

Supporting Information

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Spectroscopic and structural study of the newly synthesized Pyrrolo[1,2-a] perimidin-10-one derivatives

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(8-acetyl-10-oxo-9,10-dihydro-7H-pyrrolo[1,2-a]perimidin-9-yl)acetic acid (2a)

Brown crystals, (in CHCl₃, R_f = 0.48), yield: 81%; mp 224-226 °C. FT-IR (ATR) ν/cm^{-1} 3165 (NH), 1759, 1707, 1643 (C=O), 1618-1438 (C=C, C=N); ¹H NMR (400 MHz, DMSO-d₆): δ 12.42, (s, 1H, OH), 11.45 (s, 1H, NH), 8.38-7.26 (m, 6H, Ar-H), 3.95 (dd, *J* 5.4, 3.6 Hz, CH, enamine form), 3.01 (dd, *J* 16.6, 3.5 Hz, 1H, Ha, CH₂, A part of ABX system), 2.91 (dd, *J* 16.6, 5.6 Hz, 1H, Hb, CH₂, B part of ABX system), 2.08 (s, 3H, CH₃) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 188.3, 175.4, 170.9 (C=O), 172.2 (NH-C=C), 134.0, 134.0, 132.2, 130.4, 128.4, 127.9, 123.6, 121.3, 114.4, 110.3, 109.7, 91.1 (C=C, C=N), 41.6 (CH), 36.0 (CH₂), 27.0 (CH₃) ppm. Anal. Calcd for C₁₈H₁₄N₂O₄ (322.31 g/mol): C, 67.07; H, 4.38; N, 8.69. Found: C, 66.77; H, 4.23; N, 8.66%.

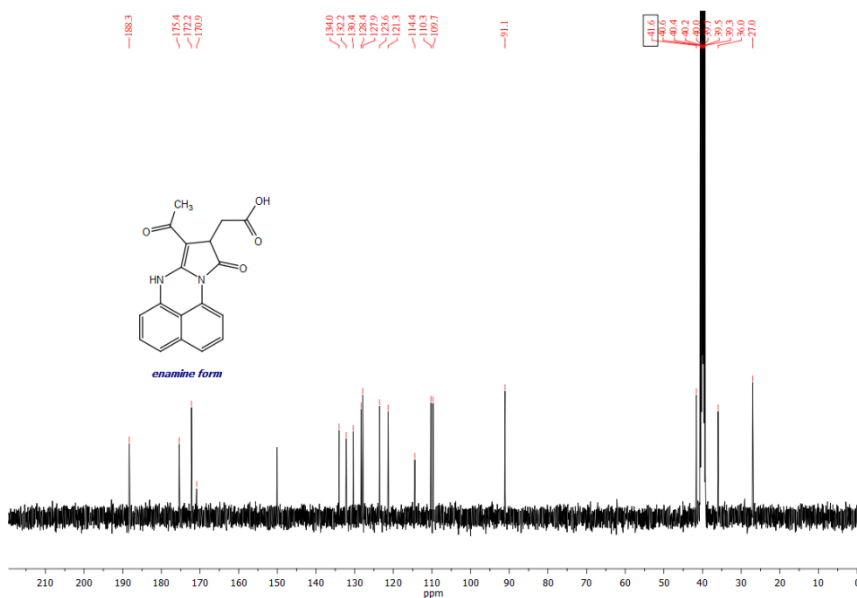


Figure S1. ¹³C NMR spectra of compound 2a

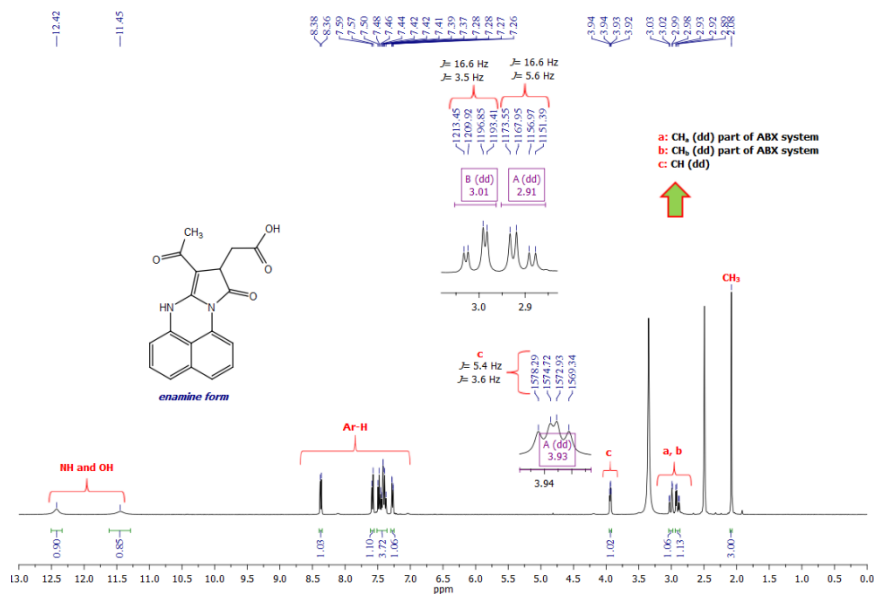


Figure S2. ^1H NMR spectra of compound **2a**

(8-benzoyl-10-oxo-9,10-dihydro-7H-pyrrolo[1,2-a]perimidin-9-yl)acetic acid (2b)

Brown crystals, (in CHCl_3 , $R_f = 0.45$), yield: 82%; mp 235-236 $^\circ\text{C}$. FT-IR (ATR) ν/cm^{-1} 3154 (NH), 1765, 1709, 1640 ($\text{C}=\text{O}$), 1611-1438 ($\text{C}=\text{C}$, $\text{C}=\text{N}$); ^1H NMR (400 MHz, DMSO-d_6): δ 12.24 (s, 1H, OH), 12.12 (s, 1H, NH), 8.40-7.35 (m, 11H, Ar-H), 5.18 (d, J 5.4 Hz, CH, imine form), 4.36 (t, J 4.2 Hz, CH, enamine form), 2.93 (broad d, CH, imine form), 2.73 (dd, J 16.9, 3.4 Hz, 1H, Ha, CH_2 , A part of ABX system), 2.13 (dd, J 16.9, 5.2 Hz, 1H, Hb, CH_2 , B part of ABX system) ppm; ^{13}C NMR(100 MHz, DMSO-d_6): δ 183.8, 175.5, 152.8 ($\text{C}=\text{O}$), 171.8 ($\text{NH}-\text{C}=\text{C}$), 140.3, 134.1, 132.2, 130.9, 130.4, 130.1, 129.2, 129.0, 128.8, 128.5, 128.0, 127.2, 123.7, 121.7, 119.0, 115.0, 110.8, 109.8, 90.9 ($\text{C}=\text{C}$, $\text{C}=\text{N}$), 41.8 (CH), 34.8 (CH_2) ppm. Anal. Calcd for $\text{C}_{23}\text{H}_{16}\text{N}_2\text{O}_4$ (384.38 g/mol): C, 71.87; H, 4.20; N, 7.29. Found: C, 71.47; H, 4.19; N, 7.19%.

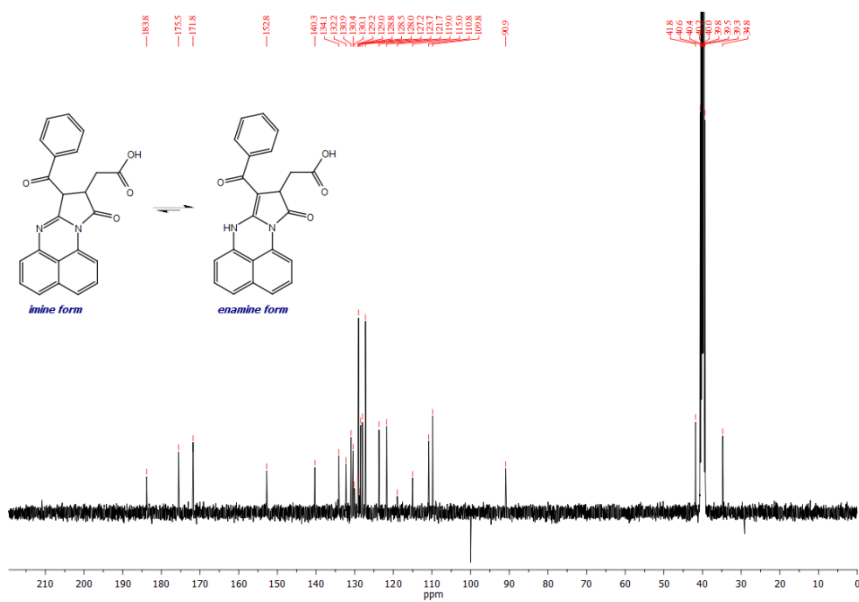


Figure S3. ^{13}C NMR spectra of compound 2b

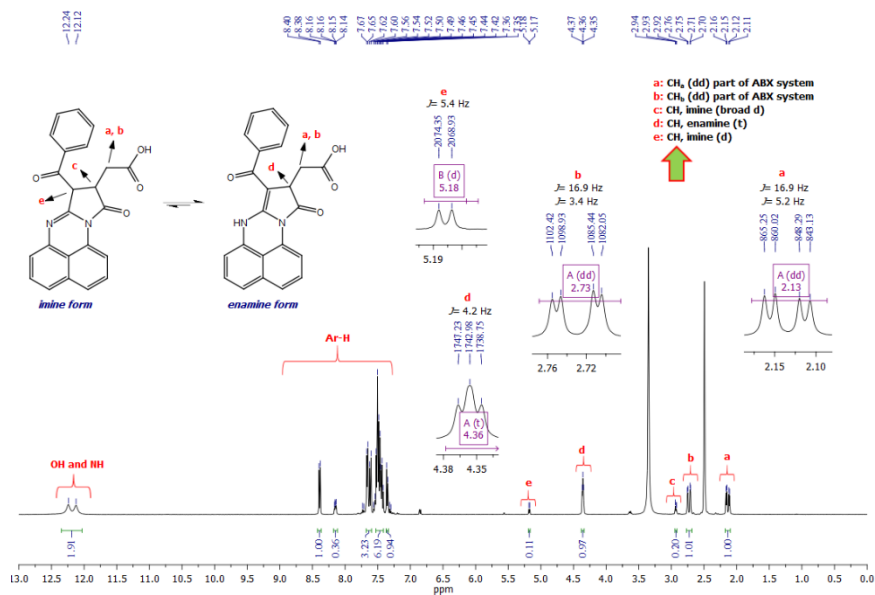


Figure S4. ^1H NMR spectra of compound 2b

[8-(3,4-dimethoxybenzoyl)-10-oxo-9,10-dihydro-7H-pyrrolo[1,2-a]perimidin-9-yl]acetic acid (2d)

Brown crystals, (in CHCl_3 , $R_f = 0.38$), yield: 83%; mp 222-223 °C. FT-IR (ATR) ν/cm^{-1} 3151 (NH, OH), 1764, 1726, 1641 (C=O), 1610-1446 C=C,C=N); ^1H NMR (400 MHz, DMSO- d_6): δ 12,27 (s, 1H, OH), 8.40-6.87 (m, 9H, Ar-H), 5.13(d, J 4.9 Hz, CH, imine form), 4.45 (broad t , CH, enamine form), 3.90, 3.85, 3.83, 3.81 ($4 \times$ s, 6H, OCH_3), 2.91 (d, J 6.1 Hz, CH, imine form), 2.78 (dd, J 17.0, 3.6 Hz, 1H, Ha, CH_2 , A part of ABX system), 2.34 (dd, J 17.0, 5.3 Hz, 1H, Hb, CH_2 , B part of ABX system) ppm; ^{13}C NMR (100 MHz, DMSO- d_6): δ 195.4, 182.7, 175.6, 175.3, 171.9, 156.1, (C=O), 172.9 NH-C=C), 154.3, 152.7, 151.3, 149.0, 148.9, 139.8, 134.4, 134.1, 132.5, 132.4, 132.2, 130.5, 128.8, 128.5, 128.0, 127.9, 125.6, 123.9, 123.7, 123.7, 121.6, 120.9, 118.9, 115.0, 111.8, 111.6, 111.4, 110.8, 110.7, 109.8, 109.0, 90.7 (C=C, C=N, aromatic), 56.4, 56.1, 56.0, 56.0 ($2 \times$ OCH_3), 49.8 (CH, imine form) 42.0 (CH), 34.8, 34.6 (CH_2) ppm. Anal. Calcd for $\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_6$ (444.44 g/mol): C, 67.56; H, 4.54; N, 6.30. Found: C, 67.84; H, 4.42; N, 6.08%.

