

### *Supplementary Information for*

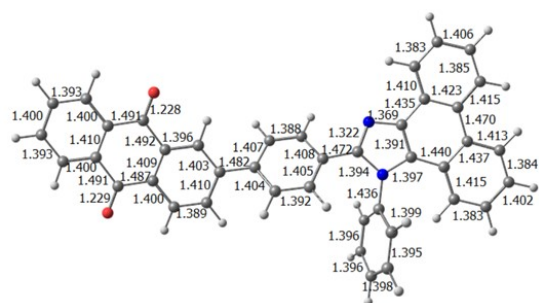
## **Insights from QM/MM-ONIOM calculations: the TADF phenomenon of phenanthro[9,10-*d*]imidazole–anthraquinone in solid state**

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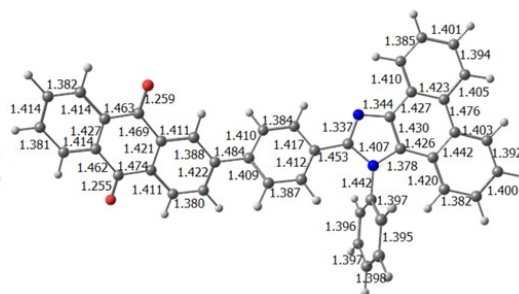
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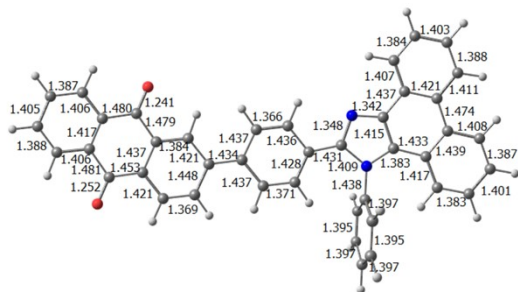
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a: Optimizatiad  $S_0$  state in toluene

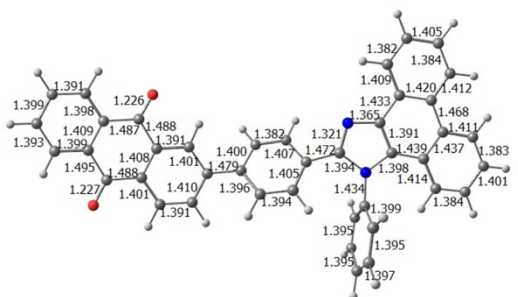


b: Optimizatiad  $S_1$  state in toluene

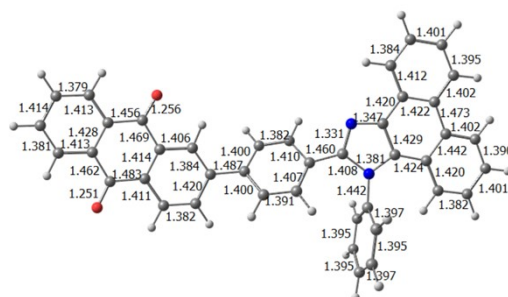


c: Optimizatiad  $T_1$  state in toluene

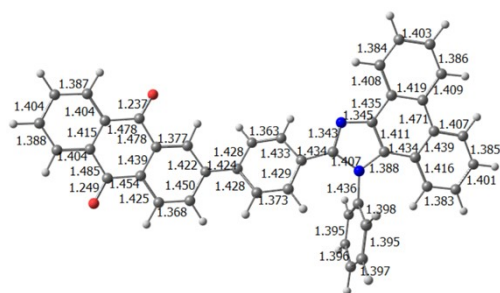
Figure S1. Bond length of the studied molecule PIPAQ in toluene by B3LYP/6-31G(d, p).



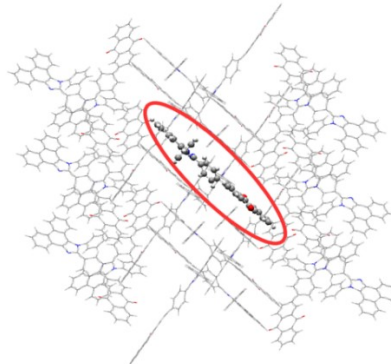
a: Optimizatiad  $S_0$  state in cluster



b: Optimizatiad  $S_1$  state in cluster



c: Optimizatiad  $T_0$  state in cluster



d: the ONIOM model

Figure S2. Bond length of the studied molecule PIPAQ in cluster (a, b, and c) by ONIOM (B3LYP/6-31G(d):UFF), the low layer omitted.

ONIOM model (d): the centered molecule is treated as a high layer and the surrounding molecules are fixed as a low layer.

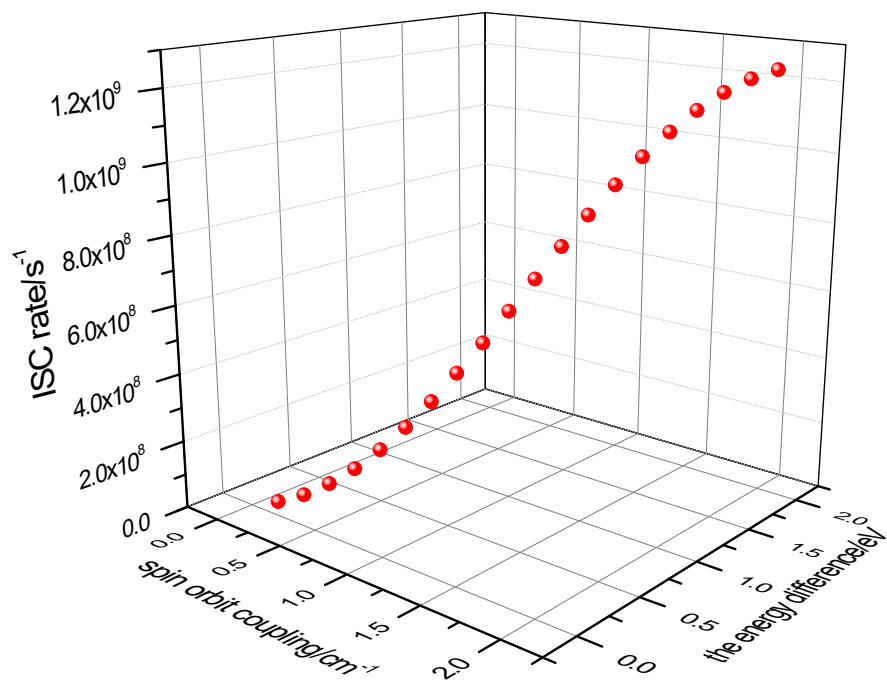


Figure S3. Three-dimensional diagram of  $k_{isc}$  and SOC and the energy difference  $\Delta E_{S1-T1}$

**Table S1.** The frequencies of the title compound according to QM and ONIOM calculations

.	In vacuum			In toluene			In cluster		
	S <sub>0</sub> state	S <sub>1</sub> state	T <sub>1</sub> state	S <sub>0</sub> state	S <sub>1</sub> state	T <sub>1</sub> state	S <sub>0</sub> state	S <sub>1</sub> state	T <sub>1</sub> state
v <sub>1</sub>	7.5	3.3	4.1	12.3	6.0	8.6	27.0	26.6	27.2
v <sub>2</sub>	13.2	12.4	11.9	15.3	15.0	14.6	32.9	33.2	33.6
v <sub>3</sub>	20.3	20.3	20.3	21.4	22.3	24.4	42.3	41.7	42.2
v <sub>4</sub>	21.5	22.8	24.1	23.8	26.0	29.1	48.7	48.1	47.8
v <sub>5</sub>	35.9	39.0	30.6	37.4	40.7	32.2	57.2	57.9	57.2
v <sub>6</sub>	41.4	41.5	35.0	43.9	43.1	38.6	58.6	59.0	60.6
v <sub>7</sub>	54.6	57.6	53.8	56.5	55.5	53.7	64.3	65.0	64.0
v <sub>8</sub>	60.3	59.1	56.0	60.2	61.7	59.5	68.1	68.4	69.1
v <sub>9</sub>	66.5	68.8	67.6	68.6	70.6	71.2	72.2	72.7	72.0
v <sub>10</sub>	74.6	77.2	85.1	74.7	79.8	84.1	80.6	76.8	79.9
v <sub>11</sub>	90.5	86.9	87.0	92.6	91.1	92.0	84.5	83.8	82.5
v <sub>12</sub>	95.5	95.1	93.1	96.6	96.2	93.9	86.9	87.9	87.8
v <sub>13</sub>	107.9	109.3	98.5	108.6	109.4	101.2	89.4	90.7	90.8
v <sub>14</sub>	123.5	125.6	128.2	124.0	126.5	128.6	94.1	95.2	94.0
v <sub>15</sub>	125.2	134.4	128.3	125.6	133.3	135.2	99.0	102.5	101.0
v <sub>16</sub>	146.9	158.3	147.1	147.3	158.1	153.7	106.8	104.6	106.3
v <sub>17</sub>	160.8	165.5	160.7	161.1	166.1	164.7	132.4	132.6	121.0
v <sub>18</sub>	172.2	175.0	175.6	173.0	175.4	177.1	136.1	136.7	136.2
v <sub>19</sub>	180.2	178.2	187.6	180.2	181.6	187.6	138.5	139.4	138.8
v <sub>20</sub>	212.1	213.6	196.5	213.1	212.9	201.6	142.2	148.9	143.4
v <sub>21</sub>	228.3	225.3	228.4	228.1	226.6	228.3	158.9	170.8	164.6
v <sub>22</sub>	230.0	232.5	238.2	230.1	235.5	239.8	172.2	178.2	167.5
v <sub>23</sub>	256.0	254.0	241.4	256.8	254.2	244.9	188.7	182.9	184.2
v <sub>24</sub>	262.0	261.7	264.8	262.0	263.0	265.4	191.1	195.6	191.1
v <sub>25</sub>	269.8	266.9	269.3	270.6	268.5	270.6	203.0	206.4	205.3
v <sub>26</sub>	290.6	281.0	276.7	291.5	281.8	281.9	230.2	228.9	230.1
v <sub>27</sub>	297.0	292.7	293.7	298.7	294.6	298.1	234.6	233.6	237.5
v <sub>28</sub>	317.6	319.7	306.9	317.4	321.1	311.2	241.4	241.3	242.4
v <sub>29</sub>	333.3	336.8	316.4	333.7	338.3	320.6	264.6	264.9	256.0
v <sub>30</sub>	375.5	372.6	361.7	376.6	373.6	365.8	272.3	271.7	273.0
v <sub>31</sub>	386.7	381.2	385.1	387.4	382.4	385.7	277.8	273.8	277.8
v <sub>32</sub>	401.6	400.7	407.4	401.9	403.5	406.3	305.8	296.4	299.7
v <sub>33</sub>	409.9	407.0	408.2	409.9	406.7	406.8	309.2	305.9	308.2
v <sub>34</sub>	413.6	409.5	410.7	413.5	409.1	413.4	325.7	327.5	317.5
v <sub>35</sub>	415.9	416.1	414.4	416.5	416.6	415.6	342.1	347.5	330.0
v <sub>36</sub>	421.2	420.7	419.9	421.6	421.5	421.6	382.1	378.4	368.7
v <sub>37</sub>	422.7	421.7	424.3	423.6	423.2	424.3	389.2	383.5	386.8
v <sub>38</sub>	440.1	431.6	430.6	440.7	433.0	433.8	410.6	408.2	407.3
v <sub>39</sub>	446.1	445.0	438.2	446.6	445.6	438.8	414.1	417.3	413.5
v <sub>40</sub>	451.5	448.6	446.1	451.3	450.1	446.7	419.0	421.5	416.3
v <sub>41</sub>	455.0	452.9	454.7	455.2	453.3	455.2	424.4	424.8	422.0
v <sub>42</sub>	462.6	464.5	454.8	462.7	465.0	459.8	429.5	427.3	428.6
v <sub>43</sub>	466.7	472.3	461.0	466.9	475.0	463.7	444.2	442.3	436.9
v <sub>44</sub>	479.1	476.3	471.8	479.9	475.7	476.1	450.5	446.3	445.3
v <sub>45</sub>	487.7	490.4	483.5	488.6	489.6	485.7	454.6	452.0	449.1
v <sub>46</sub>	498.9	499.4	484.6	499.5	500.3	493.2	460.7	458.0	458.7
v <sub>47</sub>	525.8	526.1	500.7	525.3	525.5	501.0	467.8	465.7	460.7
v <sub>48</sub>	536.1	530.7	535.0	537.1	530.6	534.7	472.1	474.2	464.1
v <sub>49</sub>	553.5	546.3	536.1	554.4	548.0	540.8	473.9	475.6	469.0

