290	0.0312
477	3319.9260	0.1974	3313.4321	0.0932

478	3319.9261	0.0000	3321.0580	0.1607
479	3331.4900	0.1670	3325.2535	15.2198
480	3331.4916	0.0000	3325.7993	0.0765
481	3332.9000	0.0000	3325.8757	14.6096
482	3332.9321	1.0174	3329.3644	0.1446
483	3333.1017	0.4386	3330.6105	0.0463
484	3333.1119	0.0000	3332.7471	0.0699
485	3339.1839	0.0000	3332.7608	0.0958
486	3339.1975	0.0385	3339.8004	0.3314