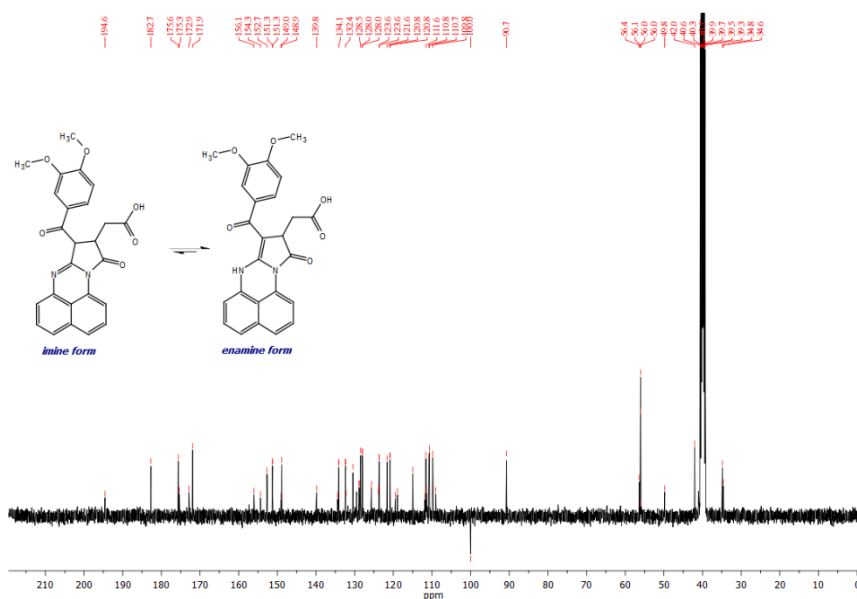


Figure S5. ^{13}C NMR spectra of compound 2d

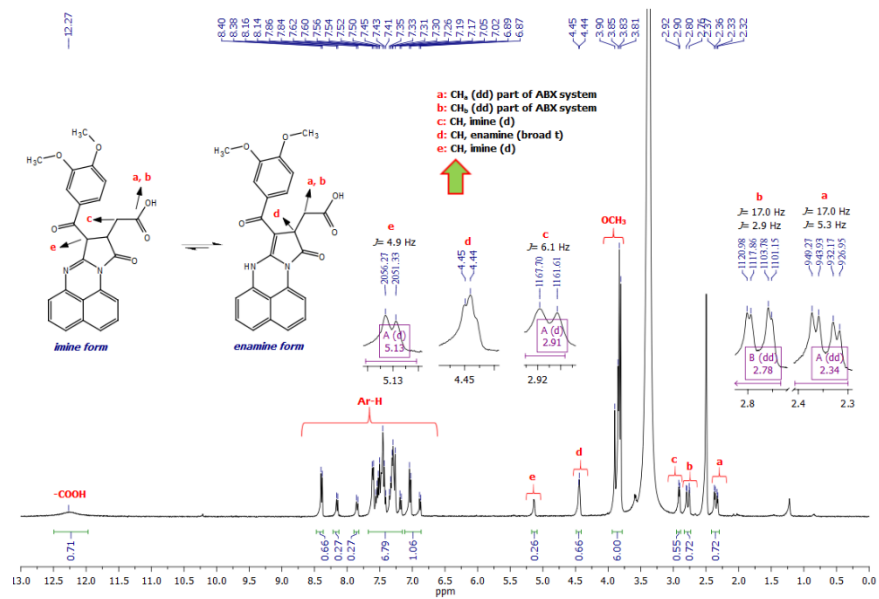


Figure S6. ¹H NMR spectra of compound 2d

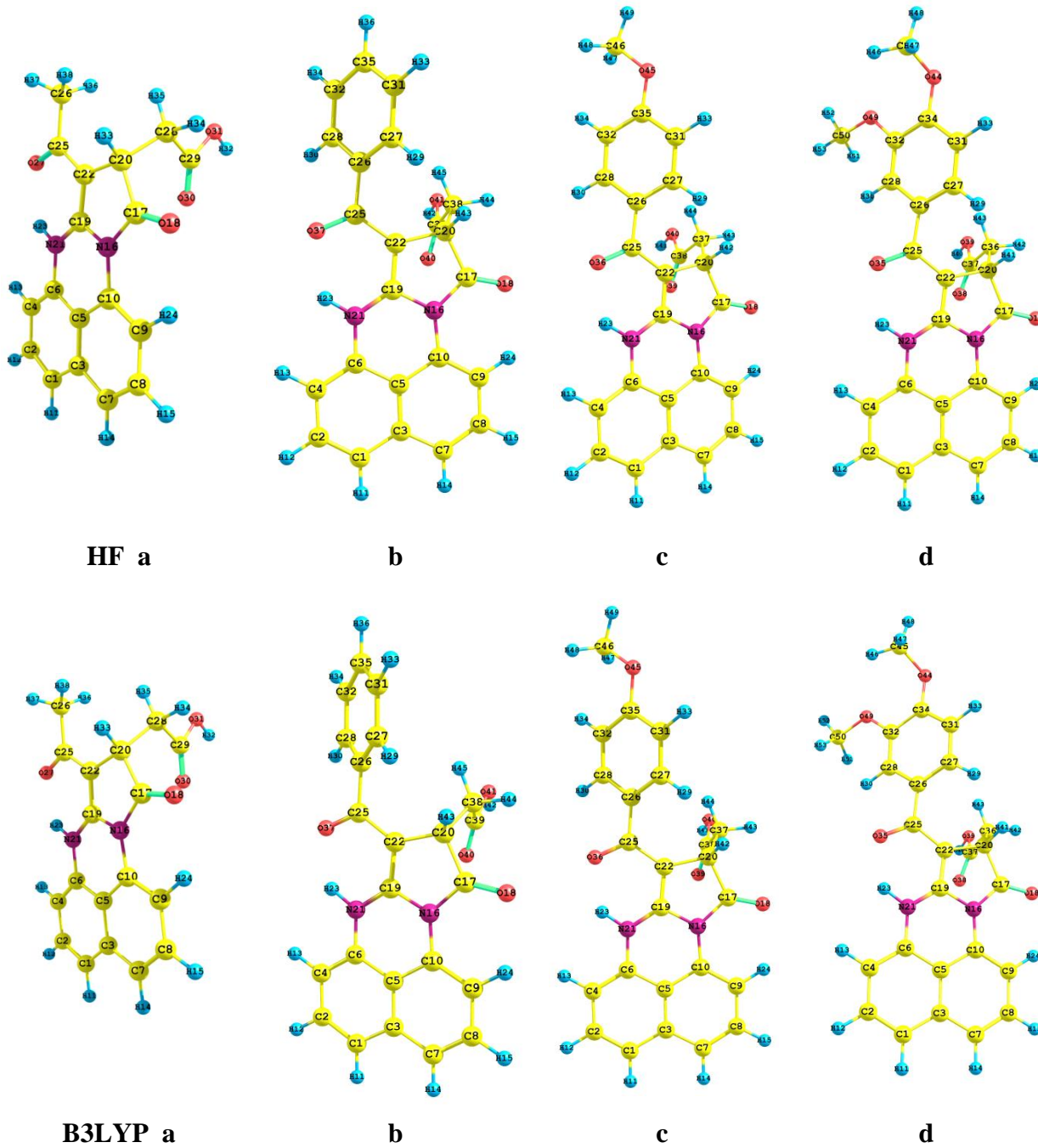


Figure S7. Geometry of 2 (a-d) A

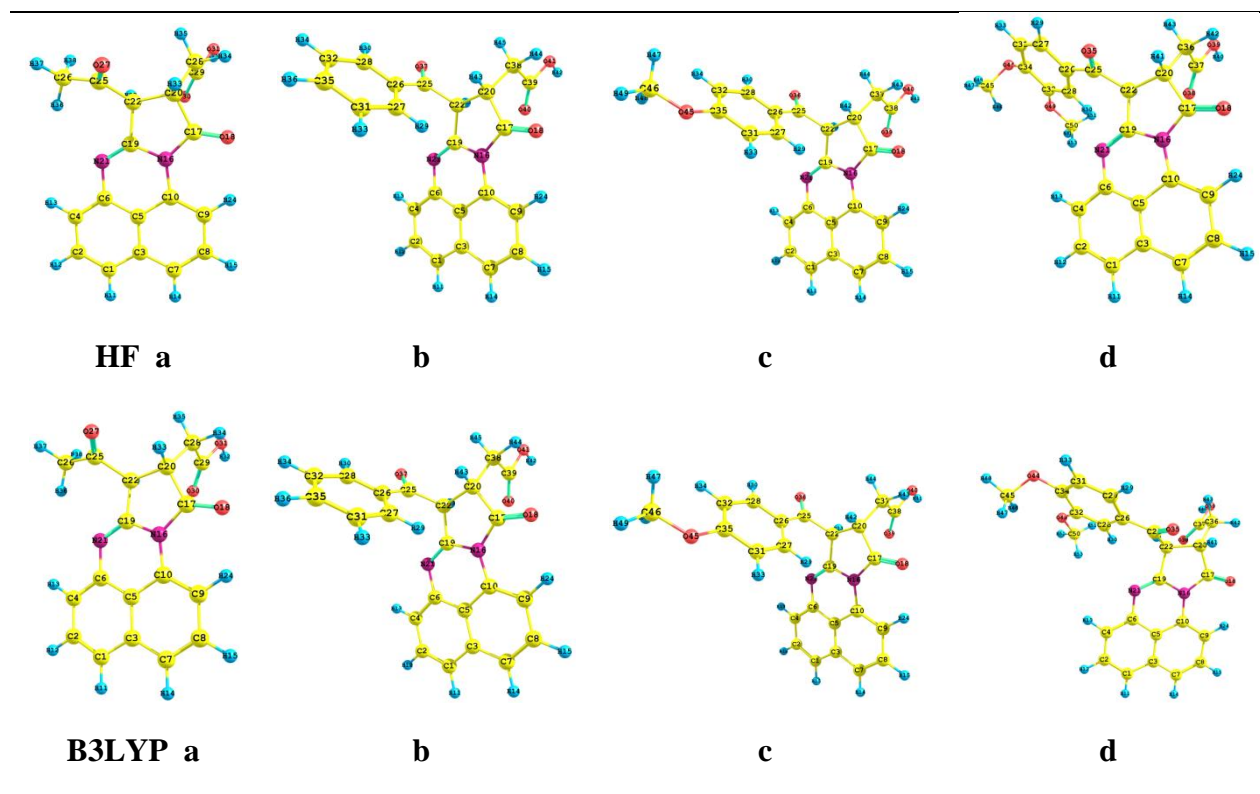
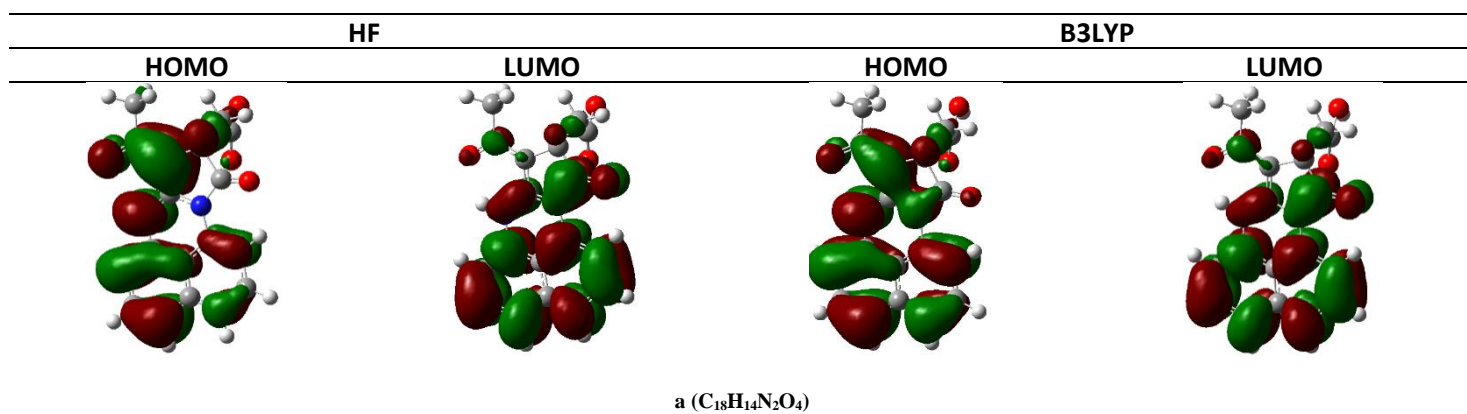
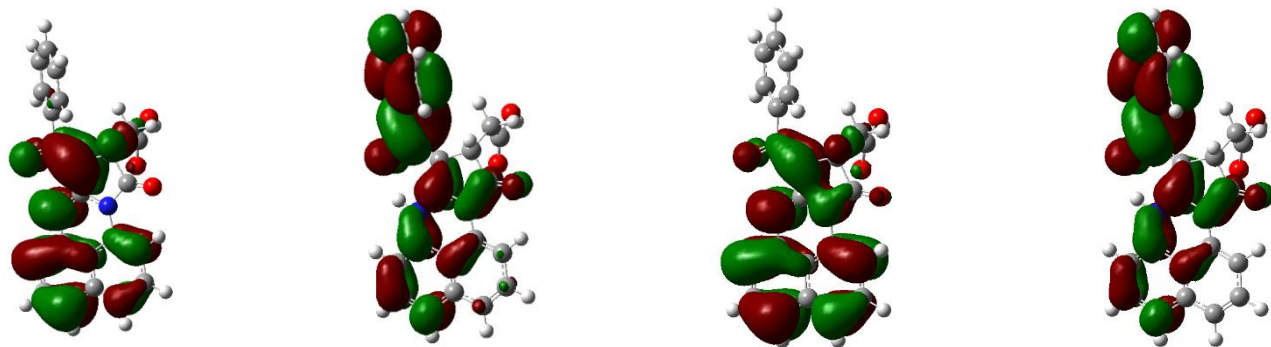
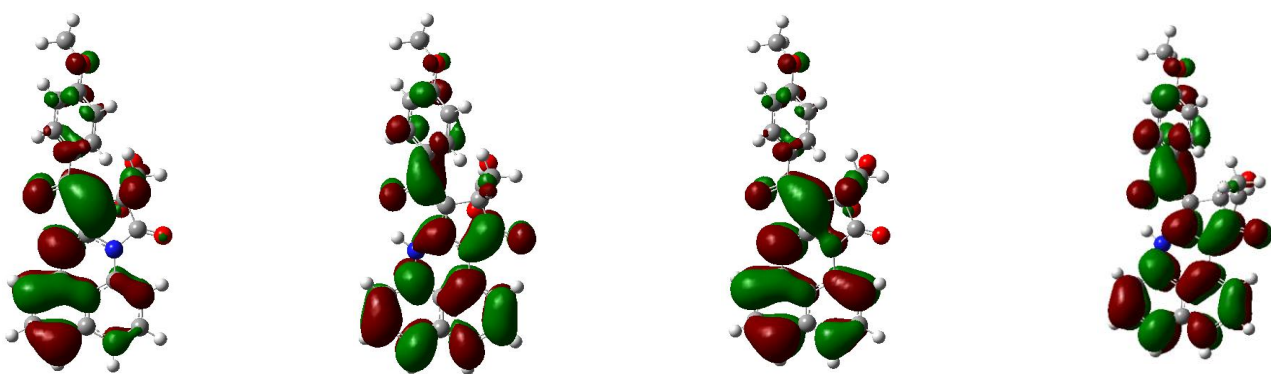


Figure S8. Geometry of 2 (a-d) B

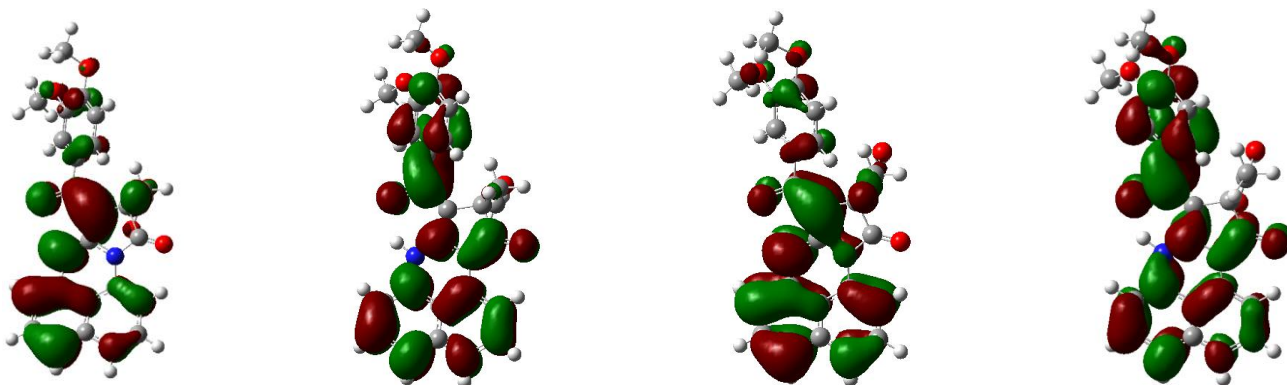




b ($C_{23}H_{16}N_2O_4$)



c ($C_{24}H_{18}N_2O_5$)



d ($C_{25}H_{20}N_2O_6$)

Figure S9. HOMO and LUMO clouds of 2 (a-d) A

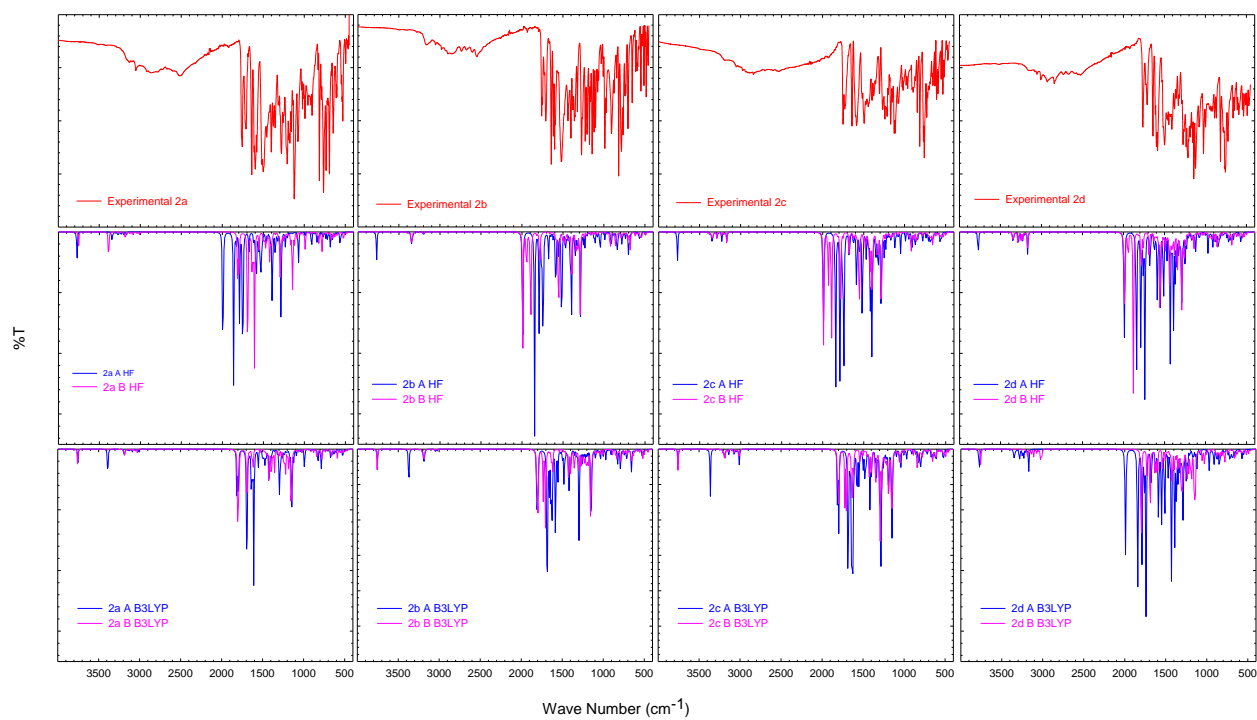


Figure S10. The comparison of the experimental and the theoretical frequencies of 2 (a-d) A and 2(a-d) B.

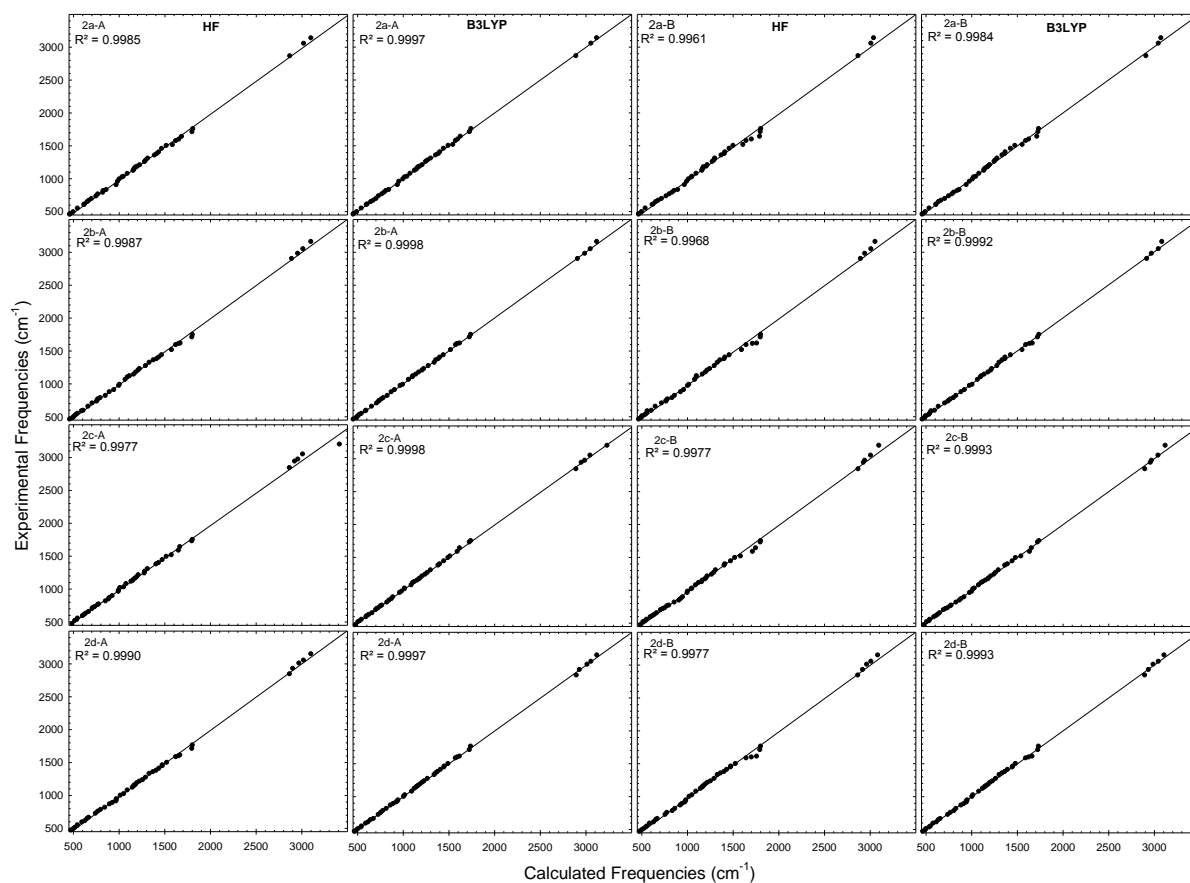


Figure S11. Correlation graphic of experimental and theoretical wavenumbers of 2c A and 2c B

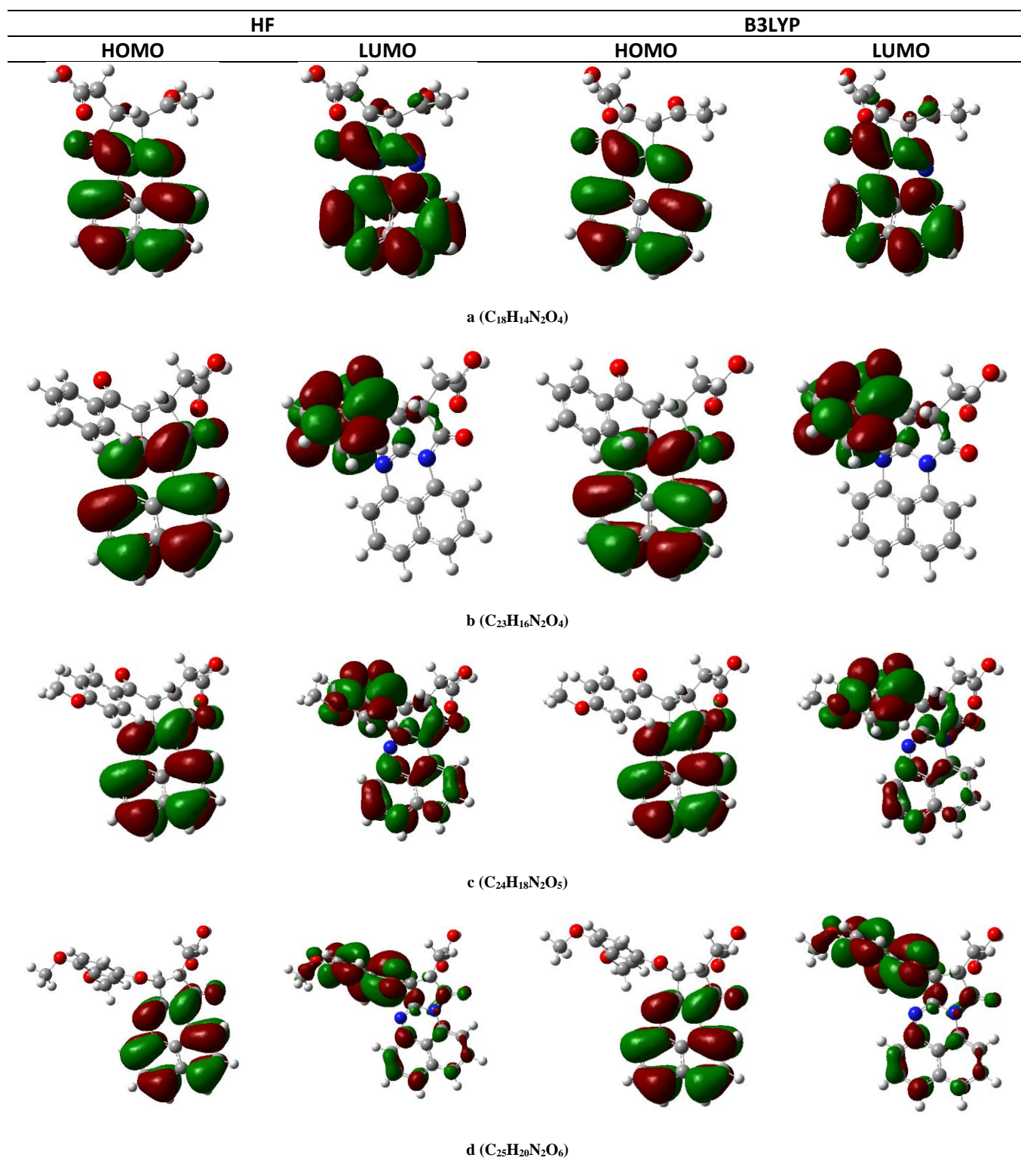


Figure S12. HOMO and LUMO clouds of 2 (a-d) B

Table S1. Calculated optimized geometries of frequencies (cm^{-1}) for 2a A and 2a B ($\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_4$)