V50	559.2	558.3	550.3	558.8	559.0	552.9	487.6	479.9	484.7
V51	574.8	558.7	560.6	575.5	559.8	561.6	492.2	495.7	491.2
V52	585.8	572.1	568.9	586.6	572.0	567.7	502.3	501.9	503.3
V53	630.4	621.3	626.0	629.9	622.2	627.0	535.1	530.5	515.2
V54	631.2	631.0	628.6	630.5	630.7	629.1	547.0	539.1	537.0
V55	646.7	638.8	629.6	646.0	638.4	629.6	557.9	548.5	551.9
V56	650.0	643.6	638.1	649.8	643.9	639.0	563.8	561.9	560.8
V57	653.2	646.9	640.3	652.5	646.6	641.8	581.6	566.0	562.5
V58	672.3	663.5	646.0	671.8	662.7	645.9	601.3	591.5	576.5
V59	680.1	670.2	670.1	680.1	670.2	670.5	632.5	623.2	629.8
V60	687.2	685.3	682.1	687.0	684.9	682.7	634.8	634.4	630.9
V61	688.9	690.7	682.8	688.4	691.4	690.8	650.3	643.5	633.3
V62	702.6	702.0	690.1	702.2	701.7	693.9	653.8	647.1	635.6
V63	705.2	703.9	694.2	705.5	703.8	695.2	661.2	656.2	642.8
V64	706.0	705.2	704.2	707.8	705.8	703.9	673.9	663.8	649.3
V65	714.9	712.6	708.2	716.2	715.4	712.2	682.7	672.1	670.9
V66	723.2	716.9	716.5	725.4	718.8	716.3	689.7	687.7	683.9
V67	729.3	724.6	717.1	729.7	725.8	718.1	694.2	696.1	691.7
V68	732.2	727.1	722.2	732.1	726.9	723.6	707.4	704.7	695.9
V69	736.7	732.4	722.2	736.9	728.9	724.4	707.9	707.8	700.2
V70	738.2	742.2	732.1	739.4	741.1	732.0	709.6	709.7	706.4
V71	755.7	756.4	740.0	755.8	755.8	746.4	723.2	714.5	716.8
V72	759.9	768.0	743.3	760.5	766.6	747.3	730.8	726.0	719.7
V73	767.4	773.9	767.4	770.6	778.2	772.2	732.6	730.2	726.5
V74	780.8	778.0	778.2	783.3	781.4	780.1	735.0	731.3	727.0
V75	788.1	785.3	780.1	788.5	788.5	788.1	740.0	742.3	729.7
V76	793.7	785.8	787.5	794.6	788.9	788.5	745.0	747.3	741.0
V77	809.0	787.7	788.2	810.7	790.0	792.6	760.3	759.8	751.0
V78	815.0	808.2	791.0	814.9	806.3	797.7	768.5	774.9	752.0
V79	819.5	821.7	807.9	819.3	821.8	806.5	773.0	778.2	775.4
V80	838.0	838.1	815.8	837.9	838.9	818.9	783.2	783.6	781.5
V81	849.0	841.7	818.5	853.0	841.2	819.8	794.0	787.1	790.0
V82	856.7	849.4	825.8	859.8	849.3	830.2	804.3	790.8	792.7
V83	861.2	857.8	834.4	861.0	862.3	846.5	810.8	793.1	800.4
V84	866.5	876.9	860.9	869.9	876.2	861.9	817.2	811.2	807.9
V85	879.3	878.6	868.1	882.8	883.9	873.4	823.4	824.8	813.2
V86	884.2	881.3	872.1	885.8	888.2	887.6	842.6	841.8	821.3
V87	922.0	892.2	884.5	924.6	896.2	912.4	862.1	845.5	826.8
V88	930.8	925.2	914.9	937.4	933.1	913.2	865.8	862.6	834.2
V89	936.6	942.3	940.2	940.4	941.6	944.0	872.1	873.9	863.9
V90	948.0	944.6	941.6	946.9	949.2	949.6	882.3	882.5	864.1
V91	948.8	953.3	944.7	954.1	950.5	951.9	887.6	883.0	875.7
V92	956.7	957.9	946.2	957.0	964.1	953.0	922.8	893.0	893.3
V93	967.0	967.7	952.9	971.1	966.8	960.4	935.2	926.4	912.2
V94	971.4	972.8	959.2	972.3	976.8	964.0	946.4	941.4	934.2
V95	973.0	975.0	962.6	973.4	977.4	967.6	948.1	942.9	945.3
V96	974.2	976.6	976.0	978.2	979.3	980.3	950.5	950.4	946.9
V97	975.5	979.7	983.7	982.0	985.5	987.1	957.8	956.2	952.5
V98	987.6	984.2	985.6	986.7	986.0	991.6	959.0	962.1	959.4
V99	988.5	986.1	986.7	992.3	987.6	992.8	974.6	973.5	962.3
V100	993.4	989.6	990.7	995.4	994.4	994.6	978.2	974.9	965.3
V101	996.2	998.4	992.7	996.3	1001.5	995.0	979.9	979.2	969.1
V102	1000.5	998.6	997.8	1003.3	1005.5	1000.9	981.3	981.5	980.9
V103	1001.3	1007.9	999.1	1007.0	1010.9	1002.7	982.3	984.4	984.7