No	2a A							2a B						
	HF			B3LYP				HF			B3LYP			
	Exp. Freq.	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	
1		34	31	1.1	33	32	0.8	19	17	0.7	18	17	0.4	
2		39	35	1.2	36	35	1.2	41	37	1.0	38	37	0.6	
3		51	46	0.5	49	47	0.3	51	46	1.0	45	43	0.7	
4		64	58	0.2	57	55	0.2	54	49	7.2	52	50	5.3	
5		89	81	0.7	82	79	0.3	80	72	1.7	73	70	2.1	
6		116	105	5.8	110	106	0.5	102	92	1.2	90	87	0.8	
7		128	116	0.2	115	110	3.0	127	115	0.7	115	111	0.8	
8		141	128	0.2	120	115	2.2	133	120	1.1	130	125	2.6	
9		155	140	3.0	143	137	2.8	135	122	1.3	155	149	0.1	
10		179	162	1.2	168	162	0.8	183	166	2.9	170	163	2.4	
11		222	201	0.6	200	192	0.6	201	182	2.2	188	181	1.6	
12		225	204	0.4	210	202	0.2	209	189	1.2	193	186	1.5	
13		245	222	8.0	226	218	6.4	235	213	6.2	218	210	5.1	
14		289	262	2.3	268	258	6.0	282	255	3.3	263	253	3.4	
15		298	270	10.2	275	265	4.9	304	275	6.8	282	271	5.6	
16		314	284	5.4	295	283	4.4	313	283	1.0	292	281	0.7	
17		333	301	1.4	312	299	1.3	336	304	6.3	310	298	4.6	
18		359	325	1.6	335	322	0.6	352	319	6.7	327	314	5.2	
19		378	342	4.8	355	342	4.5	414	375	1.1	387	372	0.8	
20		469	424	1.4	442	425	0.5	452	409	0.7	422	406	1.2	
21		474	429	0.3	444	427	0.2	495	448	10.5	462	444	7.8	
22	455.61	509	461	0.8	473	454	0.4	516	467	0.3	479	461	0.3	
23	464.41	512	463	8.9	476	458	7.4	519	470	20.5	485	466	14.5	
24		545	493	11.4	498	479	11.2	539	488	8.9	501	482	7.3	
25	493.97	551	499	3.1	513	493	3.0	553	501	31.3	514	494	19.8	
26		560	507	28.4	522	502	12.4	562	509	0.6	516	496	1.2	
27		568	514	49.7	525	504	41.2	587	531	16.1	541	520	21.6	
28	548.57	602	545	8.7	564	542	8.0	597	540	28.4	558	536	21.0	
29		630	570	20.5	578	556	3.7	625	566	40.2	576	554	15.0	
30		647	586	8.0	603	580	23.6	638	577	39.4	589	566	41.2	
31		656	594	34.0	608	584	2.7	650	588	3.1	607	584	0.9	
32	602.45	682	617	60.3	622	598	14.0	681	616	43.4	636	611	7.0	
33	610.54	685	620	18.9	632	607	19.5	693	627	3.0	637	612	6.9	
34		695	629	5.7	641	617	1.9	705	638	2.0	649	624	9.2	
35		708	641	13.5	658	633	33.2	709	642	37.2	657	632	36.5	
36	647.04	720	652	31.3	673	647	38.3	724	655	13.2	665	639	22.4	
37	666.92	739	669	32.1	701	674	12.2	753	682	12.5	693	666	7.1	
38	693.74	771	698	40.1	732	704	11.6	793	718	19.2	736	708	22.0	
39		802	726	11.6	748	720	5.1	845	765	21.1	770	740	9.4	
40	733.79	826	748	41.8	760	730	1.0	849	768	11.9	779	749	40.3	

41		843	763	36.2	768	739	1.4	857	776	44.3	783	753	20.6
42	764.95	849	768	10.0	786	756	112.9	864	782	7.5	798	767	7.2
43		849	768	26.2	799	768	6.3	888	804	16.5	819	787	12.3
44		878	795	11.0	802	771	5.2	910	824	8.5	836	804	48.2
45	790.41	909	823	5.8	826	794	71.0	923	835	81.9	839	807	18.0
46	815.85	913	826	102.7	845	813	5.9	947	857	15.9	878	844	16.0
47	831.22	950	860	5.5	878	844	4.7	990	896	14.9	901	866	0.0
48		979	886	0.1	881	847	0.1	1003	908	0.1	903	868	5.6
49		992	898	20.5	909	874	15.0	1017	920	7.2	922	886	1.5
50		1024	927	3.4	924	888	1.5	1023	926	4.1	936	900	9.2
51	905.07	1071	969	118.8	975	938	0.1	1071	969	2.3	981	943	2.5
52		1073	971	33.3	985	947	20.1	1076	974	6.1	982	944	0.1
53		1081	978	10.7	991	953	81.5	1095	991	25.8	991	953	1.3
54	955.55	1087	984	22.8	993	955	1.3	1098	994	0.1	1017	978	29.5
55		1095	991	0.2	1010	971	12.5	1105	1000	1.4	1037	997	4.1
56	991.41	1107	1002	1.5	1039	999	9.8	1120	1014	9.9	1052	1011	9.0
57	1021.70	1140	1032	11.5	1057	1016	8.6	1156	1046	17.9	1065	1024	12.4
58	1031.34	1157	1047	7.8	1085	1043	2.8	1163	1053	4.3	1090	1048	7.1
59		1176	1064	8.6	1090	1048	32.7	1203	1089	2.9	1110	1067	2.5
60	1076.89	1205	1091	24.8	1120	1077	50.5	1212	1097	17.0	1125	1082	12.1
61		1219	1103	23.9	1140	1096	130.3	1214	1099	4.3	1144	1100	233.6
62		1234	1117	67.8	1147	1102	298.0	1246	1128	29.4	1155	1110	231.5
63	1122.81	1276	1155	23.9	1169	1124	53.1	1282	1160	159.1	1181	1135	56.1
64	1139.21	1286	1164	436.8	1192	1146	5.1	1287	1165	4.9	1185	1139	44.8
65	1156.18	1290	1168	9.0	1200	1154	6.6	1295	1172	309.8	1197	1151	38.4
66	1175.45	1306	1182	8.2	1211	1165	17.4	1300	1177	4.4	1221	1174	134.9
67	1185.41	1325	1199	38.5	1231	1184	19.7	1335	1208	0.8	1230	1183	11.0
68		1334	1207	16.2	1242	1194	20.7	1340	1213	147.8	1234	1186	71.4
69	1208.07	1355	1226	156.0	1258	1210	47.2	1347	1219	125.2	1247	1199	42.6
70		1392	1260	476.5	1275	1226	15.8	1376	1245	93.5	1253	1205	12.5
71		1407	1273	12.2	1285	1235	122.2	1400	1267	41.3	1271	1222	32.8
72	1257.76	1414	1280	39.2	1298	1248	231.8	1407	1273	25.1	1298	1248	35.4
73	1278.25	1427	1292	15.9	1318	1267	18.6	1428	1292	43.1	1310	1259	17.5
74	1308.09	1452	1314	25.8	1354	1302	11.1	1437	1301	34.4	1331	1280	7.2
75		1471	1331	82.9	1384	1331	11.2	1468	1329	30.0	1354	1302	107.3
76		1506	1363	23.5	1398	1344	72.0	1484	1343	41.5	1370	1317	30.3
77		1518	1374	92.2	1403	1349	2.5	1506	1363	49.0	1387	1333	66.1
78	1355.34	1534	1388	338.5	1412	1357	63.2	1515	1371	20.8	1389	1335	10.2
79		1553	1406	109.2	1423	1368	151.1	1533	1388	50.9	1397	1343	125.0
80	1377.13	1561	1413	50.8	1442	1386	18.6	1553	1406	315.0	1420	1365	58.8
81	1402.39	1584	1434	127.4	1458	1401	34.7	1559	1411	219.5	1424	1369	154.2
82		1587	1436	34.6	1468	1412	34.6	1581	1431	3.0	1450	1394	37.2
83		1590	1439	136.0	1471	1414	51.1	1583	1433	19.5	1465	1408	7.5
84		1597	1445	53.3	1480	1423	24.4	1584	1434	26.1	1467	1410	6.2
85		1607	1454	38.4	1490	1432	29.2	1600	1448	12.4	1477	1420	13.8
86	1457.19	1620	1466	38.1	1500	1442	62.8	1612	1459	10.2	1484	1427	0.8

87	1500.81	1676	1517	119.4	1553	1493	91.9	1659	1502	14.1	1535	1476	18.0
88	1516.23	1751	1585	1026.3	1608	1545	647.9	1778	1609	36.8	1618	1556	122.8
89		1782	1613	25.7	1626	1563	116.3	1784	1615	212.4	1630	1567	46.7
90	1575.33	1791	1621	418.4	1637	1574	243.4	1817	1645	17.3	1658	1594	9.0
91	1597.86	1829	1655	67.5	1662	1598	17.1	1880	1702	785.9	1692	1627	462.6
92	1639.82	1862	1685	821.3	1692	1627	882.9	1980	1792	132.2	1785	1716	127.6
93	1710.07	1988	1799	343.6	1797	1727	309.2	1988	1799	505.1	1798	1729	351.8
94	1756.89	1998	1808	416.1	1814	1744	283.7	1994	1805	215.8	1805	1735	237.5
95	2864.30	3170	2869	13.6	3008	2892	11.9	3171	2870	10.3	3027	2910	9.2
96		3173	2872	8.8	3028	2911	6.7	3204	2900	12.6	3030	2913	11.2
97		3203	2899	12.6	3044	2926	10.8	3220	2914	2.6	3055	2937	8.1
98		3235	2928	19.6	3088	2968	13.3	3239	2932	3.2	3067	2949	3.9
99		3268	2958	10.3	3109	2989	5.0	3249	2941	8.0	3089	2970	0.9
100		3279	2968	16.5	3131	3010	10.5	3252	2943	2.0	3091	2972	5.8
101		3325	3009	6.2	3169	3046	3.9	3293	2980	9.0	3144	3023	6.1
102		3328	3012	3.5	3170	3048	0.5	3323	3008	6.0	3166	3044	3.6
103	3054.35	3338	3021	8.9	3180	3057	9.8	3326	3010	0.9	3168	3046	0.4
104		3348	3030	25.6	3187	3064	22.9	3342	3025	17.1	3182	3059	16.8
105		3352	3034	19.6	3192	3068	14.0	3347	3029	34.6	3185	3062	27.6
106	3137.50	3426	3101	3.5	3245	3119	4.2	3358	3039	10.2	3197	3074	8.1
107		3773	3415	155.7	3388	3257	177.6	3423	3098	2.4	3248	3123	3.3
108		4111	3721	133.4	3753	3608	72.9	4111	3721	147.4	3755	3610	81.8

Table S2. Calculated optimized geometries of frequencies (cm⁻¹) for 2b A and 2b B (C₂₃H₁₆N₂O₄)

No	2b A							2b B						
	HF			B3LYP				HF			B3LYP			
	Exp. Freq.	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	
1		28	25	0.7	28	26	0.5	19	17	1.1	18	17	1.0	
2		35	32	0.6	33	32	0.1	23	21	0.4	24	23	0.3	
3		37	33	0.4	36	34	0.9	38	34	0.9	36	35	0.8	
4		45	41	0.6	42	40	0.6	45	41	0.9	41	39	0.7	
5		53	48	1.1	49	47	0.6	52	47	0.3	50	48	0.4	
6		75	68	0.3	71	69	0.2	62	56	1.4	59	57	0.9	
7		85	77	0.2	79	76	0.0	99	90	2.1	90	87	1.3	
8		102	92	2.2	100	96	2.1	106	96	1.4	98	94	1.6	
9		127	115	1.1	118	113	0.9	127	115	0.3	117	112	0.3	
10		152	138	1.8	143	138	1.9	142	129	0.3	133	128	0.2	
11		179	162	1.6	169	162	1.2	172	156	0.0	157	151	0.0	
12		198	179	2.1	187	180	1.6	188	170	2.9	174	167	2.4	
13		218	197	0.7	200	192	0.5	204	185	2.2	186	179	1.4	
14		227	205	0.4	212	204	0.1	207	187	1.0	192	185	1.1	
15		253	229	3.2	235	226	5.3	237	215	7.6	221	212	7.1	
16		261	236	5.4	246	236	2.3	288	261	10.0	268	258	7.3	
17		291	263	1.3	273	262	1.9	304	275	10.6	279	268	8.8	
18		308	279	17.2	285	274	12.3	319	289	3.3	294	283	2.7	
19		332	300	0.8	310	298	0.6	332	300	3.9	306	294	2.8	
20		363	329	1.0	343	330	1.9	372	337	2.1	345	332	1.5	
21		380	344	4.2	358	344	3.0	396	358	1.0	370	356	0.7	
22		417	377	2.5	395	380	2.7	450	407	0.0	413	397	0.0	
23		452	409	0.6	414	398	0.5	459	415	0.8	428	411	0.8	
24		470	425	0.9	441	424	2.5	481	435	2.9	445	428	1.2	
25		480	434	6.4	449	432	1.7	490	443	13.9	455	437	12.3	
26		499	452	3.8	466	448	3.9	502	454	10.1	468	450	5.7	
27	459.66	509	461	1.0	473	455	0.6	516	467	1.1	479	461	0.8	
28		542	491	6.5	498	479	8.9	537	486	19.0	499	480	17.5	
29	483.73	548	496	13.8	508	488	4.2	546	494	19.1	504	485	6.3	
30	493.76	555	502	26.8	517	497	22.5	555	502	40.2	514	494	9.5	
31	511.00	570	516	47.1	526	505	32.0	558	505	3.2	517	497	30.7	
32	530.71	585	529	3.0	543	522	3.4	595	539	19.4	555	534	17.1	
33	547.97	603	546	7.9	566	544	5.7	611	553	0.1	564	542	1.8	
34	585.86	652	590	5.3	612	588	3.6	621	562	18.8	579	557	8.3	
35	594.46	673	609	0.6	619	595	10.1	671	607	6.4	620	596	18.7	
36		682	617	22.3	627	603	3.3	673	609	0.4	632	608	0.1	
37		685	620	29.4	633	609	1.4	681	616	85.8	635	610	22.0	
38		694	628	29.2	642	617	1.0	699	633	1.7	640	615	7.4	
39		701	634	59.3	653	628	44.2	704	637	21.0	651	626	43.0	
40		704	637	58.2	659	633	91.0	712	644	37.0	662	636	19.9	

41	654.87	731	662	2.6	682	656	2.3	718	650	8.0	663	637	22.4
42		738	668	29.3	689	663	3.2	741	671	8.3	685	659	7.4
43		762	690	15.6	710	682	39.9	755	683	8.1	701	674	9.6
44		780	706	34.4	718	691	26.2	776	702	20.7	710	683	31.3
45	705.18	781	707	43.6	740	712	25.4	794	719	51.7	736	708	21.9
46		800	724	4.0	745	716	7.9	826	748	10.0	761	732	12.3
47	732.93	834	755	106.1	762	733	4.1	847	767	23.8	771	741	6.2
48	744.87	843	763	33.4	770	740	1.1	850	769	7.7	781	751	46.8
49		847	767	5.8	789	759	105.6	859	777	47.7	789	759	41.4
50	766.18	849	768	30.8	794	764	4.8	865	783	44.5	801	770	6.7
51		878	795	11.3	801	770	17.1	895	810	14.2	820	788	12.4
52	785.97	879	796	10.9	815	783	7.9	920	833	49.6	835	803	56.5
53		901	815	7.2	823	792	7.4	926	838	63.8	848	815	24.2
54		913	826	106.6	827	795	71.4	929	841	1.8	860	827	0.8
55	819.36	941	852	0.9	860	827	2.9	950	860	0.8	863	830	0.6
56		953	863	1.1	872	838	0.6	965	873	21.9	885	851	24.0
57		979	886	0.3	881	847	0.1	1005	910	0.1	903	868	0.0
58	875.57	989	895	39.3	906	871	26.4	1023	926	4.2	921	885	1.5
59		1024	927	3.3	924	888	1.5	1045	946	2.8	949	912	0.7
60	907.48	1044	945	66.1	943	906	6.0	1060	959	2.0	960	923	2.9
61		1053	953	39.2	969	932	45.4	1074	972	7.9	983	945	0.0
62		1073	971	1.3	976	938	0.1	1084	981	7.5	990	952	1.3
63		1082	979	26.4	992	953	1.1	1084	981	15.8	1001	962	0.2
64		1082	979	0.4	993	955	1.4	1098	994	0.0	1005	966	28.1
65		1095	991	0.1	1000	961	26.8	1105	1000	1.3	1016	977	1.5
66	971.92	1104	999	1.5	1008	969	0.1	1110	1005	5.1	1017	978	0.5
67		1107	1002	1.5	1017	977	1.1	1111	1006	5.7	1039	999	19.3
68	988.10	1110	1005	70.2	1035	995	59.9	1123	1016	0.1	1048	1008	5.2
69		1118	1012	0.2	1051	1010	1.2	1129	1022	9.8	1057	1016	9.3
70		1123	1016	31.7	1058	1017	7.1	1157	1047	18.4	1072	1031	13.3
71		1163	1053	12.7	1090	1048	15.8	1163	1053	2.4	1084	1042	15.8
72		1165	1054	9.0	1096	1054	24.9	1176	1064	0.7	1102	1059	6.1
73	1063.73	1181	1069	6.6	1102	1060	10.8	1195	1082	9.6	1109	1066	3.6
74		1207	1092	5.6	1139	1095	62.3	1206	1092	10.3	1122	1079	11.7
75	1102.39	1209	1094	18.2	1147	1103	293.0	1213	1098	7.6	1143	1099	113.1
76	1119.35	1232	1115	73.5	1152	1108	128.0	1216	1101	7.4	1153	1108	382.2
77		1253	1134	70.2	1182	1137	0.4	1242	1124	32.0	1184	1138	43.5
78	1142.78	1284	1162	17.3	1185	1139	17.3	1287	1165	9.4	1185	1139	14.7
79		1287	1165	338.9	1198	1152	19.3	1290	1168	314.7	1196	1150	61.6
80		1290	1168	75.3	1199	1153	6.5	1293	1170	117.4	1203	1157	34.2
81		1302	1178	19.6	1210	1163	11.6	1300	1177	0.5	1213	1166	69.4
82	1175.45	1308	1184	48.6	1218	1171	35.9	1324	1198	131.2	1228	1181	41.3
83		1326	1200	10.1	1232	1185	16.6	1335	1208	5.8	1236	1188	24.0
84		1327	1201	92.7	1241	1193	23.5	1337	1210	66.2	1246	1198	15.8
85	1205.08	1337	1210	18.8	1257	1208	54.7	1345	1217	95.3	1260	1211	62.4
86	1227.29	1353	1225	166.7	1276	1227	10.1	1376	1245	3.5	1271	1222	73.8

87		1398	1265	593.4	1291	1241	108.6	1390	1258	178.7	1292	1242	76.9
88		1412	1278	8.9	1297	1247	342.4	1397	1264	84.5	1302	1252	39.1
89		1414	1280	108.2	1318	1267	18.6	1417	1283	23.7	1314	1263	12.1
90	1272.13	1427	1292	11.3	1328	1276	19.7	1432	1296	25.8	1330	1279	14.8
91		1451	1313	24.2	1348	1296	4.3	1436	1300	52.1	1339	1287	3.7
92		1454	1316	21.8	1353	1301	19.8	1459	1321	9.8	1350	1298	97.3
93	1323.37	1471	1331	131.9	1396	1342	83.6	1468	1329	25.6	1354	1302	19.7
94		1512	1369	255.6	1400	1346	24.1	1483	1342	79.2	1361	1308	22.3
95	1359.95	1521	1377	310.4	1413	1358	58.4	1500	1358	28.8	1388	1334	3.7
96		1554	1407	78.6	1419	1364	199.8	1507	1364	23.4	1397	1343	120.8
97	1377.89	1559	1411	68.7	1441	1385	11.4	1551	1404	317.3	1421	1366	57.2
98	1401.81	1585	1435	117.4	1458	1401	15.9	1560	1412	177.0	1422	1367	159.3
99		1588	1437	65.0	1468	1411	38.7	1581	1431	4.0	1449	1393	35.4
100		1589	1438	17.6	1472	1415	16.7	1585	1435	44.4	1467	1410	4.2
101		1591	1440	184.6	1480	1423	131.4	1592	1441	19.5	1477	1420	15.1
102	1437.58	1620	1466	29.2	1499	1441	47.9	1612	1459	12.4	1484	1427	1.2
103		1649	1493	19.0	1522	1463	10.6	1650	1493	0.4	1522	1463	0.4
104		1676	1517	153.8	1553	1493	125.1	1659	1502	10.8	1535	1476	14.3
105	1515.73	1742	1577	838.6	1582	1521	454.0	1762	1595	8.5	1617	1555	92.1
106		1760	1593	234.2	1620	1557	195.1	1778	1609	37.9	1618	1556	33.2
107		1782	1613	39.0	1626	1563	177.8	1784	1615	204.8	1630	1567	46.6
108		1789	1619	45.2	1637	1574	299.8	1786	1617	22.1	1637	1574	29.3
109	1591.90	1791	1621	429.5	1639	1576	4.6	1817	1645	19.7	1658	1594	12.6
110	1610.10	1827	1654	2.6	1657	1593	168.2	1894	1714	746.0	1702	1636	449.5
111	1615.48	1846	1671	1021.0	1684	1619	955.3	1945	1760	307.4	1733	1666	223.4
112	1708.65	1988	1799	365.4	1796	1727	326.6	1989	1800	376.0	1793	1724	278.4
113	1748.24	1994	1805	426.7	1810	1740	284.0	1992	1803	243.9	1808	1738	260.6
114	2901.39	3194	2891	8.9	3026	2909	9.7	3200	2896	7.2	3035	2918	4.5
115		3207	2903	14.7	3048	2930	8.9	3212	2907	6.1	3057	2939	5.8
116	2979.40	3267	2957	3.6	3109	2989	1.1	3252	2943	1.6	3089	2970	0.8
117		3320	3005	0.5	3163	3041	0.9	3274	2963	0.8	3091	2972	0.4
118		3325	3009	6.6	3169	3046	3.9	3323	3008	6.0	3166	3044	3.8
119		3328	3012	3.8	3170	3048	0.7	3325	3009	0.6	3168	3046	0.4
120	3049.00	3331	3015	6.9	3172	3049	5.7	3326	3010	0.7	3168	3046	0.7
121		3338	3021	9.3	3180	3057	10.4	3339	3022	9.4	3179	3056	7.2
122		3343	3026	30.1	3182	3059	23.3	3342	3025	18.1	3182	3059	17.6
123		3348	3030	26.2	3186	3063	24.5	3347	3029	35.9	3185	3062	28.9
124		3352	3034	14.9	3190	3067	14.0	3350	3032	22.5	3189	3066	16.1
125		3352	3034	19.9	3192	3068	14.5	3360	3041	7.2	3198	3075	5.5
126		3359	3040	6.7	3197	3074	7.8	3376	3056	14.6	3204	3080	8.0
127	3160.53	3427	3102	3.5	3245	3120	4.2	3376	3056	1.4	3208	3084	6.1
128		3773	3415	159.9	3371	3241	196.4	3422	3097	2.2	3246	3121	3.0
129		4113	3723	132.6	3755	3610	72.4	4110	3720	156.1	3756	3611	88.6

Table S3. Calculated optimized geometries of frequencies (cm^{-1}) for 2c A and 2c B ($\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}_5$)

No	2c A							2c B						
	HF			B3LYP				HF			B3LYP			
	Exp. Freq.	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	
1		21	19	0.7	20	19	0.6	16	14	1.1	16	15	0.9	
2		29	26	0.4	27	26	0.2	22	20	0.2	23	22	0.2	
3		35	32	0.8	34	32	0.7	36	33	1.1	34	33	0.9	
4		43	39	1.4	40	39	1.3	43	39	0.4	39	37	0.4	
5		51	46	0.5	48	46	0.4	49	44	0.5	46	44	0.3	
6		65	59	0.6	59	56	0.3	61	55	1.3	56	54	0.9	
7		76	69	2.4	73	70	1.1	74	67	0.5	75	72	0.0	
8		87	79	1.0	86	82	1.4	99	90	4.7	89	85	1.4	
9		100	91	1.8	99	95	1.2	103	93	1.2	94	91	3.3	
10		127	115	1.8	118	113	1.5	118	107	1.4	111	106	1.1	
11		136	123	1.3	130	125	2.0	135	122	0.6	126	121	0.4	
12		164	148	4.5	154	148	4.5	141	128	2.9	136	130	3.1	
13		179	162	1.4	167	161	0.9	177	160	2.1	165	158	2.6	
14		190	172	0.5	180	173	0.4	188	170	6.2	175	168	5.2	
15		215	195	1.3	200	192	1.0	205	186	1.0	189	182	0.7	
16		225	204	0.1	210	202	0.2	208	188	2.9	192	185	2.7	
17		251	227	9.4	225	216	1.9	249	225	0.3	223	214	0.2	
18		257	233	1.9	235	226	7.4	282	255	8.5	262	252	6.0	
19		290	262	1.6	270	260	2.7	292	264	5.3	270	260	4.8	
20		297	269	11.2	274	264	9.9	303	274	7.0	279	269	4.9	
21		315	285	2.5	295	283	1.3	319	289	1.6	294	283	1.2	
22		332	300	1.3	309	297	4.2	331	300	6.4	304	292	4.8	
23		336	304	6.3	310	298	0.3	338	306	4.4	311	299	3.5	
24		364	329	1.1	345	332	1.3	362	328	0.7	336	323	0.4	
25		376	340	4.0	358	344	3.3	389	352	0.4	363	349	0.3	
26		426	386	2.1	398	383	1.2	434	393	1.5	406	390	1.5	
27		464	420	1.0	426	410	0.7	463	419	0.1	426	410	0.1	
28		471	426	0.0	445	428	0.3	475	430	5.7	443	426	5.1	
29		480	434	0.3	449	432	0.0	497	450	20.9	463	446	12.2	
30		509	461	0.8	473	455	0.4	516	467	0.5	479	460	0.4	
31		514	465	5.2	480	462	5.7	527	477	29.3	492	473	30.4	
32	471.42	539	488	4.3	498	478	6.4	538	487	12.3	499	479	12.6	
33		547	495	16.3	503	484	9.4	545	493	13.8	501	482	1.4	
34		552	500	14.2	510	491	9.7	556	503	16.6	513	493	12.8	
35		558	505	26.8	518	498	27.6	568	514	22.1	519	499	12.3	
36	516.73	571	517	42.9	526	506	25.0	569	515	6.4	528	508	13.7	
37	532.36	594	538	9.1	547	526	7.2	596	539	19.0	557	535	17.3	
38	554.42	604	547	8.2	567	545	6.3	612	554	0.7	565	543	1.9	
39		648	587	35.6	606	583	34.8	621	562	18.1	579	557	8.9	
40	592.72	665	602	62.0	618	594	19.0	658	596	73.5	611	588	67.7	

41		682	617	24.2	620	596	22.5	672	608	7.8	626	602	4.4
42	609.45	684	619	18.8	628	604	18.2	685	620	53.5	635	610	9.1
43		690	625	27.4	642	617	0.6	690	625	2.3	640	615	10.8
44		695	629	10.8	645	620	6.9	700	634	5.4	647	622	5.3
45	628.98	703	636	11.6	650	625	46.2	706	639	28.0	653	628	47.4
46		713	645	53.6	667	641	43.0	718	650	8.9	662	636	11.2
47	653.94	738	668	31.8	687	660	2.1	734	664	5.6	676	650	1.6
48		766	693	7.4	718	690	28.0	767	694	10.5	703	676	9.7
49	701.13	781	707	44.8	729	701	12.0	782	708	18.8	722	694	14.3
50	718.25	791	716	3.4	738	710	2.0	808	731	3.4	744	715	4.0
51	729.29	814	737	12.0	758	729	5.6	833	754	18.6	766	736	16.2
52		842	762	16.4	769	739	0.0	849	768	12.7	770	740	2.4
53		843	763	26.5	778	747	11.8	850	769	6.8	781	751	48.4
54	759.70	849	768	20.1	784	754	27.5	858	777	46.0	799	768	12.3
55	770.12	859	777	15.1	799	768	95.7	882	798	8.1	809	778	17.4
56		873	790	85.7	804	773	8.0	893	808	42.3	825	793	0.8
57		881	797	13.2	806	775	17.6	915	828	25.0	826	794	25.1
58		894	809	17.8	826	794	63.6	917	830	44.0	835	802	54.0
59		913	826	105.9	826	795	14.8	923	835	77.2	842	809	59.6
60		921	834	2.9	833	800	7.3	929	841	12.4	857	824	11.0
61	814.93	942	853	2.2	856	823	28.4	947	857	27.4	864	830	2.3
62		950	860	32.4	873	839	0.5	966	874	19.5	886	852	23.6
63	845.35	978	885	0.3	880	846	0.1	1004	909	0.1	903	868	0.0
64	867.45	990	896	41.9	907	872	29.7	1023	926	4.4	921	886	1.7
65	895.52	1024	927	3.4	923	888	1.5	1048	949	4.7	956	919	4.1
66		1049	949	104.6	965	928	19.0	1073	971	10.6	973	935	0.9
67		1073	971	1.5	970	932	36.2	1079	977	9.3	982	944	0.0
68		1077	975	2.7	975	937	0.1	1086	983	11.3	990	951	1.3
69		1082	979	23.5	980	942	4.3	1094	990	0.5	993	954	0.6
70		1094	990	0.1	993	955	1.4	1097	993	0.0	1006	967	29.0
71	961.83	1097	993	8.5	1000	962	31.2	1104	999	1.4	1019	980	1.9
72	981.19	1101	997	0.5	1023	983	6.5	1108	1003	1.6	1044	1003	29.6
73		1107	1002	1.5	1039	999	70.0	1127	1020	18.5	1051	1010	55.9
74	1018.42	1117	1011	111.5	1056	1015	41.5	1153	1044	28.8	1057	1016	7.2
75	1028.72	1162	1052	25.3	1058	1017	8.4	1161	1051	6.2	1072	1031	14.5
76		1170	1059	29.7	1090	1048	16.5	1174	1063	45.4	1084	1043	14.2
77		1181	1069	10.8	1096	1054	24.3	1196	1082	6.4	1101	1059	4.8
78	1078.86	1191	1078	19.1	1133	1089	13.6	1206	1092	8.3	1121	1078	9.4
79		1209	1094	21.4	1139	1095	57.5	1208	1093	9.3	1141	1097	78.7
80		1232	1115	92.5	1147	1103	263.3	1215	1100	11.5	1143	1099	78.4
81	1114.80	1252	1133	147.0	1151	1107	188.4	1242	1124	32.1	1152	1107	397.1
82	1126.33	1271	1150	0.1	1167	1122	0.8	1279	1158	3.6	1168	1123	0.6
83		1280	1159	2.0	1185	1139	86.6	1280	1159	66.4	1184	1138	108.3
84		1284	1162	111.6	1190	1144	147.3	1284	1162	305.4	1190	1144	171.4
85	1149.28	1287	1165	375.4	1199	1153	4.7	1287	1165	19.0	1197	1151	40.1
86		1290	1168	45.9	1201	1154	2.6	1292	1169	269.1	1203	1157	0.6

87		1303	1179	6.4	1211	1164	15.5	1300	1177	0.5	1214	1167	83.1
88	1169.25	1308	1184	14.7	1220	1173	29.0	1320	1195	80.7	1227	1180	38.6
89	1182.41	1321	1196	133.8	1233	1186	12.6	1331	1205	61.6	1236	1188	23.8
90		1328	1202	94.4	1241	1193	26.8	1337	1210	73.5	1247	1198	16.2
91	1213.19	1339	1212	19.8	1257	1208	66.3	1345	1217	101.5	1260	1212	39.3
92		1354	1226	185.1	1276	1227	32.2	1376	1245	3.0	1272	1222	153.8
93		1398	1265	681.5	1280	1230	564.8	1392	1260	194.8	1291	1241	354.1
94	1239.42	1412	1278	1.3	1291	1242	96.4	1399	1266	233.9	1296	1245	27.8
95		1414	1280	142.5	1297	1247	241.6	1417	1283	136.8	1304	1253	39.5
96	1266.78	1417	1283	493.7	1317	1266	17.8	1425	1290	218.8	1314	1263	12.1
97		1427	1292	8.9	1329	1278	22.8	1432	1296	25.3	1330	1279	29.8
98		1442	1305	61.6	1337	1285	102.2	1436	1300	53.1	1335	1283	5.3
99	1306.16	1450	1312	23.9	1353	1301	46.0	1446	1309	30.0	1346	1294	89.6
100		1471	1331	122.3	1395	1341	76.0	1468	1329	25.5	1350	1297	92.5
101		1513	1369	215.4	1400	1346	56.5	1482	1341	85.7	1359	1307	29.9
102		1520	1376	327.1	1413	1358	61.6	1500	1358	26.6	1388	1334	3.5
103		1551	1404	59.1	1416	1361	234.0	1507	1364	24.2	1396	1342	120.0
104	1377.08	1554	1407	40.9	1439	1383	11.0	1551	1404	313.1	1420	1365	67.3
105		1559	1411	46.9	1444	1388	10.0	1557	1409	3.9	1423	1368	151.3
106	1396.69	1584	1434	165.5	1456	1400	15.0	1559	1411	179.0	1449	1393	1.9
107		1588	1437	131.5	1465	1409	79.5	1581	1431	3.9	1450	1394	36.0
108		1589	1438	86.4	1474	1417	38.9	1585	1435	46.1	1467	1411	4.3
109		1606	1454	7.3	1478	1421	117.4	1607	1454	12.6	1477	1420	4.4
110		1619	1465	29.1	1493	1435	9.5	1611	1458	12.1	1484	1426	1.1
111		1622	1468	8.1	1497	1440	60.2	1622	1468	8.5	1495	1437	10.0
112	1442.24	1629	1474	33.1	1504	1445	37.3	1629	1474	31.5	1503	1445	42.8
113		1675	1516	195.0	1540	1481	44.0	1658	1501	11.0	1535	1476	14.8
114	1493.13	1678	1519	22.3	1552	1492	134.1	1679	1520	106.6	1541	1482	55.4
115	1516.87	1739	1574	621.6	1574	1514	300.5	1749	1583	21.9	1604	1542	11.0
116		1754	1588	483.9	1611	1549	103.6	1778	1609	41.3	1617	1555	118.2
117		1782	1613	76.4	1625	1562	439.1	1783	1614	270.7	1630	1567	44.9
118		1789	1619	761.5	1636	1573	490.1	1785	1616	265.0	1637	1574	348.4
119		1793	1623	5.6	1642	1578	303.0	1817	1645	19.9	1657	1593	12.9
120	1586.66	1825	1652	20.6	1657	1593	56.0	1893	1713	744.5	1701	1636	445.1
121	1640.95	1842	1667	983.4	1683	1618	900.1	1932	1749	320.3	1723	1656	223.8
122	1729.08	1986	1798	362.3	1795	1725	331.4	1988	1799	359.5	1793	1723	273.8
123	1750.18	1994	1805	438.2	1811	1741	286.9	1991	1802	260.9	1808	1738	262.4
124	2842.36	3168	2867	58.5	3009	2893	67.2	3171	2870	56.0	3014	2898	59.2
125		3194	2891	9.3	3024	2907	10.7	3199	2895	7.5	3036	2919	4.5
126		3206	2902	15.3	3047	2929	8.9	3212	2907	6.3	3058	2939	6.1
127	2941.20	3230	2923	43.8	3070	2951	33.2	3235	2928	40.0	3077	2958	28.9
128	2972.00	3269	2959	3.9	3109	2989	1.1	3251	2942	1.7	3090	2970	0.7
129		3287	2975	41.3	3137	3016	23.7	3274	2963	0.9	3092	2973	0.4
130		3325	3009	6.9	3168	3046	3.9	3291	2979	34.3	3142	3021	18.0
131	3049.00	3327	3011	3.9	3170	3047	0.5	3322	3007	6.2	3165	3042	3.8
132		3338	3021	9.6	3180	3057	11.6	3326	3010	0.7	3167	3045	0.5

133		3344	3027	11.6	3183	3060	8.5	3342	3025	18.4	3181	3058	18.6
134		3348	3030	27.1	3186	3063	26.1	3346	3028	36.5	3184	3061	29.4
135		3352	3034	21.0	3191	3068	1.1	3354	3036	7.1	3191	3068	5.1
136		3353	3035	2.1	3192	3068	14.6	3360	3041	7.4	3195	3071	0.1
137		3362	3043	7.7	3199	3075	6.4	3363	3044	2.1	3198	3074	5.6
138		3373	3053	10.3	3207	3083	10.5	3376	3056	12.5	3208	3085	9.1
139		3427	3102	3.5	3246	3121	4.1	3379	3058	6.1	3210	3086	6.0
140	3199.10	3772	3414	168.5	3362	3233	216.8	3422	3097	2.2	3246	3121	2.9
141		4113	3723	131.5	3756	3611	71.3	4111	3721	156.9	3756	3611	88.8

Table S4. Calculated optimized geometries of frequencies (cm^{-1}) for 2d A and 2d B ($\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_6$)

No	2d A							2d B					
	HF			B3LYP				HF			B3LYP		
	Exp. Freq.	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity	Freq.	Scale Freq.	IR Intensity
1		20	18	0.4	21	20	0.2	10	9	0.3	13	12	0.2
2		22	20	0.0	23	22	0.0	23	21	0.6	17	16	0.2
3		34	31	0.5	34	32	0.4	27	24	0.8	20	19	1.0
4		41	37	1.6	39	38	1.3	42	38	1.4	35	34	1.4
5		46	42	0.2	44	43	0.2	43	39	0.1	38	37	1.4
6		55	50	1.0	52	50	0.7	61	55	1.4	42	40	1.5
7		76	69	1.5	67	65	3.0	69	62	1.1	55	53	1.9
8		80	72	3.1	76	73	0.9	85	77	3.6	70	67	0.4
9		92	83	3.7	94	90	2.7	88	80	2.2	85	82	0.9
10		100	91	1.6	99	95	3.3	102	92	1.4	89	86	1.8
11		120	109	2.9	111	107	2.0	106	96	3.9	92	88	3.7
12		127	115	0.7	119	114	0.4	123	111	1.7	114	110	1.0
13		143	129	0.3	135	130	0.8	135	122	0.8	125	120	0.9
14		160	145	1.0	153	147	2.2	156	141	1.4	152	146	3.3
15		165	149	5.0	168	162	5.9	182	165	1.0	170	163	1.5
16		179	162	1.3	169	162	0.7	186	168	2.2	174	167	1.1
17		209	189	3.7	191	183	2.6	201	182	1.4	185	178	4.1
18		213	193	0.6	199	191	0.8	205	186	5.2	188	181	2.9
19		225	204	0.2	210	202	0.1	212	192	0.6	197	189	4.1
20		239	216	2.8	218	210	0.8	229	207	4.0	208	200	0.5
21		258	234	7.4	236	227	8.7	262	237	3.5	241	232	1.8
22		284	257	2.1	262	252	1.4	288	261	2.3	255	245	1.0
23		292	264	1.0	274	263	1.5	298	270	4.6	279	268	3.6
24		299	271	13.8	278	267	14.6	310	281	7.2	286	275	2.5
25		315	285	6.1	298	286	2.6	310	281	3.2	288	277	5.6
26		332	300	0.7	310	298	0.4	323	292	7.7	299	287	6.3
27		359	325	5.2	332	319	4.2	352	319	8.4	323	311	5.9
28		362	328	2.6	343	330	2.8	371	336	4.6	342	329	7.1
29		382	346	1.2	358	344	0.3	390	353	1.8	362	348	1.1
30		388	351	3.8	367	353	4.0	412	373	4.1	383	368	5.7
31		458	415	4.0	427	410	3.9	458	415	0.2	428	411	0.7
32		471	426	0.1	446	428	0.4	481	435	2.4	447	430	4.7
33		492	445	2.3	459	441	3.0	502	454	14.6	468	450	12.1
34		509	461	0.9	473	455	0.5	516	467	0.4	479	461	0.3
35	469.58	524	474	0.8	486	467	0.5	527	477	24.8	485	466	2.5
36		543	491	4.9	499	479	5.4	530	480	6.0	491	472	18.3
37		547	495	17.4	503	484	9.3	542	491	4.1	502	483	3.5
38	490.55	554	501	22.6	512	492	11.6	552	500	36.6	514	494	26.3
39		565	511	10.9	518	498	15.8	565	511	1.3	518	498	2.3