V104	1012.9	1012.8	1004.3	1016.7	1014.2	1010.0	992.4	987.8	986.9
V105	1017.9	1014.4	1009.8	1017.9	1017.3	1011.2	997.9	991.0	989.9
V106	1021.3	1021.5	1010.3	1020.1	1020.2	1014.4	1000.3	993.7	991.7
V107	1035.3	1032.6	1015.5	1034.3	1029.2	1015.2	1004.9	1008.2	1005.4
V108	1052.3	1047.4	1019.4	1051.4	1047.1	1018.5	1012.4	1015.0	1006.8
V109	1061.6	1050.4	1047.9	1061.8	1050.0	1047.0	1014.3	1023.3	1012.5
V110	1068.2	1059.1	1057.8	1068.7	1058.1	1056.1	1019.4	1024.3	1015.9
V111	1071.5	1071.2	1066.0	1070.9	1071.5	1066.9	1025.7	1026.2	1019.0
V112	1077.2	1078.4	1074.0	1076.8	1078.7	1074.7	1050.5	1047.8	1025.2
V113	1088.6	1087.8	1082.3	1088.1	1088.7	1083.3	1058.1	1056.1	1033.6
V114	1106.8	1110.0	1104.6	1106.8	1111.8	1104.8	1072.6	1057.9	1055.0
V115	1116.2	1119.9	1112.0	1116.8	1119.4	1111.4	1074.5	1070.2	1066.0
V116	1130.8	1125.4	1114.8	1131.1	1126.9	1117.2	1078.9	1076.4	1073.6
V117	1136.4	1130.9	1126.9	1136.3	1135.5	1132.1	1084.8	1085.3	1084.0
V118	1152.4	1143.8	1132.9	1151.8	1147.5	1146.5	1092.0	1091.7	1089.7
V119	1157.3	1151.1	1149.8	1156.5	1155.3	1150.3	1114.1	1117.4	1106.2
V120	1173.9	1156.3	1158.6	1174.1	1159.6	1161.4	1119.7	1123.0	1114.8
V121	1183.5	1163.1	1167.8	1184.4	1166.4	1169.2	1132.0	1126.0	1121.3
V122	1192.4	1176.1	1180.7	1192.0	1178.2	1178.3	1136.7	1132.0	1133.0
V123	1193.3	1195.7	1189.7	1192.7	1196.0	1189.0	1152.7	1144.5	1139.4
V124	1196.3	1197.4	1193.4	1195.2	1196.8	1192.1	1160.2	1157.1	1152.9
V125	1200.7	1202.1	1197.2	1199.7	1203.3	1196.5	1179.0	1159.9	1157.8
V126	1203.8	1206.8	1198.6	1203.1	1206.7	1198.0	1192.7	1167.3	1175.1
V127	1204.8	1207.1	1204.7	1204.7	1208.8	1208.2	1193.4	1185.9	1192.2
V128	1216.2	1209.9	1212.1	1214.9	1210.6	1213.3	1196.6	1195.4	1197.9
V129	1229.7	1222.5	1224.3	1228.2	1225.2	1226.2	1197.4	1197.5	1198.3
V130	1247.2	1230.2	1245.7	1247.2	1231.6	1241.4	1201.5	1200.6	1200.0
V131	1271.5	1236.4	1249.7	1270.3	1235.2	1264.0	1209.3	1209.4	1211.0
V132	1285.7	1261.8	1265.8	1285.4	1263.1	1264.5	1210.5	1210.8	1212.1
V133	1294.7	1264.1	1276.1	1293.9	1266.1	1277.8	1214.6	1215.2	1214.4
V134	1304.9	1275.4	1285.5	1304.0	1274.0	1280.8	1222.2	1217.8	1221.3
V135	1309.5	1302.4	1292.7	1308.5	1303.1	1293.2	1259.1	1227.0	1247.3
V136	1315.6	1306.5	1296.8	1315.1	1309.8	1298.0	1274.7	1248.8	1257.7
V137	1329.9	1316.9	1306.8	1327.5	1317.6	1312.1	1278.1	1261.5	1274.9
V138	1331.9	1325.4	1322.2	1331.4	1325.8	1331.0	1299.8	1268.8	1281.6
V139	1337.8	1340.4	1330.8	1337.4	1340.2	1332.6	1305.5	1278.7	1291.3
V140	1342.2	1343.7	1331.2	1342.0	1343.5	1333.0	1313.0	1289.3	1304.5
V141	1344.1	1352.1	1348.1	1344.1	1351.7	1347.4	1317.3	1308.3	1306.3
V142	1357.8	1352.9	1353.1	1357.0	1354.6	1352.6	1324.3	1319.9	1309.8
V143	1359.7	1361.4	1355.7	1359.4	1363.3	1355.6	1341.6	1325.3	1336.3
V144	1360.7	1365.5	1363.0	1360.2	1363.6	1356.1	1341.7	1339.5	1341.8
V145	1368.6	1372.5	1368.9	1368.2	1374.2	1367.7	1345.7	1347.1	1343.3
V146	1380.5	1379.0	1381.1	1379.8	1379.9	1378.3	1352.2	1352.4	1344.0
V147	1382.9	1384.0	1382.7	1381.8	1381.8	1383.4	1362.2	1357.7	1359.2
V148	1412.0	1420.7	1403.2	1411.6	1423.2	1399.9	1363.4	1368.2	1363.1
V149	1446.8	1434.9	1427.2	1445.6	1435.4	1425.5	1366.8	1370.7	1367.2
V150	1464.5	1448.7	1452.7	1463.7	1442.1	1453.2	1366.9	1376.4	1370.8
V151	1467.0	1460.1	1455.1	1465.9	1460.3	1458.3	1383.1	1378.0	1380.9
V152	1469.8	1463.0	1462.7	1469.5	1465.2	1468.2	1387.0	1386.6	1389.1
V153	1484.2	1485.0	1475.4	1483.0	1484.4	1477.3	1391.5	1389.6	1402.4
V154	1497.2	1487.3	1485.7	1496.5	1486.6	1481.5	1419.3	1422.5	1414.0
V155	1498.1	1491.6	1488.9	1497.9	1492.0	1488.1	1456.6	1441.6	1430.1
V156	1498.7	1497.5	1491.8	1498.0	1495.8	1491.7	1471.2	1457.3	1451.6
V157	1517.1	1499.8	1492.5	1515.9	1499.6	1497.5	1473.0	1463.4	1461.5

V158	1520.2	1504.9	1503.9	1519.7	1505.7	1500.1	1485.8	1480.9	1468.8
V159	1531.7	1515.7	1506.0	1531.9	1515.1	1505.2	1494.8	1489.7	1485.0
V160	1545.9	1542.6	1516.7	1544.9	1542.2	1509.3	1500.3	1491.4	1493.5
V161	1562.0	1546.8	1525.0	1561.2	1546.2	1529.7	1500.7	1496.0	1498.2
V162	1570.5	1555.2	1539.4	1570.3	1554.1	1532.7	1503.1	1502.3	1500.7
V163	1574.5	1564.1	1548.0	1573.5	1557.6	1537.9	1519.3	1503.1	1503.5
V164	1601.7	1576.0	1552.4	1600.3	1569.6	1550.4	1524.4	1508.0	1512.6
V165	1617.9	1577.2	1565.6	1616.8	1571.9	1565.6	1535.2	1519.3	1515.3
V166	1625.2	1590.1	1584.4	1623.5	1583.5	1573.5	1550.1	1547.6	1522.6
V167	1627.4	1595.4	1603.7	1625.5	1592.1	1585.5	1567.6	1555.8	1539.6
V168	1632.2	1605.1	1612.5	1630.3	1602.5	1604.9	1576.3	1563.5	1548.6
V169	1644.4	1608.6	1617.0	1642.3	1609.0	1609.6	1582.9	1571.1	1555.5
V170	1645.4	1635.3	1620.0	1643.1	1632.4	1616.9	1607.6	1578.5	1566.2
V171	1650.5	1642.8	1640.0	1647.9	1642.8	1636.7	1625.9	1584.4	1569.3
V172	1657.4	1646.6	1642.9	1654.8	1643.9	1640.1	1627.3	1592.8	1580.4
V173	1666.5	1649.4	1647.3	1664.7	1645.2	1644.7	1632.1	1600.2	1600.6
V174	1667.2	1653.4	1652.5	1665.2	1651.1	1649.5	1635.5	1610.5	1612.9
V175	1672.1	1658.0	1660.4	1669.9	1654.4	1653.3	1646.4	1617.8	1618.4
V176	1743.3	1666.9	1662.5	1735.3	1660.2	1657.2	1649.2	1642.3	1624.6
V177	1754.5	1691.1	1716.7	1746.0	1681.3	1690.0	1654.3	1645.2	1646.4
V178	3190.0	3175.1	3180.3	3186.4	3174.1	3181.2	1659.9	1649.0	1647.1
V179	3192.3	3182.2	3187.4	3188.9	3188.0	3192.2	1668.5	1651.9	1654.8
V180	3197.2	3192.5	3190.0	3194.4	3190.4	3194.9	1675.6	1657.2	1658.1
V181	3197.8	3207.0	3191.2	3197.3	3204.0	3195.4	1682.4	1664.0	1663.2
V182	3200.6	3211.4	3196.0	3197.8	3208.4	3196.2	1743.9	1670.1	1666.2
V183	3204.3	3211.6	3199.8	3200.0	3210.2	3202.9	1758.0	1699.5	1711.6
V184	3206.0	3213.4	3201.6	3201.9	3211.4	3205.3	3187.5	3177.3	3192.7
V185	3206.2	3213.7	3204.9	3202.9	3212.1	3209.2	3192.8	3177.9	3195.8
V186	3208.1	3218.0	3207.2	3204.0	3213.7	3209.5	3194.1	3205.4	3198.2
V187	3209.0	3219.5	3207.7	3207.3	3216.2	3209.9	3201.2	3212.2	3198.9
V188	3212.5	3220.5	3214.5	3210.6	3217.4	3215.4	3201.4	3213.9	3202.5
V189	3214.9	3222.6	3214.7	3211.2	3217.5	3216.3	3203.6	3214.8	3207.4
V190	3218.6	3223.7	3216.7	3214.5	3220.7	3217.9	3203.7	3219.0	3210.3
V191	3222.1	3225.4	3217.7	3217.6	3221.1	3218.1	3215.6	3220.3	3219.9
V192	3225.3	3226.2	3218.8	3218.7	3221.6	3218.4	3216.7	3222.3	3223.3
V193	3226.8	3228.1	3219.4	3222.6	3222.5	3221.0	3217.9	3225.5	3224.5
V194	3229.2	3228.1	3220.1	3227.3	3224.9	3221.5	3227.1	3225.6	3225.0
V195	3230.1	3232.7	3220.2	3227.9	3228.5	3222.3	3232.9	3228.2	3227.1
V196	3230.6	3233.3	3231.0	3228.7	3230.5	3233.2	3234.9	3237.1	3230.4
V197	3232.4	3240.5	3234.3	3230.4	3235.2	3235.1	3235.4	3237.9	3234.8
V198	3236.5	3242.7	3234.6	3231.5	3244.2	3236.0	3238.3	3238.0	3237.9
V199	3237.8	3249.2	3244.6	3233.0	3248.7	3244.1	3239.5	3240.3	3237.9
V200	3249.7	3261.1	3260.9	3243.9	3269.6	3263.8	3243.8	3246.4	3244.2
V201	3262.0	3279.3	3267.6	3258.3	3277.4	3272.3	3244.5	3246.8	3246.2

**Table S2.** Absorption and emission wavelength/nm of the title compound according to TDDFT calculations

	Absorption data			Emission data		
	monomer	In toluene	In cluster	monomer	In toluene	In cluster
B3LYP	553.9	560.0	570.9	683.9	697.6	703.2
PBE0	867.4	887.4	900.4	1144.4	1159.7	1181.1
CAM-B3LYP	348.7	370.6	398.8	399.7	403.2	408.8
M08	380.0	383.5	413.7	414.9	416.4	424.7
M06	490.7	494.9	505.9	601.2	604.4	609.2
$\omega$ B97XD	375.0	372.6	374.4	394.9	398.4	399.9
CAM-B3LYP*	411.4	414.6	561.8	567.9	575.1	610.4

(B3LYP/6-31g(d):uff method is employed in cluster)

**Table S3.** Vertical excitation energies ( $E_{\perp}$ , eV), wavelength (nm) and singly occupied orbitals involved in the  $S_0 \rightarrow S_n$  or  $T_n$  electronic transitions in vacuum, solution, and cluster, which are computed by TD-B3LYP.