40	508.32	570	516	38.8	526	506	27.9	575	520	4.8	521	501	6.3
41		580	525	6.0	541	520	4.1	597	540	18.2	556	535	17.2
42	534.32	599	542	5.1	560	539	6.9	602	545	7.7	559	537	9.8
43	548.93	604	547	6.9	568	546	3.7	617	558	31.6	572	550	15.0
44		642	581	7.1	599	576	7.0	636	576	5.0	581	559	7.6
45	592.24	658	596	39.0	615	591	12.8	648	587	12.4	603	580	14.9
46		684	619	31.3	621	597	14.1	677	613	95.0	626	602	18.9
47		685	620	49.1	628	604	4.8	682	617	2.6	640	615	17.7
48	611.35	694	628	14.2	642	617	1.4	698	632	3.2	641	616	13.0
49		701	634	12.0	646	621	60.9	706	639	21.6	656	631	50.0
50		712	644	36.3	656	631	24.1	713	645	24.1	662	636	7.3
51	645.56	720	652	35.8	670	644	46.5	724	655	18.3	665	639	28.1
52	662.97	739	669	28.3	702	675	0.8	741	671	7.7	684	658	4.3
53		776	702	13.6	717	689	17.7	766	693	7.2	697	670	5.2
54		786	711	19.1	734	706	12.4	799	723	18.2	736	708	24.6
55		798	722	4.2	745	716	14.8	826	748	5.9	750	721	2.3
56	724.98	822	744	32.2	758	729	2.4	837	758	42.3	770	740	4.3
57		835	756	51.4	768	738	41.7	850	769	8.6	776	746	33.3
58		843	763	33.5	769	740	21.9	855	774	29.7	781	751	14.1
59		849	768	19.3	778	748	12.9	856	775	8.6	783	753	52.1
60	756.36	850	769	38.1	788	757	27.2	859	777	53.6	800	769	14.2
61		869	787	11.3	799	768	90.3	891	806	47.9	815	784	28.8
62		874	791	64.9	806	775	21.0	917	830	9.1	838	806	46.4
63	782.96	883	799	29.5	809	778	16.5	925	837	67.3	840	808	13.5
64		913	826	106.1	826	794	70.5	938	849	19.0	853	820	11.4
65	815.96	934	845	12.8	849	816	8.0	955	864	46.7	863	830	26.2
66		952	862	9.6	867	834	5.9	965	873	10.9	878	844	29.8
67		970	878	100.1	880	846	0.3	989	895	7.0	889	855	22.8
68		979	886	0.0	892	857	10.5	1005	910	0.1	902	867	0.1
69	867.04	991	897	4.5	897	862	80.4	1019	922	12.8	921	885	1.4
70		1000	905	12.6	914	879	6.8	1023	926	3.4	933	897	2.5
71	888.66	1025	928	3.3	925	889	1.5	1039	940	14.8	951	914	12.7
72	912.43	1070	968	19.7	959	922	4.0	1074	972	6.9	982	944	0.1
73	929.84	1072	970	0.4	975	938	0.1	1084	981	21.5	982	944	0.0
74	945.05	1075	973	4.2	983	945	4.5	1088	985	0.5	991	953	1.1
75		1083	980	29.4	993	955	1.5	1097	993	0.0	1002	963	22.8
76		1094	990	0.1	1005	966	21.0	1105	1000	1.4	1021	982	24.3
77		1107	1002	1.5	1026	986	86.8	1113	1007	13.4	1029	989	66.7
78	998.32	1122	1016	104.7	1046	1006	47.7	1127	1020	1.2	1046	1006	14.4
79		1142	1034	34.9	1058	1017	8.2	1141	1033	85.5	1055	1014	27.4
80	1022.92	1163	1053	27.2	1060	1019	26.8	1161	1051	11.8	1056	1015	27.4
81		1166	1055	47.8	1091	1049	16.1	1165	1054	50.0	1090	1048	13.2
82		1181	1069	12.8	1097	1054	22.5	1203	1089	3.2	1110	1067	6.0
83	1077.78	1206	1092	34.8	1139	1095	71.9	1209	1094	8.8	1124	1081	7.4
84		1211	1096	6.8	1141	1097	107.6	1214	1099	5.8	1139	1095	152.6
85		1232	1115	85.7	1146	1101	178.4	1217	1102	6.1	1144	1100	209.1

86		1248	1130	190.5	1149	1104	228.2	1242	1124	68.4	1153	1108	234.2
87	1120.48	1268	1148	34.3	1168	1123	9.4	1264	1144	229.0	1166	1121	0.4
88		1277	1156	8.1	1169	1124	0.8	1277	1156	8.7	1167	1122	8.3
89		1280	1159	1.7	1177	1132	88.3	1278	1157	7.5	1183	1137	87.1
90	1141.36	1287	1165	252.4	1190	1144	6.4	1287	1165	9.6	1188	1142	103.7
91	1153.87	1290	1168	142.6	1200	1153	7.6	1291	1168	363.4	1196	1150	44.1
92		1295	1172	76.3	1202	1155	1.7	1300	1177	11.7	1203	1157	50.6
93	1163.10	1306	1182	19.0	1209	1162	13.5	1304	1180	154.0	1208	1161	6.3
94		1311	1187	26.3	1219	1172	51.1	1313	1188	25.3	1221	1174	113.7
95	1186.35	1320	1195	18.1	1233	1185	13.7	1321	1196	12.3	1232	1184	39.2
96		1327	1201	122.7	1241	1193	31.0	1336	1209	4.6	1236	1188	112.1
97		1337	1210	20.6	1248	1200	108.7	1342	1215	172.3	1248	1200	53.1
98	1212.64	1353	1225	203.8	1257	1208	82.0	1348	1220	114.7	1250	1202	47.9
99		1372	1242	252.8	1277	1227	16.9	1377	1246	117.3	1270	1221	12.7
100	1234.77	1391	1259	467.7	1279	1230	39.6	1385	1254	58.8	1279	1230	59.3
101		1407	1273	10.9	1291	1241	154.8	1400	1267	43.5	1296	1246	265.5
102		1410	1276	28.9	1295	1245	34.7	1411	1277	47.4	1298	1248	33.0
103		1414	1280	28.7	1302	1252	802.1	1416	1282	62.5	1308	1258	106.0
104	1272.51	1427	1292	9.4	1317	1266	42.2	1430	1294	51.8	1315	1264	179.2
105		1431	1295	632.7	1337	1285	18.9	1436	1300	127.0	1335	1283	67.1
106		1450	1312	26.4	1351	1299	20.4	1442	1305	210.3	1344	1292	17.4
107	1330.50	1471	1331	127.1	1395	1341	75.5	1468	1329	35.6	1355	1303	83.3
108		1512	1369	300.2	1399	1345	53.3	1487	1346	114.8	1375	1322	57.0
109	1355.69	1516	1372	136.0	1412	1357	85.3	1507	1364	39.9	1388	1334	5.0
110		1551	1404	314.5	1413	1358	62.0	1528	1383	57.8	1396	1342	133.6
111	1377.21	1554	1407	63.6	1433	1377	169.7	1550	1403	64.6	1419	1364	59.2
112		1564	1416	60.2	1444	1388	72.7	1554	1407	297.6	1424	1369	161.6
113		1586	1435	195.3	1456	1400	16.7	1560	1412	257.4	1432	1377	39.8
114	1409.31	1588	1437	164.7	1465	1409	79.8	1581	1431	2.7	1449	1393	35.8
115		1589	1438	92.6	1468	1411	4.7	1583	1433	32.1	1467	1410	4.4
116		1599	1447	8.8	1477	1420	140.4	1600	1448	16.5	1469	1412	4.4
117		1612	1459	12.5	1484	1427	60.8	1612	1459	6.8	1483	1426	11.1
118		1616	1463	19.5	1488	1431	23.9	1612	1459	7.9	1484	1427	1.1
119		1620	1466	42.9	1494	1436	9.9	1617	1464	4.5	1487	1430	1.7
120		1621	1467	10.1	1498	1440	59.2	1622	1468	10.2	1493	1435	10.2
121	1446.45	1629	1474	16.9	1505	1447	57.3	1629	1474	12.4	1505	1447	46.7
122	1459.69	1630	1475	35.4	1510	1452	10.7	1631	1476	27.5	1510	1452	19.7
123		1676	1517	205.3	1537	1478	143.9	1658	1501	12.4	1535	1476	18.4
124	1498.28	1683	1523	93.6	1552	1492	107.0	1687	1527	167.2	1541	1482	105.5
125		1739	1574	865.1	1574	1513	459.9	1758	1591	88.0	1600	1538	131.1
126		1762	1595	210.8	1611	1549	16.5	1778	1609	35.6	1617	1555	128.1
127		1782	1613	47.4	1625	1562	385.7	1784	1615	196.2	1629	1566	44.0
128		1790	1620	387.5	1632	1569	128.3	1787	1617	82.2	1632	1569	77.2
129	1583.66	1791	1621	150.3	1636	1573	255.8	1817	1645	15.0	1657	1593	7.4
130	1597.55	1825	1652	14.0	1656	1592	211.9	1880	1702	766.8	1691	1626	467.2
131	1610.41	1843	1668	1006.7	1682	1617	950.0	1944	1760	198.3	1730	1663	155.9

132	1710.36	1987	1798	369.5	1795	1726	338.3	1984	1796	440.8	1796	1727	374.6
133	1762.92	1993	1804	432.8	1810	1740	284.9	1992	1803	250.7	1803	1733	202.9
134	2843.47	3168	2867	56.6	3013	2896	46.4	3167	2866	47.9	3013	2897	40.4
135		3170	2869	63.3	3017	2901	82.8	3172	2871	59.0	3024	2907	66.0
136		3197	2894	7.7	3027	2910	9.7	3203	2899	11.1	3031	2914	19.2
137	2927.97	3208	2904	14.6	3048	2931	8.6	3226	2920	4.8	3055	2937	7.5
138		3230	2923	40.2	3074	2956	28.7	3229	2923	38.5	3075	2956	24.1
139		3247	2939	42.7	3099	2979	35.1	3251	2942	33.1	3089	2970	0.6
140		3268	2958	3.3	3108	2988	0.9	3252	2943	8.5	3095	2976	3.1
141	3007.77	3282	2971	38.2	3135	3014	17.3	3275	2964	4.9	3109	2989	35.2
142		3285	2973	44.0	3136	3015	26.5	3286	2974	23.4	3137	3016	19.1
143		3325	3009	6.8	3168	3046	4.0	3288	2976	52.7	3141	3020	14.6
144		3328	3012	3.9	3170	3048	0.8	3323	3008	5.6	3165	3043	3.7
145	3052.80	3338	3021	9.4	3180	3057	10.5	3326	3010	1.1	3168	3046	0.6
146		3341	3024	11.1	3184	3061	7.9	3343	3026	18.0	3181	3058	18.0
147		3348	3030	26.6	3186	3063	25.7	3347	3029	36.4	3185	3062	29.9
148		3352	3034	20.9	3192	3068	15.2	3347	3029	8.0	3189	3066	3.5
149		3361	3042	7.8	3203	3079	5.8	3357	3038	10.8	3196	3073	7.8
150		3387	3066	2.7	3218	3093	4.6	3375	3055	2.6	3208	3084	3.2
151	3149.00	3427	3102	3.6	3247	3121	4.2	3408	3085	1.5	3233	3108	1.2
152		3774	3416	164.5	3364	3234	215.4	3423	3098	3.2	3247	3122	3.2
153		4114	3724	130.6	3757	3611	70.8	4111	3721	146.4	3756	3611	79.6

Table S5. Calculated optimized geometries of bond lengths (Å) for 2a A and 2a B (C₁₈H₁₄N₂O₄)

2a A			2a B		
Bond Lengths	HF	B3LYP	Bond Lengths	HF	B3LYP
R(1-2)	1.358	1.375	R(1-2)	1.360	1.376
R(1-3)	1.419	1.420	R(1-3)	1.419	1.420
R(1-11)	1.075	1.084	R(1-11)	1.075	1.084
R(2-4)	1.412	1.410	R(2-4)	1.411	1.409
R(2-12)	1.075	1.084	R(2-12)	1.075	1.084
R(3-5)	1.404	1.425	R(3-5)	1.404	1.425
R(3-7)	1.418	1.419	R(3-7)	1.419	1.419
R(4-6)	1.361	1.379	R(4-6)	1.362	1.381
R(4-13)	1.075	1.084	R(4-13)	1.074	1.083
R(5-6)	1.418	1.423	R(5-6)	1.422	1.426
R(5-10)	1.424	1.426	R(5-10)	1.422	1.423
R(6-21)	1.393	1.397	R(6-21)	1.403	1.405
R(7-8)	1.356	1.374	R(7-8)	1.357	1.374
R(7-14)	1.075	1.084	R(7-14)	1.075	1.084
R(8-9)	1.415	1.412	R(8-9)	1.415	1.412
R(8-15)	1.075	1.084	R(8-15)	1.075	1.084
R(9-10)	1.361	1.380	R(9-10)	1.361	1.381
R(9-24)	1.068	1.079	R(9-24)	1.068	1.078
R(10-16)	1.416	1.417	R(10-16)	1.418	1.421
R(16-17)	1.390	1.406	R(16-17)	1.383	1.401
R(16-19)	1.381	1.393	R(16-19)	1.386	1.399
R(17-18)	1.183	1.207	R(17-18)	1.184	1.208
R(17-20)	1.524	1.537	R(17-20)	1.515	1.523
R(19-21)	1.332	1.342	R(19-21)	1.252	1.274
R(19-22)	1.367	1.380	R(19-22)	1.516	1.521
R(20-22)	1.511	1.512	R(20-22)	1.531	1.534
R(20-28)	1.535	1.540	R(20-28)	1.524	1.528
R(20-33)	1.088	1.098	R(20-33)	1.085	1.097
R(21-23)	1.000	1.024	R(22-23)	1.083	1.093
R(22-25)	1.439	1.434	R(22-25)	1.535	1.547
R(25-26)	1.514	1.517	R(25-26)	1.505	1.505
R(25-27)	1.213	1.246	R(25-27)	1.187	1.210
R(26-36)	1.087	1.095	R(26-36)	1.083	1.093
R(26-37)	1.081	1.090	R(26-37)	1.081	1.089
R(26-38)	1.085	1.093	R(26-38)	1.088	1.096
R(28-29)	1.507	1.512	R(28-29)	1.507	1.512
R(28-34)	1.087	1.096	R(28-34)	1.084	1.094
R(28-35)	1.082	1.090	R(28-35)	1.086	1.094
R(29-30)	1.183	1.205	R(29-30)	1.185	1.207
R(29-31)	1.327	1.354	R(29-31)	1.324	1.351
R(31-32)	0.947	0.970	R(31-32)	0.947	0.970

Table S6 Calculated optimized geometries of bond angles (°) for 2a A and 2a B (C₁₈H₁₄N₂O₄)

2a A			2a B		
Bond Angles	HF	B3LYP	Bond Angles	HF	B3LYP
A(2-1-3)	120.2	120.6	A(2-1-3)	120.4	120.7
A(2-1-11)	120.7	120.6	A(2-1-11)	120.6	120.5
A(1-2-4)	121.1	121.1	A(1-2-4)	121.0	121.0
A(1-2-12)	120.1	120.0	A(1-2-12)	119.9	119.8
A(3-1-11)	119.0	118.9	A(3-1-11)	119.0	118.8
A(1-3-5)	119.0	118.8	A(1-3-5)	118.6	118.3
A(1-3-7)	122.4	122.8	A(1-3-7)	122.7	123.1
A(4-2-12)	118.8	118.9	A(4-2-12)	119.1	119.2
A(2-4-6)	119.5	119.6	A(2-4-6)	120.0	120.1
A(2-4-13)	120.3	120.5	A(2-4-13)	120.8	121.0
A(5-3-7)	118.6	118.5	A(5-3-7)	118.7	118.5
A(3-5-6)	119.2	119.1	A(3-5-6)	120.0	119.9
A(3-5-10)	120.0	119.6	A(3-5-10)	119.6	119.4
A(3-7-8)	120.0	120.4	A(3-7-8)	120.1	120.4
A(3-7-14)	119.2	118.9	A(3-7-14)	119.2	119.0
A(6-4-13)	120.2	120.0	A(6-4-13)	119.2	118.8
A(4-6-5)	120.9	120.9	A(4-6-5)	120.0	119.9
A(4-6-21)	121.4	121.5	A(4-6-21)	119.7	119.7
A(6-5-10)	120.8	121.2	A(6-5-10)	120.4	120.6
A(5-6-21)	117.7	117.6	A(5-6-21)	120.2	120.4
A(5-10-9)	120.4	120.6	A(5-10-9)	120.9	121.0
A(5-10-16)	116.1	116.3	A(5-10-16)	114.8	115.1
A(6-21-19)	123.5	123.1	A(6-21-19)	118.1	118.0
A(6-21-23)	121.5	123.8	A(8-7-14)	120.7	120.5
A(8-7-14)	120.8	120.6	A(7-8-9)	121.8	121.7
A(7-8-9)	121.9	121.7	A(7-8-15)	120.0	119.9
A(7-8-15)	120.0	119.9	A(9-8-15)	118.2	118.4
A(9-8-15)	118.2	118.4	A(8-9-10)	118.9	118.9
A(8-9-10)	119.2	119.2	A(8-9-24)	120.1	120.7
A(8-9-24)	120.0	120.7	A(10-9-24)	121.0	120.4
A(10-9-24)	120.8	120.1	A(9-10-16)	124.4	123.9
A(9-10-16)	123.6	123.1	A(10-16-17)	127.5	127.7
A(10-16-17)	127.8	128.6	A(10-16-19)	120.1	120.0
A(10-16-19)	122.7	122.1	A(17-16-19)	112.4	112.3
A(17-16-19)	109.4	109.3	A(16-17-18)	126.2	125.9
A(16-17-18)	126.0	125.9	A(16-17-20)	108.1	107.9
A(16-17-20)	107.9	107.4	A(16-19-21)	126.3	125.8
A(16-19-21)	119.1	119.6	A(16-19-22)	109.0	109.1
A(16-19-22)	112.6	112.7	A(18-17-20)	125.7	126.2
A(18-17-20)	126.0	126.7	A(17-20-22)	104.7	105.4
A(17-20-22)	102.6	103.3	A(17-20-28)	112.9	112.7
A(17-20-28)	110.7	110.8	A(17-20-33)	105.2	105.8

A(17-20-33)	105.6	105.8	A(21-19-22)	124.7	125.1
A(21-19-22)	128.2	127.7	A(19-22-20)	103.4	104.1
A(19-21-23)	115.0	113.1	A(19-22-23)	106.3	106.5
A(19-22-20)	107.5	107.3	A(19-22-25)	112.0	111.8
A(19-22-25)	121.9	121.3	A(22-20-28)	117.9	117.8
A(22-20-28)	118.3	118.0	A(22-20-33)	107.9	107.3
A(22-20-33)	112.2	111.8	A(20-22-23)	111.4	111.8
A(20-22-25)	130.5	131.3	A(20-22-25)	114.3	113.8
A(28-20-33)	106.6	106.6	A(28-20-33)	107.5	107.2
A(20-28-29)	114.3	113.8	A(20-28-29)	114.2	114.2
A(20-28-34)	109.3	108.9	A(20-28-34)	109.8	109.5
A(20-28-35)	111.0	111.1	A(20-28-35)	110.6	110.8
A(22-25-26)	119.2	119.6	A(23-22-25)	109.1	108.6
A(22-25-27)	121.8	121.3	A(22-25-26)	116.8	116.3
A(26-25-27)	119.0	119.0	A(22-25-27)	120.4	120.5
A(25-26-36)	109.2	109.7	A(26-25-27)	122.8	123.1
A(25-26-37)	108.7	108.8	A(25-26-36)	110.0	109.3
A(25-26-38)	112.5	112.7	A(25-26-37)	109.7	110.2
A(36-26-37)	108.3	107.9	A(25-26-38)	108.9	109.3
A(36-26-38)	108.3	108.0	A(36-26-37)	110.8	111.1
A(37-26-38)	109.8	109.7	A(36-26-38)	107.9	107.1
A(29-28-34)	106.4	106.8	A(37-26-38)	109.5	109.7
A(29-28-35)	108.9	109.2	A(29-28-34)	107.4	107.4
A(28-29-30)	125.5	125.8	A(29-28-35)	108.0	108.5
A(28-29-31)	111.9	111.5	A(28-29-30)	125.4	125.8
A(34-28-35)	106.7	106.6	A(28-29-31)	111.8	111.4
A(30-29-31)	122.6	122.7	A(34-28-35)	106.4	106.0
A(29-31-32)	108.9	107.3	A(30-29-31)	122.8	122.7
			A(29-31-32)	109.1	107.4

Table S7. Calculated optimized geometries of Dihedral angles ($^{\circ}$) for 2a A and 2a B ($C_{18}H_{14}N_2O_4$)

2a A			2a B		
Dihedral Angles	HF	B3LYP	Dihedral Angles	HF	B3LYP
D(3-1-2-4)	0.1	0.0	D(3-1-2-4)	0.2	0.1
D(3-1-2-12)	180.0	180.0	D(3-1-2-12)	-180.0	180.0
D(11-1-2-4)	-179.9	-179.9	D(11-1-2-4)	-179.8	-179.9
D(11-1-2-12)	0.0	0.0	D(11-1-2-12)	0.0	0.0
D(2-1-3-5)	0.1	0.0	D(2-1-3-5)	0.1	0.1
D(2-1-3-7)	-179.9	-179.9	D(2-1-3-7)	-179.9	-180.0
D(11-1-3-5)	-180.0	180.0	D(11-1-3-5)	-179.9	-180.0
D(11-1-3-7)	0.1	0.0	D(11-1-3-7)	0.1	0.0
D(1-2-4-6)	0.0	0.0	D(1-2-4-6)	-0.2	-0.1
D(1-2-4-13)	179.8	179.8	D(1-2-4-13)	179.6	179.8
D(12-2-4-6)	-179.9	-179.9	D(12-2-4-6)	180.0	180.0
D(12-2-4-13)	-0.1	-0.1	D(12-2-4-13)	-0.2	-0.1
D(1-3-5-6)	-0.3	-0.2	D(1-3-5-6)	-0.4	-0.1
D(1-3-5-10)	179.8	180.0	D(1-3-5-10)	179.7	179.9
D(7-3-5-6)	179.7	179.8	D(7-3-5-6)	179.6	179.9
D(7-3-5-10)	-0.2	-0.1	D(7-3-5-10)	-0.3	-0.1
D(1-3-7-8)	179.9	179.9	D(1-3-7-8)	180.0	180.0
D(1-3-7-14)	0.0	0.0	D(1-3-7-14)	0.0	0.0
D(5-3-7-8)	0.0	0.0	D(5-3-7-8)	0.0	0.0
D(5-3-7-14)	-179.9	-180.0	D(5-3-7-14)	-180.0	-180.0
D(2-4-6-5)	-0.2	-0.1	D(2-4-6-5)	-0.1	0.0
D(2-4-6-21)	179.6	179.7	D(2-4-6-21)	179.4	179.7
D(13-4-6-5)	-180.0	-179.9	D(13-4-6-5)	-179.9	-179.9
D(13-4-6-21)	-0.2	-0.2	D(13-4-6-21)	-0.4	-0.2
D(3-5-6-4)	0.3	0.2	D(3-5-6-4)	0.4	0.1
D(3-5-6-21)	-179.4	-179.6	D(3-5-6-21)	-179.1	-179.6
D(10-5-6-4)	-179.8	-179.9	D(10-5-6-4)	-179.7	-179.9
D(10-5-6-21)	0.4	0.3	D(10-5-6-21)	0.8	0.4
D(3-5-10-9)	0.3	0.1	D(3-5-10-9)	0.5	0.2
D(3-5-10-16)	-179.3	-179.6	D(3-5-10-16)	-179.0	-179.5
D(6-5-10-9)	-179.6	-179.7	D(6-5-10-9)	-179.5	-179.8
D(6-5-10-16)	0.8	0.6	D(6-5-10-16)	1.0	0.6
D(4-6-21-19)	179.9	-179.9	D(4-6-21-19)	179.4	179.7
D(4-6-21-23)	-0.4	0.1	D(5-6-21-19)	-1.1	-0.5
D(5-6-21-19)	-0.3	-0.2	D(3-7-8-9)	0.2	0.1
D(5-6-21-23)	179.4	179.9	D(3-7-8-15)	-179.9	-179.9
D(3-7-8-9)	0.2	0.1	D(14-7-8-9)	-179.9	-180.0
D(3-7-8-15)	-179.9	-179.9	D(14-7-8-15)	0.1	0.1
D(14-7-8-9)	-179.9	-180.0	D(7-8-9-10)	0.0	0.0
D(14-7-8-15)	0.0	0.1	D(7-8-9-24)	180.0	-179.8
D(7-8-9-10)	-0.1	0.0	D(15-8-9-10)	-180.0	180.0
D(7-8-9-24)	179.9	-179.9	D(15-8-9-24)	0.0	0.2

D(15-8-9-10)	179.9	179.9	D(8-9-10-5)	-0.3	-0.2
D(15-8-9-24)	0.0	0.0	D(8-9-10-16)	179.2	179.5
D(8-9-10-5)	-0.1	-0.1	D(24-9-10-5)	179.7	179.6
D(8-9-10-16)	179.5	179.6	D(24-9-10-16)	-0.8	-0.7
D(24-9-10-5)	179.8	179.8	D(5-10-16-17)	177.2	-179.7
D(24-9-10-16)	-0.6	-0.5	D(5-10-16-19)	-2.6	-1.4
D(5-10-16-17)	-179.4	-179.2	D(9-10-16-17)	-2.3	0.6
D(5-10-16-19)	-2.3	-1.6	D(9-10-16-19)	177.9	179.0
D(9-10-16-17)	1.0	1.1	D(10-16-17-18)	4.2	3.0
D(9-10-16-19)	178.1	178.7	D(10-16-17-20)	-173.2	-174.9
D(10-16-17-18)	-2.8	-2.0	D(19-16-17-18)	-176.0	-175.5
D(10-16-17-20)	178.5	179.1	D(19-16-17-20)	6.6	6.6
D(19-16-17-18)	179.7	-179.8	D(10-16-19-21)	2.6	1.4
D(19-16-17-20)	1.0	1.3	D(10-16-19-22)	-176.5	-177.7
D(10-16-19-21)	2.5	1.8	D(17-16-19-21)	-177.2	179.9
D(10-16-19-22)	-178.9	-179.3	D(17-16-19-22)	3.6	0.8
D(17-16-19-21)	-179.9	179.8	D(16-17-20-22)	-13.7	-11.2
D(17-16-19-22)	-1.3	-1.4	D(16-17-20-28)	-143.2	-140.9
D(16-17-20-22)	-0.5	-0.8	D(16-17-20-33)	99.9	102.3
D(16-17-20-28)	-127.7	-128.1	D(18-17-20-22)	168.8	171.0
D(16-17-20-33)	117.3	116.8	D(18-17-20-28)	39.3	41.2
D(18-17-20-22)	-179.1	-179.7	D(18-17-20-33)	-77.6	-75.6
D(18-17-20-28)	53.7	53.0	D(16-19-21-6)	-0.6	-0.3
D(18-17-20-33)	-61.4	-62.1	D(22-19-21-6)	178.4	178.6
D(16-19-21-6)	-1.1	-0.9	D(16-19-22-20)	-11.9	-7.7
D(16-19-21-23)	179.2	179.1	D(16-19-22-23)	105.6	110.6
D(22-19-21-6)	-179.5	-179.5	D(16-19-22-25)	-135.4	-130.9
D(22-19-21-23)	0.8	0.4	D(21-19-22-20)	168.9	173.1
D(16-19-22-20)	0.9	0.8	D(21-19-22-23)	-73.6	-68.6
D(16-19-22-25)	-174.6	-175.5	D(21-19-22-25)	45.4	49.9
D(21-19-22-20)	179.4	179.5	D(17-20-22-19)	15.0	11.1
D(21-19-22-25)	3.9	3.2	D(17-20-22-23)	-98.7	-103.5
D(17-20-22-19)	-0.3	0.0	D(17-20-22-25)	137.0	133.1
D(17-20-22-25)	174.8	175.9	D(28-20-22-19)	141.5	137.8
D(28-20-22-19)	121.9	122.7	D(28-20-22-23)	27.7	23.2
D(28-20-22-25)	-63.1	-61.5	D(28-20-22-25)	-96.5	-100.3
D(33-20-22-19)	-113.2	-113.3	D(33-20-22-19)	-96.7	-101.3
D(33-20-22-25)	61.9	62.6	D(33-20-22-23)	149.5	144.2
D(17-20-28-29)	61.0	62.6	D(33-20-22-25)	25.3	20.7
D(17-20-28-34)	-58.1	-56.4	D(17-20-28-29)	60.0	62.7
D(17-20-28-35)	-175.5	-173.6	D(17-20-28-34)	-60.7	-57.8
D(22-20-28-29)	-57.0	-56.2	D(17-20-28-35)	-177.9	-174.4
D(22-20-28-34)	-176.1	-175.2	D(22-20-28-29)	-62.4	-60.3
D(22-20-28-35)	66.5	67.7	D(22-20-28-34)	176.9	179.2
D(33-20-28-29)	175.4	177.2	D(22-20-28-35)	59.7	62.6
D(33-20-28-34)	56.3	58.2	D(33-20-28-29)	175.5	178.7

D(33-20-28-35)	-61.1	-58.9	D(33-20-28-34)	54.8	58.2
D(19-22-25-26)	175.2	176.2	D(33-20-28-35)	-62.3	-58.4
D(19-22-25-27)	-5.1	-4.0	D(19-22-25-26)	-83.0	-77.8
D(20-22-25-26)	0.8	0.8	D(19-22-25-27)	98.5	102.9
D(20-22-25-27)	-179.5	-179.4	D(20-22-25-26)	159.8	164.7
D(22-25-26-37)	-157.4	-155.5	D(20-22-25-27)	-18.7	-14.6
D(22-25-26-38)	-35.5	-33.7	D(22-25-26-36)	52.3	52.9
D(27-25-26-37)	22.9	24.7	D(22-25-26-37)	174.4	175.4
D(27-25-26-38)	144.8	146.5	D(22-25-26-38)	-65.7	-64.0
D(20-28-29-30)	-20.5	-22.1	D(23-25-26-36)	67.9	70.7
D(20-28-29-31)	161.2	159.4	D(23-25-26-37)	-170.0	-166.8
D(34-28-29-30)	100.1	98.2	D(23-25-26-38)	-50.2	-46.2
D(34-28-29-31)	-78.2	-80.4	D(27-25-26-36)	-129.3	-127.8
D(35-28-29-30)	-145.2	-146.9	D(27-25-26-37)	-7.1	-5.3
D(35-28-29-31)	36.5	34.6	D(27-25-26-38)	112.7	115.3
D(28-29-31-32)	177.2	177.3	D(20-28-29-30)	3.4	0.9
D(30-29-31-32)	-1.2	-1.3	D(20-28-29-31)	-177.0	-179.2
			D(34-28-29-30)	125.5	122.6
			D(34-28-29-31)	-55.0	-57.5
			D(35-28-29-30)	-120.1	-123.2
			D(35-28-29-31)	59.5	56.7
			D(28-29-31-32)	179.1	179.0
			D(30-29-31-32)	-1.3	-1.1

Table S8. Charges of molecules 2 (a and b) A and B

2a A		2a B		2b A		2b B			
HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP		
C1	-0.399913	-0.257148	-0.428967	-0.286292	C1	-0.399857	-0.260985	-0.456380	-0.274841
C2	-0.357897	-0.369729	-0.268005	-0.281624	C2	-0.357645	-0.368978	-0.142861	-0.162346
C3	0.586215	0.417237	0.451823	0.305238	C3	0.612335	0.445896	0.446425	0.310914
C4	-0.437932	-0.398038	-0.190994	-0.181700	C4	-0.388774	-0.358854	-0.202804	-0.214103
C5	-0.367980	-0.367868	0.035452	-0.072851	C5	-0.254285	-0.294501	0.261565	0.080713
C6	0.512686	0.491291	0.260237	0.215350	C6	0.511451	0.494978	0.038051	0.074180
C7	-0.309708	-0.169224	-0.451070	-0.264177	C7	-0.319075	-0.177648	-0.468588	-0.308987
C8	-0.400948	-0.416816	-0.372996	-0.408706	C8	-0.355596	-0.398983	-0.362434	-0.399460
C9	-0.153662	-0.142560	-0.119822	-0.148019	C9	-0.095807	-0.095592	-0.089248	-0.068706
C10	0.544302	0.515444	0.588568	0.522614	C10	0.489767	0.494044	0.489043	0.348979
H11	0.162494	0.128843	0.159453	0.124680	H11	0.161226	0.128177	0.159657	0.126693
H12	0.219854	0.181948	0.216310	0.180654	H12	0.220972	0.182378	0.216416	0.177839
H13	0.176083	0.143418	0.203630	0.158935	H13	0.179460	0.146671	0.211594	0.175069
H14	0.164693	0.129887	0.163640	0.130349	H14	0.164712	0.129508	0.165416	0.131106
H15	0.220765	0.184894	0.217643	0.181657	H15	0.220935	0.184880	0.219401	0.182812
N16	0.021836	0.149649	0.070814	0.207192	N16	0.040808	0.165706	0.270834	0.389287
C17	0.037475	-0.065035	-0.564491	-0.476007	C17	0.422279	0.163658	-0.795630	-0.701268
O18	-0.333026	-0.243751	-0.340846	-0.245094	O18	-0.337234	-0.243861	-0.302147	-0.210215
C19	0.077171	-0.082373	-1.352781	-0.906019	C19	-0.106298	-0.173956	-1.132380	-0.913208
C20	-0.004017	-0.092772	0.605289	0.364703	C20	0.246021	0.065330	0.353254	0.300788
N21	-0.367683	-0.136525	0.050756	0.111959	N21	-0.348428	-0.135518	0.215679	0.249589
C22	-0.023035	0.159561	0.217136	0.099864	C22	-0.252125	-0.042273	-0.078025	-0.028361
H23	0.482266	0.422158	0.340124	0.302752	H23	0.484375	0.424607	0.400283	0.341616
H24	0.280408	0.223819	0.288849	0.231109	H24	0.282454	0.225634	0.272637	0.216271
C25	0.408206	0.051161	0.375624	0.132580	C25	-0.506802	-0.729049	0.108679	-0.026700
C26	-0.779588	-0.681905	-0.649243	-0.560451	C26	0.714405	0.718841	0.067454	0.098678
O27	-0.422289	-0.329965	-0.307393	-0.231265	C27	-0.810937	-0.537420	-0.686439	-0.615901
C28	-0.822954	-0.679255	-0.624415	-0.491871	C28	0.471843	0.316480	0.457738	0.413629
C29	0.223217	0.065909	0.233851	0.037175	H29	0.200355	0.136220	0.181266	0.130280
O30	-0.352910	-0.249185	-0.346017	-0.260962	H30	0.251110	0.207144	0.272247	0.225310
O31	-0.215108	-0.131087	-0.232514	-0.145824	C31	-0.242736	-0.266131	0.228969	0.179170
H32	0.315103	0.287626	0.314750	0.287557	C32	-0.395297	-0.416353	-0.678895	-0.642322
H33	0.320584	0.294483	0.365745	0.315106	H33	0.226437	0.187205	0.230678	0.194031
H34	0.242248	0.226435	0.270140	0.253453	H34	0.216202	0.175494	0.205770	0.172180
H35	0.236722	0.231436	0.260116	0.243072	C35	-0.411355	-0.249558	-0.293170	-0.181333
H36	0.189494	0.185703	0.213052	0.220121	H36	0.202600	0.170812	0.202966	0.169228
H37	0.195270	0.187752	0.193609	0.184918	O37	-0.353495	-0.265276	-0.289773	-0.211216
H38	0.131560	0.134583	0.152943	0.149825	C38	-1.193638	-0.885398	-0.513406	-0.466147
					C39	0.235310	0.069029	0.260776	0.088480
					O40	-0.346895	-0.251298	-0.329400	-0.241758
					O41	-0.197802	-0.121263	-0.233806	-0.144276
					H42	0.313205	0.286644	0.316676	0.289399
					H43	0.297877	0.285655	0.258343	0.237991
					H44	0.245709	0.230382	0.267242	0.248890
					H45	0.262232	0.237524	0.276327	0.258026