	In vacuum			In toluene			In cluster		
	$E_{\perp}$ (eV)	$\lambda$ (nm)	Assignments	$E_{\perp}$ (eV)	$\lambda$ (nm)	Assignments	$E_{\perp}$ (eV)	$\lambda$ (nm)	Assignments
$S_1$	2.24	554	HOMO $\rightarrow$ LUMO	1.88	658	HOMO $\rightarrow$ LUMO	1.95	633	HOMO $\rightarrow$ LUMO
$S_2$	2.91	426	HOMO-1 $\rightarrow$ LUMO	2.78	446	HOMO-1 $\rightarrow$ LUMO	2.73	454	HOMO-1 $\rightarrow$ LUMO
$S_3$	2.94	421	HOMO-4 $\rightarrow$ LUMO	2.79	444	HOMO-4 $\rightarrow$ LUMO	2.74	451	HOMO-9 $\rightarrow$ LUMO
$S_4$	3.21	386	HOMO-8 $\rightarrow$ LUMO	2.84	437	HOMO $\rightarrow$ LUMO+1	2.78	446	HOMO-4 $\rightarrow$ LUMO
$S_5$	3.26	380	HOMO $\rightarrow$ LUMO+1	2.89	429	HOMO-7 $\rightarrow$ LUMO	2.93	422	HOMO $\rightarrow$ LUMO+1
$T_1$	2.10	589	HOMO $\rightarrow$ LUMO	1.51	821	HOMO $\rightarrow$ LUMO	1.57	787	HOMO $\rightarrow$ LUMO
$T_2$	2.51	494	HOMO-4 $\rightarrow$ LUMO	2.24	553	HOMO $\rightarrow$ LUMO+1	2.32	535	HOMO $\rightarrow$ LUMO+1
$T_3$	2.65	468	HOMO $\rightarrow$ LUMO+2	2.37	522	HOMO-4 $\rightarrow$ LUMO+1	2.35	527	HOMO-4 $\rightarrow$ LUMO
$T_4$	2.73	454	HOMO-2 $\rightarrow$ LUMO	2.41	514	HOMO-2 $\rightarrow$ LUMO	2.39	518	HOMO-2 $\rightarrow$ LUMO
$T_5$	2.75	450	HOMO-8 $\rightarrow$ LUMO	2.62	474	HOMO-9 $\rightarrow$ LUMO	2.61	475	HOMO-8 $\rightarrow$ LUMO

**Table S4.** Spin-orbital coupling (SOC)/ $\text{cm}^{-1}$ , intersystem crossing rate ( $k_{\text{isc}}$ ), and reverse intersystem crossing rate ( $k_{\text{risc}}$ ) of the title compound at the  $S_1$  and  $T_1$  minima.

	In vacuum		In toluene		In cluster	
	$S_1 \rightarrow T_1$	$T_1 \rightarrow S_1$	$S_1 \rightarrow T_1$	$T_1 \rightarrow S_1$	$S_1 \rightarrow T_1$	$T_1 \rightarrow S_1$
SOC	1.65	0.047	1.53	0.31	1.07	0.938
$k_{\text{isc}}$ or $k_{\text{risc}}/ \text{S}^{-1}$	$1.545 \times 10^6$	$5.69 \times 10^{-15}$	$9.49 \times 10^7$	$2.16 \times 10^{-9}$	$5.085 \times 10^8$	$4.399 \times 10^4$

the  $\lambda_{\text{reorg}}$  is from NMA method with Cartesian coordinate, the temperature is 300K.





**Table S5.** The reorganization energy ( $\text{cm}^{-1}$ ) between  $S_1$  and  $T_1$  minima vs each frequency of the title compound by NMA method with internal coordinate

frequency.	In vacuum		In toluene		In cluster	
	$S_1 \rightarrow T_1$	$T_1 \rightarrow S_1$	$S_1 \rightarrow T_1$	$T_1 \rightarrow S_1$	$S_1 \rightarrow T_1$	$T_1 \rightarrow S_1$
$\nu_1$	1.49	7.93	4.97	14.19	15.37	20.34
$\nu_2$	23.89	12.77	12.44	1.10	0.05	0.87
$\nu_3$	63.61	76.04	23.06	4.61	0.00	40.47
$\nu_4$	5.70	32.41	0.61	128.94	1.42	48.39
$\nu_5$	40.93	49.70	7.02	112.70	5.40	22.32
$\nu_6$	402.86	5.23	309.23	14.35	0.07	6.27
$\nu_7$	178.54	15.15	72.13	1.07	1.30	29.77
$\nu_8$	318.22	13.92	128.14	11.14	2.65	8.14
$\nu_9$	16.92	11.25	0.01	2.69	7.01	0.49
$\nu_{10}$	89.46	7.65	32.21	0.17	37.70	0.25
$\nu_{11}$	32.96	1.07	11.84	0.26	12.02	14.92
$\nu_{12}$	21.71	44.04	10.66	19.98	39.39	1.15
$\nu_{13}$	45.00	1.03	15.24	2.34	91.00	0.01
$\nu_{14}$	48.16	34.34	23.47	0.05	0.01	2.39
$\nu_{15}$	18.87	3.19	10.33	9.57	88.40	0.16
$\nu_{16}$	20.35	2.52	28.09	3.93	1.51	47.98
$\nu_{17}$	23.08	2.57	13.47	6.43	7.02	87.76
$\nu_{18}$	6.95	9.52	3.82	3.23	6.91	1.84
$\nu_{19}$	1.62	0.75	0.39	0.22	32.67	0.71
$\nu_{20}$	9.30	40.13	10.74	17.10	7.90	22.23
$\nu_{21}$	1.11	2.14	2.45	4.50	82.69	13.23
$\nu_{22}$	10.29	6.55	4.88	0.48	1.82	45.16
$\nu_{23}$	9.61	2.28	5.72	0.01	3.76	0.47
$\nu_{24}$	9.09	2.54	0.70	2.35	0.30	5.80
$\nu_{25}$	0.01	3.95	0.18	1.70	0.02	4.76
$\nu_{26}$	0.01	3.48	0.00	0.92	1.92	1.88
$\nu_{27}$	0.04	0.27	0.14	0.00	0.00	98.34
$\nu_{28}$	9.01	2.52	0.18	0.09	0.47	28.45
$\nu_{29}$	2.38	0.37	0.76	0.84	0.01	7.78
$\nu_{30}$	1.19	4.67	0.10	1.43	4.16	8.48
$\nu_{31}$	8.15	0.00	2.01	0.00	3.01	0.80
$\nu_{32}$	1.18	17.42	2.35	3.60	19.06	5.07
$\nu_{33}$	6.98	2.32	0.03	14.60	64.61	0.00
$\nu_{34}$	14.35	0.92	19.65	9.79	8.78	2.10
$\nu_{35}$	71.35	41.70	31.37	27.52	12.98	0.01
$\nu_{36}$	14.70	0.08	14.36	0.74	0.05	2.08
$\nu_{37}$	1.85	0.03	0.97	0.21	0.67	0.00
$\nu_{38}$	2.04	0.81	0.79	0.19	0.07	49.37
$\nu_{39}$	0.96	0.14	0.37	0.08	3.33	47.27
$\nu_{40}$	0.03	0.03	0.00	0.01	2.86	11.31
$\nu_{41}$	0.08	0.25	0.06	0.25	13.50	1.18
$\nu_{42}$	5.25	6.15	0.86	0.22	8.38	0.00
$\nu_{43}$	0.24	11.24	6.30	5.98	2.60	3.74
$\nu_{44}$	7.71	0.41	0.19	0.62	17.75	0.16
$\nu_{45}$	0.00	1.07	0.00	0.15	0.02	3.01
$\nu_{46}$	1.30	1.26	0.16	0.06	0.62	4.96
$\nu_{47}$	0.27	0.18	0.00	0.29	0.06	4.80
$\nu_{48}$	1.45	0.02	0.51	0.39	0.13	10.29