Table S9. Charges of molecules 2 (c and d) A and B

2c A		2c B		2d A		2d B			
HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP		
C1	-0.427280	-0.269479	-0.379835	-0.237046	C1	-0.423545	-0.253944	-0.457788	-0.328904
C2	-0.370829	-0.375676	-0.163495	-0.172925	C2	-0.380624	-0.385511	-0.282760	-0.245519
C3	0.605345	0.456831	0.459524	0.323601	C3	0.603570	0.456851	0.352675	0.202541
C4	-0.375223	-0.349258	-0.198595	-0.198849	C4	-0.374346	-0.344727	-0.117819	-0.131807
C5	-0.174754	-0.253193	0.170724	0.023037	C5	-0.171427	-0.277152	0.145306	0.032000
C6	0.501192	0.471371	0.087355	0.093404	C6	0.505718	0.476867	0.317786	0.192374
C7	-0.350388	-0.195817	-0.472050	-0.300117	C7	-0.340362	-0.168738	-0.449632	-0.228857
C8	-0.414495	-0.432093	-0.365905	-0.405042	C8	-0.405803	-0.400106	-0.408646	-0.462581
C9	-0.141918	-0.141573	-0.074455	-0.070533	C9	-0.133174	-0.177046	-0.138518	-0.189282
C10	0.657182	0.616019	0.452750	0.337452	C10	0.632363	0.584484	0.711646	0.717824
H11	0.162062	0.128348	0.159728	0.125709	H11	0.162035	0.128378	0.159049	0.123547
H12	0.219688	0.181008	0.214727	0.176314	H12	0.220049	0.180850	0.216003	0.179557
H13	0.178714	0.145480	0.210154	0.173735	H13	0.179455	0.145683	0.219336	0.159576
H14	0.164293	0.128837	0.164672	0.130962	H14	0.164630	0.129003	0.161960	0.129217
H15	0.220303	0.184149	0.218784	0.181964	H15	0.220875	0.184648	0.217775	0.180778
N16	0.044003	0.166613	0.302210	0.405182	N16	0.038298	0.160379	0.135369	0.282606
C17	0.161133	-0.020133	-0.799632	-0.708317	C17	0.175398	-0.046160	-0.760680	-0.647689
O18	-0.331578	-0.240601	-0.296389	-0.207233	O18	-0.332025	-0.240396	-0.331033	-0.234946
C19	-0.254875	-0.282160	-1.130926	-0.922339	C19	-0.331674	-0.300583	-2.023109	-1.644172
C20	0.211713	0.041390	0.397190	0.339484	C20	0.321098	0.133635	1.017114	0.732069
N21	-0.357622	-0.142550	0.229686	0.259149	N21	-0.349479	-0.133225	0.217925	0.259324
C22	0.100151	0.136772	-0.065225	-0.109142	C22	0.000434	0.191060	1.055574	0.925811
H23	0.488652	0.432074	0.402456	0.342406	H23	0.484172	0.435020	0.193075	0.113859
H24	0.282091	0.224814	0.272763	0.216607	H24	0.282635	0.225015	0.287693	0.231174
C25	-0.635635	-0.750265	-0.215792	-0.356103	C25	-0.391446	-0.608628	-0.060080	-0.231745
C26	0.854902	0.953597	0.171346	0.379123	C26	0.903312	0.818823	0.448564	0.630439
C27	-0.714684	-0.419460	-0.247249	-0.151574	C27	-0.693228	-0.372135	-0.043330	-0.155254
C28	0.419284	0.206664	0.106933	0.022131	C28	0.586915	0.514334	0.325216	0.343984
H29	0.212137	0.135369	0.198875	0.153949	H29	0.204240	0.132546	0.261740	0.219398
H30	0.262087	0.209597	0.274938	0.223416	H30	0.307266	0.250389	0.311790	0.224082
C31	-0.398556	-0.347819	-0.344867	-0.304371	C31	0.148030	0.044861	0.174957	0.015692
C32	0.192617	0.072908	0.332026	0.216435	C32	-0.610606	-0.712591	-0.676782	-0.698379
H33	0.244593	0.204339	0.249948	0.210762	H33	0.249562	0.205059	0.249028	0.202638
H34	0.225606	0.187185	0.224882	0.190156	C34	-0.561706	-0.544391	-1.226369	-0.942688
C35	-0.720991	-0.718609	-0.453281	-0.429093	O35	-0.363607	-0.274588	-0.310460	-0.220826
O36	-0.351486	-0.264252	-0.305853	-0.222705	C36	-1.161390	-0.884097	-0.755778	-0.618424
C37	-1.112405	-0.837462	-0.519794	-0.474240	C37	0.186515	0.049023	0.275389	0.106444
C38	0.199991	0.052962	0.241600	0.074411	O38	-0.344691	-0.250195	-0.334475	-0.256969
O39	-0.349081	-0.252536	-0.326631	-0.241565	O39	-0.195883	-0.121770	-0.225458	-0.139236
O40	-0.198388	-0.123051	-0.234958	-0.145531	H40	0.312563	0.285568	0.312958	0.284790
H41	0.311923	0.285587	0.316914	0.289238	H41	0.297493	0.292698	0.374396	0.320765
H42	0.290337	0.286287	0.261620	0.239817	H42	0.238306	0.227462	0.270117	0.252476
H43	0.240227	0.228561	0.264117	0.246152	H43	0.286413	0.261401	0.255986	0.241516
H44	0.283598	0.254306	0.277403	0.258520	O44	-0.223984	-0.164749	-0.213100	-0.162855
O45	-0.230832	-0.145189	-0.231619	-0.143462	C45	-0.267318	-0.294804	-0.272818	-0.284696
C46	-0.296251	-0.320712	-0.312961	-0.330258	H46	0.145438	0.161987	0.151013	0.163632
H47	0.145506	0.154767	0.146899	0.157031	H47	0.115431	0.132414	0.115548	0.131644
H48	0.150149	0.158651	0.149426	0.159248	H48	0.160590	0.156195	0.166932	0.162849
H49	0.177790	0.177405	0.179863	0.181047	O49	-0.249318	-0.175812	-0.247687	-0.161329
					C50	-0.309626	-0.334196	-0.264062	-0.293789
					H51	0.146418	0.156276	0.152750	0.161937
					H52	0.178664	0.175750	0.188560	0.184913
					H53	0.157376	0.168886	0.157157	0.170491

Table S10. Calculated optimized geometries of bond lengths (Å) for 2b A and 2b B (C₂₃H₁₆N₂O₄)

2b A			2b B		
Bond Lengths	HF	B3LYP	Bond Lengths	HF	B3LYP
R(1-2)	1.358	1.375	R(1-2)	1.360	1.376
R(1-3)	1.419	1.420	R(1-3)	1.419	1.420
R(1-11)	1.075	1.084	R(1-11)	1.075	1.084
R(2-4)	1.412	1.410	R(2-4)	1.411	1.409
R(2-12)	1.075	1.084	R(2-12)	1.075	1.084
R(3-5)	1.404	1.425	R(3-5)	1.404	1.425
R(3-7)	1.418	1.419	R(3-7)	1.420	1.419
R(4-6)	1.361	1.379	R(4-6)	1.362	1.382
R(4-13)	1.075	1.084	R(4-13)	1.074	1.083
R(5-6)	1.418	1.423	R(5-6)	1.422	1.427
R(5-10)	1.424	1.426	R(5-10)	1.423	1.424
R(6-21)	1.393	1.397	R(6-21)	1.402	1.404
R(7-8)	1.356	1.374	R(7-8)	1.357	1.374
R(7-14)	1.075	1.084	R(7-14)	1.075	1.084
R(8-9)	1.415	1.412	R(8-9)	1.416	1.412
R(8-15)	1.075	1.084	R(8-15)	1.075	1.084
R(9-10)	1.361	1.380	R(9-10)	1.361	1.381
R(9-24)	1.068	1.079	R(9-24)	1.068	1.078
R(10-16)	1.416	1.418	R(10-16)	1.418	1.421
R(16-17)	1.391	1.406	R(16-17)	1.381	1.398
R(16-19)	1.380	1.392	R(16-19)	1.390	1.405
R(17-18)	1.183	1.207	R(17-18)	1.184	1.209
R(17-20)	1.523	1.535	R(17-20)	1.521	1.530
R(19-21)	1.331	1.341	R(19-21)	1.250	1.272
R(19-22)	1.370	1.384	R(19-22)	1.509	1.511
R(20-22)	1.513	1.515	R(20-22)	1.540	1.548
R(20-38)	1.535	1.539	R(20-38)	1.526	1.529
R(20-43)	1.086	1.096	R(20-43)	1.086	1.096
R(21-23)	0.999	1.025	R(22-23)	1.080	1.091
R(22-25)	1.439	1.435	R(22-25)	1.530	1.538
R(25-26)	1.504	1.502	R(25-26)	1.503	1.499
R(25-37)	1.215	1.250	R(25-37)	1.190	1.216
R(26-27)	1.388	1.399	R(26-27)	1.390	1.401
R(26-28)	1.390	1.401	R(26-28)	1.394	1.404
R(27-29)	1.075	1.084	R(27-29)	1.072	1.082
R(27-31)	1.386	1.394	R(27-31)	1.385	1.393
R(28-30)	1.074	1.083	R(28-30)	1.073	1.083
R(28-32)	1.384	1.391	R(28-32)	1.381	1.389
R(31-33)	1.075	1.084	R(31-33)	1.075	1.084
R(31-35)	1.385	1.394	R(31-35)	1.383	1.393

R(32-34)	1.075	1.084	R(32-34)	1.075	1.084
R(32-35)	1.387	1.395	R(32-35)	1.387	1.396
R(35-36)	1.075	1.084	R(35-36)	1.075	1.084
R(38-39)	1.507	1.511	R(38-39)	1.507	1.512
R(38-44)	1.087	1.096	R(38-44)	1.084	1.094
R(38-45)	1.082	1.091	R(38-45)	1.085	1.094
R(39-40)	1.184	1.206	R(39-40)	1.184	1.206
R(39-41)	1.326	1.354	R(39-41)	1.323	1.350
R(41-42)	0.946	0.970	R(41-42)	0.947	0.970

Table S11. Calculated optimized geometries of bond angles (°) for 2b A and 2b B (C₂₃H₁₆N₂O₄)

2b A			2b B		
Bond Angles	HF	B3LYP	Bond Angles	HF	B3LYP
A(2-1-3)	120.3	120.6	A(2-1-3)	120.4	120.7
A(2-1-11)	120.7	120.6	A(2-1-11)	120.6	120.5
A(1-2-4)	121.1	121.1	A(1-2-4)	121.0	121.0
A(1-2-12)	120.1	120.0	A(1-2-12)	119.9	119.8
A(3-1-11)	119.0	118.9	A(3-1-11)	119.0	118.8
A(1-3-5)	119.0	118.7	A(1-3-5)	118.6	118.3
A(1-3-7)	122.4	122.8	A(1-3-7)	122.7	123.1
A(4-2-12)	118.8	118.9	A(4-2-12)	119.1	119.2
A(2-4-6)	119.5	119.6	A(2-4-6)	120.0	120.1
A(2-4-13)	120.3	120.5	A(2-4-13)	120.9	121.2
A(5-3-7)	118.6	118.4	A(5-3-7)	118.7	118.5
A(3-5-6)	119.2	119.1	A(3-5-6)	119.9	119.9
A(3-5-10)	120.0	119.7	A(3-5-10)	119.6	119.4
A(3-7-8)	120.0	120.4	A(3-7-8)	120.2	120.5
A(3-7-14)	119.2	119.0	A(3-7-14)	119.2	119.0
A(6-4-13)	120.3	120.0	A(6-4-13)	119.1	118.7
A(4-6-5)	121.0	120.9	A(4-6-5)	120.1	119.9
A(4-6-21)	121.4	121.5	A(4-6-21)	119.7	119.6
A(6-5-10)	120.8	121.2	A(6-5-10)	120.5	120.7
A(5-6-21)	117.7	117.6	A(5-6-21)	120.2	120.5
A(5-10-9)	120.3	120.5	A(5-10-9)	120.9	121.0
A(5-10-16)	116.1	116.4	A(5-10-16)	114.7	115.1
A(6-21-19)	123.6	123.2	A(6-21-19)	118.1	117.8
A(6-21-23)	121.4	123.8	A(8-7-14)	120.7	120.5
A(8-7-14)	120.8	120.6	A(7-8-9)	121.8	121.7
A(7-8-9)	121.9	121.7	A(7-8-15)	120.0	119.9
A(7-8-15)	120.0	119.9	A(9-8-15)	118.3	118.4
A(9-8-15)	118.2	118.4	A(8-9-10)	118.9	118.9
A(8-9-10)	119.2	119.2	A(8-9-24)	120.1	120.7
A(8-9-24)	120.0	120.7	A(10-9-24)	121.0	120.4
A(10-9-24)	120.8	120.1	A(9-10-16)	124.4	123.9
A(9-10-16)	123.6	123.1	A(10-16-17)	127.5	127.7
A(10-16-17)	127.7	128.4	A(10-16-19)	120.0	119.9
A(10-16-19)	122.8	122.2	A(17-16-19)	112.5	112.4
A(17-16-19)	109.4	109.3	A(16-17-18)	126.4	126.2
A(16-17-18)	125.9	125.9	A(16-17-20)	108.4	108.0
A(16-17-20)	108.0	107.4	A(16-19-21)	126.5	126.0
A(16-19-21)	119.1	119.5	A(16-19-22)	109.2	109.2
A(16-19-22)	112.6	112.8	A(18-17-20)	125.1	125.7
A(18-17-20)	126.1	126.7	A(17-20-22)	104.5	104.8
A(17-20-22)	102.6	103.5	A(17-20-38)	112.9	112.9
A(17-20-38)	111.0	111.0	A(17-20-43)	105.1	105.3

A(17-20-43)	105.2	105.2	A(21-19-22)	124.3	124.8
A(21-19-22)	128.3	127.7	A(19-22-20)	104.0	104.2
A(19-21-23)	115.0	112.9	A(19-22-23)	106.2	106.5
A(19-22-20)	107.3	107.0	A(19-22-25)	117.3	117.5
A(19-22-25)	121.2	120.5	A(22-20-38)	116.7	116.7
A(22-20-38)	117.9	117.7	A(22-20-43)	110.2	109.8
A(22-20-43)	112.9	112.4	A(20-22-23)	110.2	109.8
A(20-22-25)	131.4	132.5	A(20-22-25)	114.2	114.0
A(38-20-43)	106.5	106.5	A(38-20-43)	106.9	106.8
A(20-38-39)	114.4	114.0	A(20-38-39)	113.8	113.8
A(20-38-44)	109.4	109.1	A(20-38-44)	109.9	109.7
A(20-38-45)	110.6	110.8	A(20-38-45)	110.4	110.7
A(21-23-37)	127.6	131.1	A(23-22-25)	104.7	104.6
A(22-25-26)	120.1	121.1	A(22-25-26)	122.5	121.8
A(22-25-37)	121.8	121.1	A(22-25-37)	117.2	117.5
A(26-25-37)	118.1	117.8	A(26-25-37)	120.2	120.6
A(25-26-27)	122.2	122.7	A(25-26-27)	124.0	123.9
A(25-26-28)	118.4	118.2	A(25-26-28)	117.1	117.3
A(25-37-23)	105.7	106.4	A(27-26-28)	118.9	118.8
A(27-26-28)	119.3	119.0	A(26-27-29)	121.4	121.1
A(26-27-29)	120.2	120.1	A(26-27-31)	120.6	120.6
A(26-27-31)	120.4	120.5	A(26-28-30)	118.8	118.3
A(26-28-30)	119.2	118.7	A(26-28-32)	120.6	120.6
A(26-28-32)	120.3	120.5	A(29-27-31)	118.0	118.3
A(29-27-31)	119.4	119.4	A(27-31-33)	119.7	119.7
A(27-31-33)	119.8	119.8	A(27-31-35)	120.0	120.1
A(27-31-35)	120.0	120.1	A(30-28-32)	120.5	121.0
A(30-28-32)	120.5	120.8	A(28-32-34)	119.9	119.9
A(28-32-34)	119.8	119.8	A(28-32-35)	120.0	120.0
A(28-32-35)	120.1	120.1	A(33-31-35)	120.3	120.2
A(33-31-35)	120.2	120.1	A(31-35-32)	119.9	119.9
A(31-35-32)	119.9	119.8	A(31-35-36)	120.0	120.0
A(31-35-36)	120.0	120.1	A(34-32-35)	120.1	120.1
A(34-32-35)	120.1	120.0	A(32-35-36)	120.1	120.1
A(32-35-36)	120.1	120.1	A(39-38-44)	107.4	107.4
A(39-38-44)	106.5	106.9	A(39-38-45)	108.1	108.5
A(39-38-45)	108.8	109.1	A(38-39-40)	125.2	125.7
A(38-39-40)	125.7	126.0	A(38-39-41)	111.8	111.4
A(38-39-41)	111.8	111.4	A(44-38-45)	106.8	106.4
A(44-38-45)	106.8	106.6	A(40-39-41)	123.0	122.9
A(40-39-41)	122.5	122.6	A(39-41-42)	109.1	107.5
A(39-41-42)	108.8	107.2			

Table S12. Calculated optimized geometries of Dihedral angles (°) for 2b A and 2b B (C₂₃H₁₆N₂O₄)

2b A			2b B		
Dihedral Angles	HF	B3LYP	Dihedral Angles	HF	B3LYP
D(3-1-2-4)	0.0	-0.1	D(3-1-2-4)	0.0	0.2
D(3-1-2-12)	180.0	179.9	D(3-1-2-12)	180.0	179.9
D(11-1-2-4)	-179.9	-179.9	D(11-1-2-4)	-179.9	-179.7
D(11-1-2-12)	0.0	0.0	D(11-1-2-12)	0.0	0.1
D(2-1-3-5)	0.1	0.1	D(2-1-3-5)	0.1	0.1
D(2-1-3-7)	-179.8	-179.8	D(2-1-3-7)	-179.8	-179.8
D(11-1-3-5)	-180.0	180.0	D(11-1-3-5)	-180.0	180.0
D(11-1-3-7)	0.1	0.1	D(11-1-3-7)	0.1	0.1
D(1-2-4-6)	0.0	0.0	D(1-2-4-6)	0.0	-0.2
D(1-2-4-13)	179.9	180.0	D(1-2-4-13)	179.9	179.6
D(12-2-4-6)	-179.9	-180.0	D(12-2-4-6)	-179.9	-179.9
D(12-2-4-13)	-0.1	0.0	D(12-2-4-13)	-0.1	-0.2
D(1-3-5-6)	-0.2	-0.1	D(1-3-5-6)	-0.2	-0.4
D(1-3-5-10)	-179.9	-179.8	D(1-3-5-10)	-179.9	179.7
D(7-3-5-6)	179.7	179.8	D(7-3-5-6)	179.7	179.5
D(7-3-5-10)	-0.1	0.1	D(7-3-5-10)	-0.1	-0.3
D(1-3-7-8)	179.8	179.8	D(1-3-7-8)	179.8	179.9
D(1-3-7-14)	-0.1	-0.1	D(1-3-7-14)	-0.1	0.1
D(5-3-7-8)	-0.1	-0.1	D(5-3-7-8)	-0.1	0.0
D(5-3-7-14)	-180.0	180.0	D(5-3-7-14)	-180.0	-179.9
D(2-4-6-5)	-0.1	0.0	D(2-4-6-5)	-0.1	-0.2
D(2-4-6-21)	179.7	179.8	D(2-4-6-21)	179.7	179.3
D(13-4-6-5)	180.0	-180.0	D(13-4-6-5)	180.0	-179.9
D(13-4-6-21)	-0.2	-0.1	D(13-4-6-21)	-0.2	-0.4
D(3-5-6-4)	0.2	0.0	D(3-5-6-4)	0.2	0.4
D(3-5-6-21)	-179.7	-179.8	D(3-5-6-21)	-179.7	-179.0
D(10-5-6-4)	180.0	179.8	D(10-5-6-4)	180.0	-179.7
D(10-5-6-21)	0.1	-0.1	D(10-5-6-21)	0.1	0.8
D(3-5-10-9)	0.1	0.0	D(3-5-10-9)	0.1	0.5
D(3-5-10-16)	-179.4	-179.7	D(3-5-10-16)	-179.4	-179.1
D(6-5-10-9)	-179.7	-179.7	D(6-5-10-9)	-179.7	-179.4
D(6-5-10-16)	0.8	0.6	D(6-5-10-16)	0.8	1.0
D(4-6-21-19)	179.7	-180.0	D(4-6-21-19)	179.7	179.3
D(4-6-21-23)	-2.9	-2.7	D(5-6-21-23)	176.9	-1.3
D(5-6-21-19)	-0.4	-0.1	D(3-7-8-9)	0.1	0.2
D(5-6-21-23)	176.9	177.1	D(3-7-8-15)	-179.9	-179.7
D(3-7-8-9)	0.1	0.1	D(14-7-8-9)	-180.0	-179.9
D(3-7-8-15)	-179.9	-179.9	D(14-7-8-15)	0.0	0.1
D(14-7-8-9)	-180.0	180.0	D(7-8-9-10)	-0.1	-0.1
D(14-7-8-15)	0.0	0.0	D(7-8-9-24)	-179.9	180.0
D(7-8-9-10)	-0.1	0.0	D(15-8-9-10)	179.9	179.9
D(7-8-9-24)	-179.9	-179.8	D(15-8-9-24)	0.1	0.0