V49	0.04	4.73	0.04	0.31	0.22	22.08
V50	2.19	0.10	1.34	0.01	1.07	0.00
V51	0.32	10.01	0.10	1.18	0.07	14.32
V52	2.98	0.14	0.43	0.02	2.25	2.53
V53	0.16	4.48	0.04	0.19	0.17	2.70
V54	0.02	1.44	0.00	0.02	0.01	0.01
V55	5.77	0.00	1.67	2.32	6.30	0.43
V56	0.01	1.03	0.14	0.74	2.33	1.19
V57	3.14	4.53	1.66	0.19	0.01	0.26
V58	0.15	1.22	0.00	0.95	1.20	0.11
V59	1.04	1.01	0.50	0.32	0.33	8.49
V60	2.40	2.47	0.70	0.92	0.18	5.14
V61	0.20	1.20	0.10	0.22	0.00	0.07
V62	4.26	0.04	3.49	0.00	1.21	0.17
V63	0.45	1.36	0.26	3.96	1.42	0.08
V64	0.48	1.76	0.08	0.98	8.25	1.06
V65	0.53	1.28	0.54	0.00	0.90	0.61
V66	2.03	2.55	0.72	0.61	2.46	2.13
V67	0.05	1.39	0.44	0.21	4.08	0.53
V68	3.30	3.12	2.42	2.09	1.07	11.99
V69	0.17	0.33	0.48	1.20	0.02	0.44
V70	1.35	0.06	0.39	0.01	0.17	1.03
V71	14.43	5.59	6.04	4.19	3.31	2.92
V72	0.56	4.82	0.43	0.00	0.07	0.02
V73	0.02	0.23	0.00	0.03	0.24	2.35
V74	0.02	1.76	0.01	0.02	0.00	6.11
V75	0.00	208.47	0.25	0.01	0.01	0.28
V76	0.00	0.03	0.46	3.55	0.21	0.12
V77	0.72	4.40	0.01	2.98	1.15	1.68
V78	7.11	32.73	0.85	79.70	0.34	8.47
V79	5.57	7.64	1.73	3.46	2.26	0.04
V80	1.91	17.05	0.54	16.70	0.22	0.02
V81	0.04	1.26	0.80	0.14	1.32	1.81
V82	35.75	0.96	5.04	0.59	0.04	1.08
V83	2.44	3.09	0.04	0.58	0.41	0.15
V84	0.69	0.05	0.03	0.01	0.03	0.20
V85	0.00	0.02	0.00	0.00	0.01	11.02
V86	0.00	1.91	0.00	0.01	0.02	0.71
V87	0.00	0.02	0.00	0.09	0.67	17.97
V88	0.02	0.67	0.15	0.31	12.18	2.06
V89	0.91	31.63	0.14	0.04	0.02	0.03
V90	0.75	0.30	1.26	10.78	0.08	0.05
V91	15.89	0.01	2.19	11.99	1.22	0.03
V92	0.00	4.81	0.00	0.01	0.00	0.01
V93	4.60	4.53	2.15	2.44	0.31	0.16
V94	0.01	3.90	0.00	1.04	0.18	16.47
V95	0.10	0.00	0.01	0.00	0.00	0.00
V96	2.01	3.23	0.41	2.60	0.10	0.45
V97	0.00	0.02	0.42	0.00	0.02	0.87
V98	0.83	22.18	2.29	0.00	2.03	1.74
V99	15.30	0.00	2.24	0.05	0.01	0.33
V100	0.05	0.46	0.00	9.00	0.01	2.94
V101	0.14	0.25	0.53	0.00	0.01	0.01
V102	3.26	2.08	0.00	0.59	0.01	0.06

V103	0.00	0.25	0.00	0.01	0.07	1.11
V104	0.04	5.40	0.00	0.02	0.06	0.07
V105	0.05	0.00	0.04	0.32	0.57	0.00
V106	1.10	0.01	0.81	0.01	7.41	0.01
V107	11.14	0.47	8.53	0.25	10.83	1.96
V108	9.90	1.06	3.07	1.17	0.69	8.80
V109	1.02	17.72	0.04	9.09	1.79	0.00
V110	0.04	7.44	0.42	4.17	0.15	0.00
V111	2.05	10.87	2.12	6.04	0.10	0.48
V112	0.39	1.40	0.26	1.58	4.98	0.74
V113	5.94	12.57	5.03	11.68	0.17	2.91
V114	0.07	0.00	0.05	0.01	6.20	14.95
V115	7.83	79.35	2.24	63.69	0.99	3.15
V116	6.87	1.05	12.05	15.59	91.39	2.43
V117	95.18	28.37	45.67	3.82	2.14	3.67
V118	0.45	39.71	0.73	2.09	1.42	8.63
V119	8.50	6.18	4.46	2.35	10.21	24.06
V120	2.31	0.03	9.82	0.79	23.16	0.80
V121	4.41	10.98	2.71	5.95	3.65	0.70
V122	24.21	17.55	6.59	9.54	5.70	6.25
V123	1.39	0.00	0.39	0.01	4.40	42.42
V124	0.08	0.00	0.02	0.02	0.23	4.08
V125	0.03	1.08	0.17	1.67	0.56	5.76
V126	0.03	0.27	0.01	0.00	4.29	12.94
V127	1.64	9.56	2.95	4.34	0.28	9.38
V128	4.35	0.28	1.65	0.30	1.49	2.86
V129	6.54	24.51	0.01	41.68	21.81	18.60
V130	132.13	154.04	35.18	124.20	13.59	0.53
V131	43.81	187.61	72.54	7.71	39.05	0.03
V132	0.58	0.65	0.01	2.93	0.24	5.28
V133	0.31	114.60	1.55	0.36	20.64	1.39
V134	96.36	19.90	72.83	53.04	89.53	1.59
V135	0.44	1.92	0.02	1.36	0.01	6.59
V136	122.86	0.92	77.17	0.42	227.00	54.05
V137	0.08	13.74	0.04	0.41	27.87	1.31
V138	32.03	18.69	26.78	9.96	0.00	11.88
V139	0.31	27.26	0.05	0.00	0.05	26.34
V140	1.60	0.08	0.56	31.78	0.01	137.17
V141	3.20	5.08	5.54	93.83	5.77	2.83
V142	6.81	3.44	0.14	0.23	0.06	0.54
V143	0.00	0.00	1.39	0.72	21.09	16.94
V144	19.60	100.40	9.50	16.69	87.23	5.77
V145	105.41	10.33	62.09	3.38	0.30	0.31
V146	56.90	0.46	36.21	49.05	33.22	5.42
V147	13.47	155.52	0.68	14.16	29.62	13.89
V148	24.59	215.93	12.22	27.65	20.35	129.10
V149	1.75	81.98	0.04	14.13	9.75	0.09
V150	76.51	2.55	50.88	2.46	21.14	3.01
V151	13.20	0.07	2.78	0.99	8.87	0.14
V152	2.11	2.83	0.07	4.62	0.00	178.48
V153	5.09	1.45	0.11	5.40	2.93	108.73
V154	3.36	0.04	2.62	4.22	2.02	2.40
V155	0.04	1.88	0.04	0.03	5.88	14.74
V156	2.81	0.02	0.70	0.00	0.23	5.47

V157	0.29	13.04	0.07	1.39	0.08	5.64
V158	0.25	28.62	0.07	9.42	0.51	1.78
V159	34.64	1.52	8.40	9.82	26.83	4.88
V160	1.70	30.22	1.69	0.21	3.76	0.05
V161	0.12	25.66	0.84	16.68	26.86	3.79
V162	12.54	4.11	6.06	0.68	0.01	0.03
V163	1.55	1.86	7.63	3.11	2.46	4.55
V164	83.35	10.92	84.02	8.46	78.88	15.17
V165	0.00	17.36	8.33	7.51	19.21	6.60
V166	129.32	47.06	38.17	0.98	124.82	10.43
V167	1.22	100.29	5.52	138.63	0.10	39.89
V168	6.57	148.02	0.01	2.57	18.21	3.05
V169	13.81	83.12	13.75	0.73	13.89	23.06
V170	155.38	111.98	130.28	0.00	80.51	27.39
V171	8.30	0.00	0.22	4.50	43.18	10.21
V172	0.07	23.54	70.67	0.00	0.00	0.00
V173	177.93	2.42	0.02	10.16	149.09	280.88
V174	13.51	1.19	0.42	4.37	1.20	14.75
V175	32.92	23.57	1.10	17.80	29.39	17.49
V176	108.55	47.91	15.34	0.00	63.68	0.03
V177	296.11	3.87	167.74	19.26	306.78	3.09
V178	0.01	0.01	0.01	0.00	0.47	19.07
V179	0.73	0.00	0.59	0.00	0.06	13.26
V180	0.01	0.01	0.11	0.00	0.00	5.70
V181	0.00	0.01	0.01	0.00	0.00	58.36
V182	0.98	0.01	0.00	0.06	0.02	0.10
V183	0.00	0.00	0.00	0.00	0.00	27.28
V184	0.00	0.03	0.00	0.00	0.00	0.01
V185	0.00	0.15	0.30	0.17	0.00	0.01
V186	0.00	0.92	0.03	0.00	0.02	0.01
V187	0.00	0.04	0.03	0.01	0.03	0.03
V188	0.02	0.00	0.35	0.00	0.04	0.26
V189	0.01	0.00	0.06	0.00	0.35	0.00
V190	0.33	0.00	0.08	0.06	0.00	0.08
V191	0.00	0.04	0.00	0.12	0.14	0.04
V192	0.00	0.01	0.61	0.00	0.02	0.20
V193	0.09	0.01	0.00	0.15	0.00	0.00
V194	0.00	0.18	0.01	0.00	0.13	0.03
V195	0.01	0.01	0.16	0.23	0.00	0.06
V196	0.00	0.17	0.00	0.04	0.02	0.02
V197	0.03	0.18	0.01	0.00	0.05	0.00
V198	0.05	3.71	0.12	0.65	0.00	0.03
V199	0.04	1.48	0.01	0.40	0.00	0.01
V200	0.83	0.09	0.03	0.00	0.14	0.02
V201	0.00	3.93	0.02	0.90	0.18	0.08

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**Table S6.** The reorganization energy (cm<sup>-1</sup>) between S<sub>1</sub> and T<sub>1</sub> minima vs each frequency of the title compound by NMA method with Cartesian coordinate

.	In vacuum		In toluene		In cluster	
	S <sub>1</sub> →T <sub>1</sub>	T <sub>1</sub> →S <sub>1</sub>	S <sub>1</sub> →T <sub>1</sub>	T <sub>1</sub> →S <sub>1</sub>	S <sub>1</sub> →T <sub>1</sub>	T <sub>1</sub> →S <sub>1</sub>
v <sub>1</sub>	1.6	7.5	5.1	13.8	29.9	14.7
v <sub>2</sub>	22.2	12.0	11.2	1.3	8.1	0.0
v <sub>3</sub>	50.2	71.6	20.9	4.8	0.8	0.0
v <sub>4</sub>	6.6	28.3	0.9	133.8	0.1	1.6
v <sub>5</sub>	32.9	76.2	5.5	101.9	14.6	5.9
v <sub>6</sub>	412.9	6.2	308.8	16.4	0.9	0.0
v <sub>7</sub>	174.0	13.8	71.0	1.0	0.0	0.7
v <sub>8</sub>	297.3	11.3	126.3	10.2	2.2	2.6
v <sub>9</sub>	19.9	10.7	0.0	2.8	0.0	6.7
v <sub>10</sub>	82.1	5.2	32.1	0.1	50.6	34.9
v <sub>11</sub>	29.0	1.9	11.5	0.3	84.2	12.8
v <sub>12</sub>	21.3	34.8	11.1	17.2	2.0	41.5
v <sub>13</sub>	50.6	1.1	16.8	1.7	1.0	88.1
v <sub>14</sub>	56.3	44.3	25.5	0.0	22.8	0.0
v <sub>15</sub>	17.0	3.7	9.8	9.8	12.8	88.6
v <sub>16</sub>	26.1	2.1	30.8	3.1	44.4	1.2
v <sub>17</sub>	22.1	2.9	13.4	6.0	0.4	6.9
v <sub>18</sub>	6.6	5.0	4.2	2.2	5.2	6.5
v <sub>19</sub>	2.3	1.6	0.6	0.0	2.7	38.4
v <sub>20</sub>	6.3	33.9	9.9	16.1	1.4	7.8
v <sub>21</sub>	0.0	6.5	0.9	7.6	91.7	85.5
v <sub>22</sub>	5.0	5.1	3.4	0.6	32.1	0.8
v <sub>23</sub>	10.1	2.4	6.2	0.0	7.3	4.4
v <sub>24</sub>	3.7	1.4	0.0	1.5	6.7	0.5
v <sub>25</sub>	0.0	4.6	0.1	2.3	0.6	0.0
v <sub>26</sub>	0.8	1.2	0.3	0.1	4.5	1.8
v <sub>27</sub>	28.2	0.3	12.0	2.0	0.1	0.1
v <sub>28</sub>	14.4	22.9	1.5	14.3	1.5	0.2
v <sub>29</sub>	0.7	3.7	0.3	0.2	0.0	0.0
v <sub>30</sub>	0.0	6.6	0.0	1.4	1.9	4.1
v <sub>31</sub>	9.2	0.2	1.8	0.2	0.0	2.3
v <sub>32</sub>	6.2	30.4	10.0	1.7	52.0	18.3
v <sub>33</sub>	0.0	1.1	1.9	19.7	52.8	57.8
v <sub>34</sub>	14.6	1.0	9.7	48.3	11.9	7.8
v <sub>35</sub>	0.1	235.8	1.1	73.9	1.1	12.5
v <sub>36</sub>	12.3	0.0	7.9	1.6	0.0	0.0
v <sub>37</sub>	1.6	0.0	0.6	0.7	3.7	0.7
v <sub>38</sub>	2.3	16.8	1.4	3.9	0.1	0.0
v <sub>39</sub>	13.4	0.5	8.7	1.2	2.8	3.7
v <sub>40</sub>	4.0	0.0	1.9	0.1	4.2	2.9
v <sub>41</sub>	4.9	0.9	3.5	6.9	5.3	14.2
v <sub>42</sub>	118.2	28.7	54.7	7.3	10.7	9.8
v <sub>43</sub>	22.0	94.3	26.9	43.1	18.6	2.7
v <sub>44</sub>	42.4	0.4	5.0	0.5	0.0	17.5
v <sub>45</sub>	178.3	203.2	74.7	86.8	17.3	0.1
v <sub>46</sub>	410.5	1.9	127.8	9.9	2.7	0.1
v <sub>47</sub>	0.1	73.8	0.0	36.1	1.8	0.0
v <sub>48</sub>	1.8	0.0	1.8	2.0	0.1	0.2
v <sub>49</sub>	0.9	4.1	0.0	0.1	0.5	0.1

V50	19.2	0.1	1.8	0.0	0.8	0.8
V51	2.6	184.5	0.1	22.6	0.2	0.0
V52	0.0	0.1	0.0	0.0	0.1	1.8
V53	0.0	12.1	0.0	0.1	14.4	0.1
V54	5.5	0.9	0.8	1.3	8.2	0.0
V55	43.8	11.9	16.8	0.2	0.0	4.9
V56	131.8	128.3	19.8	0.0	0.0	0.8
V57	32.8	7.2	18.2	9.9	0.0	0.0
V58	0.4	16.5	0.1	2.9	1.4	0.9
V59	0.1	41.0	0.1	9.9	1.5	0.1
V60	361.6	875.8	67.8	183.1	4.1	0.0
V61	43.4	0.2	5.6	1.2	0.2	0.0
V62	263.5	3.0	132.6	0.0	24.8	1.4
V63	62.7	653.0	31.1	305.6	0.0	0.9
V64	107.9	61.4	11.6	9.0	0.6	1.3
V65	0.9	2.7	0.1	0.0	3.3	0.6
V66	5.6	1.0	3.0	0.2	0.0	3.1
V67	4.1	0.0	4.0	1.1	1.1	1.9
V68	48.1	269.6	9.0	61.5	8.5	0.3
V69	5.2	10.1	0.9	5.4	0.0	0.3
V70	4.2	0.0	0.9	0.0	0.2	0.2
V71	2145.1	11.1	413.0	601.2	0.8	0.0
V72	15.3	2850.8	3.1	34.1	24.1	0.0
V73	0.2	0.1	0.0	0.0	0.0	0.2
V74	0.4	1.4	0.0	0.0	0.0	0.0
V75	1.0	195.8	1.7	0.0	2.0	0.0
V76	0.0	0.0	2.6	26.0	1.6	0.1
V77	16.9	86.1	0.1	3.4	0.1	0.6
V78	16.6	33.7	2.6	89.1	0.2	0.3
V79	226.2	8.0	33.5	4.5	10.9	2.0
V80	192.6	12.9	130.1	31.9	0.2	0.2
V81	1245.3	77.2	146.8	39.1	22.9	1.6
V82	2.8	1287.7	1.0	293.0	14.0	0.0
V83	0.9	2.5	0.0	0.5	0.0	0.7
V84	0.6	0.0	0.0	0.0	0.1	0.0
V85	0.0	0.0	0.0	0.0	0.0	0.0
V86	0.0	758.8	0.0	0.0	0.0	0.0
V87	0.0	0.0	0.0	1.4	0.2	1.3
V88	0.2	0.7	0.7	100.0	27.9	7.2
V89	7.0	28.7	0.7	4.0	0.0	3.6
V90	32.4	0.6	4.2	343.7	0.2	0.3
V91	2.6	0.0	2.6	0.0	7.2	2.9
V92	0.2	1055.8	0.1	0.0	0.7	0.0
V93	819.3	4.6	180.3	64.4	0.3	0.0
V94	0.4	165.5	0.0	0.2	1.8	0.0
V95	3.4	0.0	0.1	0.0	0.0	0.0
V96	0.4	37.8	0.5	12.5	0.1	0.0
V97	0.1	0.0	14.3	0.0	1.8	0.0
V98	17.1	168.7	68.7	0.1	0.1	0.3
V99	501.3	0.0	5.2	0.5	0.0	0.0
V100	0.0	0.2	0.0	31.0	0.0	0.2
V101	1.2	0.4	1.7	0.0	3.1	0.0
V102	11.8	3.6	0.0	1.1	14.4	0.0
V103	0.0	0.4	0.0	0.0	0.0	0.0

V104	1.3	6.5	0.1	0.0	0.0	0.0
V105	0.6	0.0	0.6	0.0	0.6	0.5
V106	46.4	0.2	10.5	0.0	0.7	2.4
V107	1.3	0.2	0.0	0.0	3.3	8.9
V108	7.9	48.9	6.6	4.2	19.1	0.7
V109	777.4	287.9	172.6	63.8	3.0	1.9
V110	239.1	197.8	24.6	55.8	2.9	0.5
V111	23.5	259.6	4.9	65.3	4.4	0.0
V112	18.8	49.5	2.2	18.3	10.2	3.4
V113	114.7	196.0	15.3	80.0	30.9	0.1
V114	9.1	2.8	0.8	0.6	1.0	3.0
V115	0.5	130.7	0.7	131.5	1.4	1.0
V116	150.0	4.4	18.0	67.0	7.0	62.3
V117	0.0	474.7	3.0	1.4	55.9	1.8
V118	14.2	67.8	3.1	39.8	3.5	1.9
V119	98.9	57.5	24.9	5.4	7.6	10.4
V120	96.0	3.2	55.8	0.0	17.3	19.7
V121	56.4	235.0	12.7	78.7	8.9	7.2
V122	0.7	42.4	0.1	6.1	3.4	4.4
V123	32.0	5.4	1.6	0.5	20.2	2.8
V124	6.0	0.0	0.9	0.0	0.6	0.2
V125	88.5	9.0	14.5	0.4	0.2	0.1
V126	11.0	6.3	0.9	0.2	5.1	4.2
V127	22.7	19.1	15.9	5.3	1.1	0.1
V128	80.8	111.5	11.2	17.2	0.7	1.1
V129	195.7	260.1	39.3	209.8	3.8	23.1
V130	835.1	1154.1	18.9	386.9	63.1	11.6
V131	181.3	803.3	49.1	43.1	1.1	29.5
V132	0.6	12.5	3.3	10.0	12.4	0.0
V133	29.3	359.7	1.3	2.3	34.1	20.6
V134	10.8	47.4	33.2	63.9	150.7	77.8
V135	1.1	24.7	0.0	0.2	2.6	0.0
V136	29.8	2.3	2.7	0.2	0.5	191.9
V137	3.0	14.9	1.6	17.4	14.3	22.9
V138	24.8	58.9	21.3	14.5	4.6	0.7
V139	0.4	126.4	0.0	0.1	1.1	0.0
V140	1.4	0.8	0.5	47.8	7.8	0.0
V141	21.2	1.7	11.5	35.9	13.1	5.5
V142	5.8	1.7	0.0	3.8	142.1	0.0
V143	0.2	0.2	1.7	0.5	0.0	20.6
V144	37.4	36.9	16.4	7.0	0.9	82.9
V145	42.6	52.1	42.5	17.3	0.0	1.5
V146	34.3	13.9	37.2	55.0	176.9	34.7
V147	46.0	212.5	6.9	2.1	119.6	24.5
V148	24.5	226.4	12.4	15.3	3.5	19.2
V149	0.0	42.3	0.2	2.2	15.3	8.3
V150	85.3	2.9	57.7	0.1	8.5	22.9
V151	2.7	0.1	0.7	0.0	4.5	7.9
V152	3.5	54.0	0.4	30.0	2.0	0.3
V153	4.1	18.4	0.2	4.2	5.1	2.1
V154	0.7	0.2	1.2	0.1	0.0	1.9
V155	0.4	0.6	0.0	0.1	3.0	5.5
V156	5.3	0.4	2.8	0.0	0.0	0.2
V157	3.3	0.4	0.4	0.0	3.6	0.0



V158	0.8	13.8	0.3	10.8	14.7	0.2
V159	25.6	10.6	3.3	1.9	6.8	23.6
V160	9.7	19.4	5.0	3.9	6.8	3.9
V161	9.6	4.5	9.0	9.8	40.7	27.5
V162	16.5	2.1	12.2	0.5	3.1	0.0
V163	0.0	0.3	1.7	1.0	20.4	2.2
V164	279.0	12.2	195.1	6.6	31.5	78.9
V165	3.4	46.1	5.1	60.5	10.2	20.0
V166	124.5	281.5	23.2	19.1	0.4	116.4
V167	12.2	14.0	13.7	56.5	272.8	0.2
V168	23.5	37.9	0.4	0.4	15.2	19.0
V169	8.7	15.7	13.2	0.0	17.0	14.2
V170	105.7	15.4	133.8	0.2	0.0	79.7
V171	6.8	2.4	0.3	0.4	3.2	43.3
V172	1.8	2.3	91.5	0.2	19.9	0.0
V173	186.9	11.4	0.1	24.6	13.0	146.6
V174	1.0	26.4	0.1	24.0	5.8	1.2
V175	53.4	59.2	12.3	67.3	61.4	30.8
V176	242.5	218.2	38.5	1.5	0.0	61.6
V177	6.1	137.5	6.5	102.4	29.4	274.1
V178	20.0	17.1	8.3	6.8	0.0	2.2
V179	23.4	0.0	5.3	0.0	0.0	0.1
V180	0.0	0.0	0.0	0.7	0.0	0.0
V181	0.3	5.8	0.1	0.0	0.0	0.0
V182	46.1	0.1	0.0	0.4	0.0	0.0
V183	0.0	6.9	1.7	0.8	0.0	0.0
V184	14.8	0.2	0.0	0.0	0.1	0.0
V185	0.0	0.2	2.3	18.1	0.0	1.0
V186	0.3	109.1	9.0	0.0	0.2	0.0
V187	11.9	2.0	2.8	0.5	0.0	0.0
V188	170.7	0.0	134.7	4.1	0.0	0.0
V189	3.8	0.0	11.1	0.0	0.8	4.5
V190	725.1	32.5	17.1	60.7	0.0	0.0
V191	0.0	119.2	1.3	8.4	0.0	0.1
V192	0.1	40.9	248.0	0.0	1.6	0.0
V193	187.3	158.3	0.0	4.5	0.2	0.0
V194	64.4	1.1	0.1	0.0	0.0	0.7
V195	36.9	1.7	8.3	0.2	0.1	0.0
V196	0.0	0.1	0.0	22.3	0.1	0.0
V197	7.7	10.5	0.0	0.6	0.0	0.0
V198	1596.1	380.0	226.1	85.1	0.0	0.0
V199	0.1	1782.3	0.2	337.5	0.3	0.0
V200	1883.2	1.2	311.8	0.1	0.1	0.0
V201	0.1	1885.3	0.0	317.8	2.2	0.3

**Table S7.** The reorganization energy (cm<sup>-1</sup>) between S<sub>0</sub> and S<sub>1</sub> minima vs each frequency of the title compound by NMA method with internal coordinate

.	In vacuum		In toluene		In cluster	
	S <sub>0</sub> →S <sub>1</sub>	S <sub>1</sub> →S <sub>0</sub>	S <sub>0</sub> →S <sub>1</sub>	S <sub>1</sub> →S <sub>0</sub>	S <sub>0</sub> →S <sub>1</sub>	S <sub>1</sub> →S <sub>0</sub>
v <sub>1</sub>	6.52	1.37	69.04	19.24	1.49	1.66
v <sub>2</sub>	4.43	2.81	21.22	3.09	0.80	0.22
v <sub>3</sub>	0.62	0.40	0.22	5.15	0.01	0.04
v <sub>4</sub>	0.06	0.02	0.11	0.15	5.81	4.30
v <sub>5</sub>	0.04	0.05	1.24	0.21	0.53	0.01
v <sub>6</sub>	1.03	2.84	3.41	0.03	1.29	3.26
v <sub>7</sub>	3.65	0.31	3.23	0.00	0.68	1.43
v <sub>8</sub>	3.53	5.20	1.97	0.02	4.34	3.01
v <sub>9</sub>	0.00	0.01	11.19	0.01	1.12	1.01
v <sub>10</sub>	0.31	0.63	2.37	0.05	0.14	0.18
v <sub>11</sub>	0.17	0.03	0.64	0.46	11.10	17.56
v <sub>12</sub>	2.23	2.60	1.89	2.84	16.70	12.38
v <sub>13</sub>	9.46	12.78	4.03	11.56	20.54	19.90
v <sub>14</sub>	14.45	55.24	57.00	61.88	2.22	0.03
v <sub>15</sub>	49.50	0.47	29.55	1.27	3.59	0.00
v <sub>16</sub>	0.00	0.15	1.40	0.14	2.28	6.40
v <sub>17</sub>	0.31	0.42	0.24	0.50	0.30	0.81
v <sub>18</sub>	0.30	0.06	0.90	0.46	0.28	0.29
v <sub>19</sub>	0.45	0.32	1.67	0.85	4.12	3.99
v <sub>20</sub>	0.01	0.04	0.23	1.13	3.16	2.13
v <sub>21</sub>	0.05	0.20	0.06	0.00	0.15	0.17
v <sub>22</sub>	2.54	2.65	2.76	8.40	3.12	3.76
v <sub>23</sub>	0.39	0.31	0.01	4.36	0.52	0.00
v <sub>24</sub>	0.58	0.02	2.11	0.01	2.51	1.76
v <sub>25</sub>	2.35	2.18	0.99	1.98	2.98	4.58
v <sub>26</sub>	0.03	0.28	0.42	0.47	0.07	0.00
v <sub>27</sub>	0.00	3.58	4.28	19.65	0.25	0.20
v <sub>28</sub>	3.26	4.50	1.15	3.97	8.06	6.09
v <sub>29</sub>	4.08	3.31	5.29	0.16	0.45	0.55
v <sub>30</sub>	0.77	0.01	2.71	0.53	0.19	0.00
v <sub>31</sub>	24.54	2.92	56.31	11.04	17.39	2.25
v <sub>32</sub>	2.98	12.42	0.06	56.40	70.72	46.05
v <sub>33</sub>	99.46	20.39	138.81	7.51	29.45	76.83
v <sub>34</sub>	6.02	25.44	48.66	19.62	0.62	4.22
v <sub>35</sub>	18.14	50.03	16.07	2.64	0.01	0.01
v <sub>36</sub>	16.41	0.05	30.19	2.24	0.05	0.02
v <sub>37</sub>	0.24	0.00	0.13	0.02	24.57	2.76
v <sub>38</sub>	2.36	3.61	0.01	5.73	0.03	5.23
v <sub>39</sub>	14.19	20.71	1.42	48.37	0.14	1.33
v <sub>40</sub>	0.50	5.26	0.10	14.59	11.94	0.57
v <sub>41</sub>	10.50	8.38	1.22	27.05	0.74	0.40
v <sub>42</sub>	2.98	97.49	4.31	254.89	7.41	63.73
v <sub>43</sub>	7.07	21.43	13.87	25.37	72.47	9.28
v <sub>44</sub>	1.83	5.03	22.07	25.66	1.79	9.46
v <sub>45</sub>	0.15	80.79	34.62	298.19	4.28	17.42
v <sub>46</sub>	0.16	66.38	4.32	258.54	0.38	23.86
v <sub>47</sub>	0.97	3.69	0.13	0.97	3.48	3.12
v <sub>48</sub>	0.15	3.30	0.01	13.67	0.13	2.93
v <sub>49</sub>	0.07	0.03	0.54	0.12	0.01	0.00

V50	0.33	0.70	2.23	0.00	0.46	0.65
V51	0.02	0.03	0.01	0.07	0.02	0.00
V52	0.04	0.00	0.51	0.08	0.02	0.05
V53	0.17	0.30	0.25	0.02	0.52	0.46
V54	0.01	0.07	0.81	0.40	0.16	0.07
V55	1.31	8.20	0.90	9.53	3.63	8.20
V56	1.11	2.11	0.18	7.64	4.65	0.64
V57	1.60	2.08	21.92	19.20	0.04	0.04
V58	0.86	2.41	0.60	0.57	1.24	0.66
V59	0.00	1.92	0.08	7.24	0.03	1.02
V60	0.06	0.17	3.14	14.83	0.04	0.00
V61	0.01	0.03	9.96	2.04	0.03	0.00
V62	46.77	0.52	344.16	166.57	5.31	6.74
V63	6.77	21.82	59.50	168.26	1.68	0.58
V64	0.55	16.81	3.94	32.00	0.43	0.22
V65	6.13	0.27	0.46	0.03	1.20	0.17
V66	0.00	12.08	4.23	22.09	0.11	6.37
V67	0.13	0.26	0.22	3.45	11.89	3.15
V68	3.79	1.45	3.81	0.41	2.99	0.26
V69	0.01	3.23	0.53	10.85	0.43	4.87
V70	0.04	0.17	0.04	2.12	0.08	4.01
V71	0.05	15.31	64.27	181.93	3.47	4.79
V72	0.06	1.80	17.50	8.53	3.19	1.01
V73	0.00	0.06	0.06	0.11	0.15	0.02
V74	0.00	0.00	0.06	0.05	0.00	0.00
V75	0.17	0.05	5.94	0.71	0.04	1.53
V76	0.01	0.19	0.02	2.56	0.02	0.01
V77	0.11	0.00	0.62	0.33	1.09	0.15
V78	0.52	0.38	1.17	2.09	0.07	0.25
V79	5.05	3.17	12.65	0.70	5.54	4.10
V80	5.58	2.73	28.69	64.02	9.49	0.06
V81	0.28	20.69	0.11	57.45	0.00	11.93
V82	0.01	0.15	0.01	0.00	0.06	0.04
V83	0.00	0.00	0.04	0.26	0.04	0.50
V84	0.00	0.08	0.02	0.43	0.57	0.01
V85	0.03	0.07	0.03	0.09	0.09	0.04
V86	0.01	0.00	0.08	0.00	0.03	0.26
V87	0.00	0.01	0.00	0.00	0.00	7.09
V88	0.02	5.90	0.03	7.32	0.01	0.33
V89	0.19	11.64	0.97	8.65	16.02	12.65
V90	10.35	3.61	0.90	0.24	0.53	0.97
V91	0.00	0.87	0.00	6.69	0.09	1.99
V92	0.17	0.00	2.92	0.03	0.05	0.00
V93	1.15	13.96	1.58	107.89	14.11	2.83
V94	13.70	0.00	24.20	0.01	1.59	1.32
V95	0.00	0.01	1.22	0.05	0.36	0.00
V96	0.10	1.15	0.07	1.29	2.97	0.05
V97	0.05	0.07	0.00	7.62	0.25	0.17
V98	0.38	0.40	0.66	30.19	0.00	15.27
V99	0.00	20.32	0.00	5.24	6.75	0.20
V100	0.09	0.01	13.04	0.06	8.76	11.02
V101	16.66	0.00	0.00	0.33	0.00	0.00
V102	0.32	0.99	0.01	0.04	0.06	0.03
V103	0.07	0.00	0.00	0.00	0.00	0.13

V104	0.02	0.03	0.10	0.08	0.09	0.00
V105	0.19	0.03	0.06	1.45	0.30	0.39
V106	0.24	3.98	30.82	44.71	1.49	0.04
V107	15.28	2.60	31.31	0.41	0.40	8.45
V108	0.26	53.19	15.31	120.63	7.59	4.68
V109	0.42	1.89	57.63	100.07	5.49	4.39
V110	0.36	13.54	33.12	27.22	1.01	4.64
V111	0.46	0.45	0.00	8.18	0.22	0.01
V112	0.31	0.13	4.61	2.81	0.14	0.06
V113	0.05	0.01	4.85	8.60	0.02	0.13
V114	0.11	0.09	1.06	0.05	0.27	0.15
V115	1.12	0.62	3.06	2.63	1.32	3.59
V116	9.53	1.82	77.69	3.51	3.52	6.29
V117	0.39	0.21	0.34	17.35	4.33	0.62
V118	2.23	0.00	6.61	0.06	0.39	9.59
V119	1.19	25.85	0.38	41.69	5.35	6.74
V120	6.36	8.76	20.03	65.14	40.23	4.79
V121	33.73	0.82	5.69	7.80	0.22	51.15
V122	0.77	67.84	0.15	62.30	0.02	0.10
V123	0.00	0.02	6.44	1.44	0.19	0.11
V124	0.73	0.07	1.57	0.98	22.40	0.31
V125	0.22	9.01	0.01	34.21	23.99	1.87
V126	0.89	1.82	3.75	9.42	1.29	16.12
V127	20.19	6.71	16.32	31.77	2.01	1.96
V128	1.85	3.17	0.38	15.33	3.18	0.00
V129	0.84	40.44	20.60	30.45	0.07	40.62
V130	6.86	4.91	61.06	0.08	0.60	1.84
V131	1.97	0.56	9.89	73.64	0.54	5.18
V132	4.00	4.78	3.79	8.28	1.68	0.22
V133	22.15	0.00	21.13	0.04	26.22	2.06
V134	15.24	0.30	0.22	2.06	6.21	1.81
V135	15.74	3.73	14.81	10.11	32.53	3.99
V136	11.00	11.69	2.39	40.44	26.80	1.28
V137	21.87	15.28	16.72	31.74	0.01	4.83
V138	0.00	2.81	0.49	0.05	0.10	7.88
V139	0.07	0.00	0.37	0.01	0.65	0.30
V140	5.52	0.20	5.60	3.41	3.40	2.63
V141	0.01	6.94	0.90	15.47	33.61	13.00
V142	71.14	13.44	70.24	4.07	0.21	0.19
V143	1.34	0.00	13.10	3.98	28.38	42.41
V144	16.75	45.36	15.93	43.38	18.43	59.88
V145	1.35	56.23	0.50	40.47	132.43	0.15
V146	134.78	0.00	105.20	5.58	15.12	58.79
V147	1.92	74.73	1.45	107.99	1.79	19.80
V148	22.04	50.41	30.04	67.93	12.65	48.99
V149	18.70	17.36	21.70	13.28	13.64	8.45
V150	1.36	13.79	0.34	17.30	30.98	6.34
V151	16.96	25.65	13.53	28.18	7.27	34.26
V152	18.46	4.33	24.19	1.31	0.29	0.42
V153	0.02	0.64	0.06	0.59	2.83	1.72
V154	1.08	0.10	1.01	0.13	1.23	1.08
V155	0.31	3.68	1.51	2.16	1.69	9.03
V156	0.53	6.82	0.52	0.04	0.00	0.37
V157	4.60	0.06	13.16	0.01	15.15	5.30

V158	73.07	2.36	61.61	0.29	33.22	2.24
V159	23.31	38.17	27.82	12.58	33.75	40.85
V160	1.46	8.03	0.77	7.08	1.46	6.17
V161	9.59	5.16	10.77	14.36	10.33	38.62
V162	0.60	25.12	0.23	37.48	23.62	0.31
V163	32.82	13.65	34.75	7.32	3.66	5.19
V164	0.65	69.33	4.09	181.89	1.04	36.08
V165	1.26	1.85	3.37	0.12	10.72	7.98
V166	31.52	15.06	17.29	1.71	38.58	16.26
V167	31.46	3.06	38.46	3.24	21.21	4.05
V168	7.85	0.01	8.21	4.96	0.22	24.73
V169	0.38	24.16	2.94	23.24	0.03	0.59
V170	12.82	66.08	0.00	106.62	19.22	68.79
V171	10.53	2.16	28.28	0.20	10.29	28.84
V172	1.94	0.18	4.48	70.24	1.54	0.05
V173	48.02	83.60	33.96	0.03	38.05	71.93
V174	1.78	0.19	2.31	0.79	25.48	0.02
V175	15.52	4.72	9.16	23.98	3.84	24.98
V176	244.83	62.47	59.51	29.32	332.37	14.91
V177	21.30	409.11	6.25	871.07	71.14	270.56
V178	0.00	1.41	0.11	13.70	0.04	0.19
V179	0.16	1.74	0.57	7.59	0.02	0.10
V180	0.18	0.11	1.68	0.05	0.02	0.02
V181	1.16	0.00	12.59	0.30	0.04	0.00
V182	0.52	5.32	9.43	0.06	0.22	0.04
V183	0.10	0.00	0.11	1.96	0.00	0.00
V184	0.30	0.11	6.24	0.14	0.28	0.01
V185	0.01	0.01	1.32	21.68	0.13	0.04
V186	0.73	0.02	2.65	11.94	0.17	0.13
V187	0.36	0.68	12.68	7.84	0.55	0.18
V188	0.26	10.82	1.22	85.55	0.06	0.15
V189	0.00	9.02	1.13	15.79	0.00	0.49
V190	0.01	2.47	0.15	60.10	0.04	0.01
V191	0.34	0.00	2.96	0.72	0.04	0.67
V192	0.26	0.07	0.79	62.36	0.05	0.15
V193	1.37	0.00	28.60	0.19	0.43	0.13
V194	0.13	0.30	12.87	0.16	0.05	0.02
V195	0.04	0.44	0.88	22.57	0.30	0.00
V196	5.10	0.00	47.34	0.01	0.00	0.10
V197	10.03	0.25	107.32	0.04	0.11	0.37
V198	0.67	0.03	72.48	35.39	0.00	0.01
V199	0.62	0.34	1.41	0.18	0.19	0.25
V200	0.24	0.05	35.87	25.42	0.28	0.27
V201	0.39	0.01	0.81	0.00	0.93	0.92

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