D(15-8-9-10)	179.9	179.9	D(8-9-10-5)	0.0	-0.3
D(15-8-9-24)	0.1	0.2	D(8-9-10-16)	179.5	179.3
D(8-9-10-5)	0.0	0.0	D(24-9-10-5)	179.8	179.7
D(8-9-10-16)	179.5	179.7	D(24-9-10-16)	-0.7	-0.8
D(24-9-10-5)	179.8	179.7	D(5-10-16-17)	-177.1	178.9
D(24-9-10-16)	-0.7	-0.6	D(5-10-16-19)	-1.5	-2.5
D(5-10-16-17)	-177.1	-176.6	D(9-10-16-17)	3.4	-0.6
D(5-10-16-19)	-1.5	-0.9	D(9-10-16-19)	179.0	178.0
D(9-10-16-17)	3.4	3.7	D(10-16-17-18)	-3.4	0.9
D(9-10-16-19)	179.0	179.4	D(10-16-17-20)	178.1	-176.4
D(10-16-17-18)	-3.4	-2.9	D(19-16-17-18)	-179.5	-177.8
D(10-16-17-20)	178.1	178.4	D(19-16-17-20)	2.1	4.9
D(19-16-17-18)	-179.5	-179.1	D(10-16-19-21)	1.3	2.3
D(19-16-17-20)	2.1	2.3	D(10-16-19-22)	-179.6	-175.6
D(10-16-19-21)	1.3	0.8	D(17-16-19-21)	177.6	-179.0
D(10-16-19-22)	-179.6	-179.4	D(17-16-19-22)	-3.3	3.2
D(17-16-19-21)	177.6	177.2	D(16-17-20-22)	-0.3	-10.6
D(17-16-19-22)	-3.3	-3.0	D(16-17-20-38)	-127.2	-138.6
D(16-17-20-22)	-0.3	-0.8	D(16-17-20-43)	118.0	105.2
D(16-17-20-38)	-127.2	-127.9	D(18-17-20-22)	-178.7	172.1
D(16-17-20-43)	118.0	117.3	D(18-17-20-38)	54.4	44.0
D(18-17-20-22)	-178.7	-179.5	D(18-17-20-43)	-60.4	-72.1
D(18-17-20-38)	54.4	53.4	D(16-19-21-6)	-0.3	-0.3
D(18-17-20-43)	-60.4	-61.4	D(16-19-21-23)	-177.8	177.3
D(16-19-21-6)	-0.3	-0.2	D(22-19-21-6)	-179.3	-9.6
D(16-19-21-23)	-177.8	-177.7	D(22-19-21-23)	3.2	106.4
D(22-19-21-6)	-179.3	-180.0	D(16-19-22-20)	3.0	-136.8
D(22-19-21-23)	3.2	2.5	D(16-19-22-25)	-178.9	172.5
D(16-19-22-20)	3.0	2.4	D(21-19-22-20)	-178.0	-71.5
D(16-19-22-25)	-178.9	-179.9	D(21-19-22-25)	0.1	45.3
D(21-19-22-20)	-178.0	-177.8	D(17-20-22-19)	-1.5	11.9
D(21-19-22-25)	0.1	-0.1	D(17-20-22-25)	-179.4	141.2
D(17-20-22-19)	-1.5	-0.9	D(38-20-22-19)	120.8	137.6
D(17-20-22-25)	-179.4	-178.2	D(38-20-22-25)	-57.0	-93.1
D(38-20-22-19)	120.8	121.9	D(43-20-22-19)	-114.2	-100.7
D(38-20-22-25)	-57.0	-55.4	D(43-20-22-25)	67.9	28.6
D(43-20-22-19)	-114.2	-113.8	D(17-20-38-39)	58.9	59.0
D(43-20-22-25)	67.9	68.8	D(17-20-38-44)	-60.5	-61.4
D(17-20-38-39)	58.9	60.6	D(17-20-38-45)	-177.9	-178.5
D(17-20-38-44)	-60.5	-58.8	D(22-20-38-39)	-59.1	-62.5
D(17-20-38-45)	-177.9	-175.9	D(22-20-38-44)	-178.5	177.1
D(22-20-38-39)	-59.1	-58.2	D(22-20-38-45)	64.1	60.0
D(22-20-38-44)	-178.5	-177.6	D(43-20-38-39)	172.9	174.3
D(22-20-38-45)	64.1	65.2	D(43-20-38-44)	53.5	53.9
D(43-20-38-39)	172.9	174.6	D(43-20-38-45)	-63.9	-63.3
D(43-20-38-44)	53.5	55.2	D(19-22-25-26)	173.6	50.5

D(43-20-38-45)	-63.9	-61.9	D(19-22-25-37)	-7.0	-133.0
D(19-22-25-26)	173.6	176.2	D(20-22-25-26)	-8.9	-71.8
D(19-22-25-37)	-7.0	-4.6	D(20-22-25-37)	170.6	104.7
D(20-22-25-26)	-8.9	-6.8	D(22-25-26-27)	-47.8	0.6
D(20-22-25-37)	170.6	172.4	D(22-25-26-28)	135.2	179.8
D(22-25-26-27)	-47.8	-42.5	D(37-25-26-27)	132.7	-175.8
D(22-25-26-28)	135.2	140.9	D(37-25-26-28)	-44.3	3.3
D(37-25-26-27)	132.7	138.2	D(25-26-27-29)	0.6	-1.5
D(37-25-26-28)	-44.3	-38.3	D(25-26-27-31)	-177.5	178.9
D(25-26-27-29)	0.6	0.6	D(28-26-27-29)	177.6	179.4
D(25-26-27-31)	-177.5	-177.2	D(28-26-27-31)	-0.6	-0.2
D(28-26-27-29)	177.6	177.1	D(25-26-28-30)	-1.0	0.9
D(28-26-27-31)	-0.6	-0.7	D(25-26-28-32)	178.8	-179.3
D(25-26-28-30)	-1.0	-1.3	D(27-26-28-30)	-178.0	-179.9
D(25-26-28-32)	178.8	178.5	D(27-26-28-32)	1.8	-0.1
D(27-26-28-30)	-178.0	-178.0	D(26-27-31-33)	178.9	-180.0
D(27-26-28-32)	1.8	1.8	D(26-27-31-35)	-0.9	0.3
D(26-27-31-33)	178.9	178.8	D(29-27-31-33)	0.8	0.4
D(26-27-31-35)	-0.9	-0.8	D(29-27-31-35)	-179.0	-179.3
D(29-27-31-33)	0.8	1.1	D(26-28-32-34)	179.1	-179.7
D(29-27-31-35)	-179.0	-178.5	D(26-28-32-35)	-1.6	0.3
D(26-28-32-34)	179.1	179.1	D(30-28-32-34)	-1.1	0.2
D(26-28-32-35)	-1.6	-1.5	D(30-28-32-35)	178.3	-179.9
D(30-28-32-34)	-1.1	-1.2	D(27-31-35-32)	1.1	-0.1
D(30-28-32-35)	178.3	178.3	D(27-31-35-36)	-179.4	179.7
D(27-31-35-32)	1.1	1.1	D(33-31-35-32)	-178.7	-179.8
D(27-31-35-36)	-179.4	-179.5	D(33-31-35-36)	0.8	0.1
D(33-31-35-32)	-178.7	-178.5	D(28-32-35-31)	0.1	-0.2
D(33-31-35-36)	0.8	0.9	D(28-32-35-36)	-179.3	180.0
D(28-32-35-31)	0.1	0.0	D(34-32-35-31)	179.4	179.8
D(28-32-35-36)	-179.3	-179.4	D(34-32-35-36)	0.0	-0.1
D(34-32-35-31)	179.4	179.5	D(20-38-39-40)	-15.3	-1.9
D(34-32-35-36)	0.0	0.0	D(20-38-39-41)	166.3	178.3
D(20-38-39-40)	-15.3	-15.8	D(44-38-39-40)	105.7	119.8
D(20-38-39-41)	166.3	165.6	D(44-38-39-41)	-72.7	-60.0
D(44-38-39-40)	105.7	104.9	D(45-38-39-40)	-139.5	-125.6
D(44-38-39-41)	-72.7	-73.7	D(45-38-39-41)	42.1	54.7
D(45-38-39-40)	-139.5	-140.2	D(38-39-41-42)	177.6	179.3
D(45-38-39-41)	42.1	41.2	D(40-39-41-42)	-0.9	-0.4
D(38-39-41-42)	177.6	177.7			
D(40-39-41-42)	-0.9	-1.0			

Table S13. Calculated optimized geometries of bond lengths (Å) for 2c A and 2c B (C₂₄H₁₈N₂O₅)

2c A			2c B		
Bond Lengths	HF	B3LYP	Bond Lengths	HF	B3LYP
R(1-2)	1.358	1.375	R(1-2)	1.360	1.377
R(1-3)	1.419	1.420	R(1-3)	1.419	1.420
R(1-11)	1.075	1.084	R(1-11)	1.075	1.084
R(2-4)	1.412	1.410	R(2-4)	1.411	1.409
R(2-12)	1.075	1.084	R(2-12)	1.076	1.084
R(3-5)	1.404	1.425	R(3-5)	1.404	1.425
R(3-7)	1.418	1.419	R(3-7)	1.420	1.419
R(4-6)	1.361	1.380	R(4-6)	1.362	1.382
R(4-13)	1.075	1.084	R(4-13)	1.074	1.083
R(5-6)	1.418	1.423	R(5-6)	1.422	1.427
R(5-10)	1.424	1.426	R(5-10)	1.423	1.424
R(6-21)	1.392	1.396	R(6-21)	1.402	1.404
R(7-8)	1.356	1.374	R(7-8)	1.357	1.374
R(7-14)	1.075	1.084	R(7-14)	1.075	1.084
R(8-9)	1.415	1.412	R(8-9)	1.416	1.412
R(8-15)	1.075	1.084	R(8-15)	1.075	1.084
R(9-10)	1.361	1.380	R(9-10)	1.361	1.381
R(9-24)	1.068	1.079	R(9-24)	1.068	1.078
R(10-16)	1.415	1.417	R(10-16)	1.418	1.421
R(16-17)	1.390	1.404	R(16-17)	1.381	1.398
R(16-19)	1.381	1.394	R(16-19)	1.391	1.405
R(17-18)	1.183	1.208	R(17-18)	1.184	1.209
R(17-20)	1.523	1.535	R(17-20)	1.520	1.530
R(19-21)	1.332	1.342	R(19-21)	1.250	1.273
R(19-22)	1.369	1.383	R(19-22)	1.509	1.511
R(20-22)	1.513	1.515	R(20-22)	1.540	1.547
R(20-37)	1.535	1.539	R(20-37)	1.526	1.529
R(20-42)	1.085	1.096	R(20-42)	1.086	1.096
R(21-23)	0.999	1.025	R(22-23)	1.080	1.091
R(22-25)	1.442	1.439	R(22-25)	1.531	1.539
R(25-26)	1.499	1.497	R(25-26)	1.494	1.490
R(25-36)	1.216	1.252	R(25-36)	1.192	1.218
R(26-27)	1.394	1.404	R(26-27)	1.396	1.406
R(26-28)	1.385	1.398	R(26-28)	1.388	1.401
R(27-29)	1.074	1.083	R(27-29)	1.073	1.082
R(27-31)	1.377	1.386	R(27-31)	1.375	1.383
R(28-30)	1.074	1.083	R(28-30)	1.073	1.083
R(28-32)	1.387	1.392	R(28-32)	1.383	1.388
R(31-33)	1.074	1.083	R(31-33)	1.074	1.083
R(31-35)	1.393	1.401	R(31-35)	1.394	1.402
R(32-34)	1.072	1.082	R(32-34)	1.072	1.081
R(32-35)	1.388	1.399	R(32-35)	1.389	1.401

R(35-45)	1.342	1.361	R(35-45)	1.337	1.356
R(37-38)	1.507	1.511	R(37-38)	1.507	1.512
R(37-43)	1.087	1.096	R(37-43)	1.084	1.094
R(37-44)	1.082	1.091	R(37-44)	1.085	1.094
R(38-39)	1.184	1.206	R(38-39)	1.184	1.206
R(38-40)	1.327	1.354	R(38-40)	1.323	1.351
R(40-41)	0.946	0.969	R(40-41)	0.947	0.969
R(45-46)	1.401	1.423	R(45-46)	1.403	1.425
R(46-47)	1.086	1.095	R(46-47)	1.085	1.095
R(46-48)	1.086	1.095	R(46-48)	1.085	1.094
R(46-49)	1.080	1.089	R(46-49)	1.080	1.088

Table S14. Calculated optimized geometries of bond angles (°) for 2c A and 2c B (C₂₄H₁₈N₂O₅)

2c A			2c B		
Bond Angles	HF	Bond Angles	HF	Bond Angles	HF
A(2-1-3)	120.2	120.5	A(2-1-3)	120.4	120.7
A(2-1-11)	120.7	120.6	A(2-1-11)	120.6	120.5
A(1-2-4)	121.2	121.1	A(1-2-4)	121.0	121.0
A(1-2-12)	120.1	120.0	A(1-2-12)	119.9	119.8
A(3-1-11)	119.1	118.9	A(3-1-11)	119.0	118.8
A(1-3-5)	119.0	118.7	A(1-3-5)	118.6	118.3
A(1-3-7)	122.4	122.8	A(1-3-7)	122.7	123.1
A(4-2-12)	118.8	118.9	A(4-2-12)	119.1	119.2
A(2-4-6)	119.5	119.6	A(2-4-6)	120.0	120.2
A(2-4-13)	120.3	120.5	A(2-4-13)	120.9	121.2
A(5-3-7)	118.6	118.4	A(5-3-7)	118.7	118.5
A(3-5-6)	119.2	119.2	A(3-5-6)	119.9	120.0
A(3-5-10)	120.0	119.7	A(3-5-10)	119.6	119.4
A(3-7-8)	120.0	120.4	A(3-7-8)	120.2	120.5
A(3-7-14)	119.2	119.0	A(3-7-14)	119.2	119.0
A(6-4-13)	120.2	119.9	A(6-4-13)	119.1	118.7
A(4-6-5)	120.9	120.8	A(4-6-5)	120.0	119.9
A(4-6-21)	121.4	121.5	A(4-6-21)	119.7	119.5
A(6-5-10)	120.7	121.1	A(6-5-10)	120.5	120.7
A(5-6-21)	117.7	117.6	A(5-6-21)	120.3	120.6
A(5-10-9)	120.3	120.5	A(5-10-9)	120.9	121.0
A(5-10-16)	116.1	116.4	A(5-10-16)	114.7	115.1
A(6-21-19)	123.6	123.3	A(6-21-19)	118.1	117.9
A(6-21-23)	121.5	124.0	A(8-7-14)	120.7	120.5
A(8-7-14)	120.8	120.6	A(7-8-9)	121.8	121.7
A(7-8-9)	121.9	121.7	A(7-8-15)	120.0	119.9
A(7-8-15)	120.0	119.9	A(9-8-15)	118.3	118.4
A(9-8-15)	118.2	118.4	A(8-9-10)	118.9	118.9
A(8-9-10)	119.2	119.2	A(8-9-24)	120.1	120.7
A(8-9-24)	120.0	120.7	A(10-9-24)	121.0	120.4
A(10-9-24)	120.8	120.1	A(9-10-16)	124.4	123.9
A(9-10-16)	123.6	123.1	A(10-16-17)	127.5	127.7
A(10-16-17)	127.7	128.4	A(10-16-19)	120.0	119.9
A(10-16-19)	122.8	122.2	A(17-16-19)	112.5	112.4
A(17-16-19)	109.4	109.3	A(16-17-18)	126.3	126.2
A(16-17-18)	126.0	126.0	A(16-17-20)	108.4	108.0
A(16-17-20)	107.9	107.4	A(16-19-21)	126.4	125.9
A(16-19-21)	119.0	119.3	A(16-19-22)	109.2	109.2
A(16-19-22)	112.7	112.9	A(18-17-20)	125.2	125.8
A(18-17-20)	126.0	126.6	A(17-20-22)	104.5	104.8
A(17-20-22)	102.7	103.5	A(17-20-37)	112.9	112.9
A(17-20-37)	111.0	111.0	A(17-20-42)	105.1	105.3

A(17-20-42)	104.9	105.0	A(21-19-22)	124.4	124.9
A(21-19-22)	128.4	127.8	A(19-22-20)	104.0	104.2
A(19-21-23)	114.8	112.7	A(19-22-23)	106.2	106.4
A(19-22-20)	107.2	106.8	A(19-22-25)	117.4	117.6
A(19-22-25)	121.2	120.4	A(22-20-37)	116.7	116.7
A(22-20-37)	117.8	117.7	A(22-20-42)	110.1	109.8
A(22-20-42)	113.1	112.5	A(20-22-23)	110.2	109.8
A(20-22-25)	131.6	132.7	A(20-22-25)	114.1	114.0
A(37-20-42)	106.5	106.5	A(37-20-42)	106.9	106.8
A(20-37-38)	114.4	114.0	A(20-37-38)	113.8	113.9
A(20-37-43)	109.4	109.1	A(20-37-43)	110.0	109.8
A(20-37-44)	110.6	110.8	A(20-37-44)	110.4	110.6
A(21-23-36)	127.7	131.4	A(23-22-25)	104.7	104.6
A(22-25-26)	120.6	121.6	A(22-25-26)	122.4	121.6
A(22-25-36)	121.2	120.5	A(22-25-36)	117.0	117.3
A(26-25-36)	118.2	117.9	A(26-25-36)	120.6	121.0
A(25-26-27)	123.2	123.7	A(25-26-27)	124.7	124.5
A(25-26-28)	118.5	118.1	A(25-26-28)	117.5	117.6
A(25-36-23)	106.1	107.0	A(27-26-28)	117.8	117.9
A(27-26-28)	118.2	118.0	A(26-27-29)	121.3	121.1
A(26-27-29)	120.2	120.2	A(26-27-31)	121.3	121.2
A(26-27-31)	121.1	121.1	A(26-28-30)	118.7	118.2
A(26-28-30)	119.0	118.5	A(26-28-32)	121.8	121.7
A(26-28-32)	121.5	121.6	A(29-27-31)	117.4	117.8
A(29-27-31)	118.6	118.6	A(27-31-33)	121.1	121.2
A(27-31-33)	121.2	121.3	A(27-31-35)	120.1	120.1
A(27-31-35)	120.1	120.1	A(30-28-32)	119.5	120.1
A(30-28-32)	119.5	119.9	A(28-32-34)	119.2	119.4
A(28-32-34)	119.2	119.4	A(28-32-35)	119.5	119.5
A(28-32-35)	119.6	119.6	A(33-31-35)	118.8	118.7
A(33-31-35)	118.7	118.6	A(31-35-32)	119.5	119.6
A(31-35-32)	119.5	119.6	A(31-35-45)	115.9	115.8
A(31-35-45)	115.9	115.8	A(34-32-35)	121.3	121.1
A(34-32-35)	121.3	121.0	A(32-35-45)	124.5	124.6
A(32-35-45)	124.5	124.6	A(35-45-46)	120.3	119.0
A(35-45-46)	120.2	118.8	A(38-37-43)	107.4	107.4
A(38-37-43)	106.5	106.9	A(38-37-44)	108.1	108.5
A(38-37-44)	108.7	109.1	A(37-38-39)	125.2	125.8
A(37-38-39)	125.7	126.1	A(37-38-40)	111.8	111.4
A(37-38-40)	111.8	111.3	A(43-37-44)	106.9	106.4
A(43-37-44)	106.9	106.7	A(39-38-40)	123.0	122.9
A(39-38-40)	122.5	122.6	A(38-40-41)	109.1	107.4
A(38-40-41)	108.8	107.2	A(45-46-47)	111.3	111.3
A(45-46-47)	111.3	111.3	A(45-46-48)	111.2	111.2
A(45-46-48)	111.3	111.3	A(45-46-49)	106.1	105.7
A(45-46-49)	106.1	105.8	A(47-46-48)	109.7	109.7

A(47-46-48)	109.6	109.6	A(47-46-49)	109.3	109.4
A(47-46-49)	109.2	109.4	A(48-46-49)	109.3	109.4
A(48-46-49)	109.2	109.4			

Table S15. Calculated optimized geometries of Dihedral angles (°) for 2c A and 2c B (C₂₄H₁₈N₂O₅)

2c A			2c B		
Dihedral Angles	HF	B3LYP	Dihedral Angles	HF	B3LYP
D(3-1-2-4)	0.0	-0.1	D(3-1-2-4)	0.1	0.1
D(3-1-2-12)	180.0	179.9	D(3-1-2-12)	180.0	179.9
D(11-1-2-4)	-179.9	-179.9	D(11-1-2-4)	-179.8	-179.8
D(11-1-2-12)	0.0	0.0	D(11-1-2-12)	0.0	0.0
D(2-1-3-5)	0.1	0.1	D(2-1-3-5)	0.1	0.1
D(2-1-3-7)	-179.8	-179.8	D(2-1-3-7)	-179.8	-179.8
D(11-1-3-5)	-180.0	180.0	D(11-1-3-5)	-180.0	180.0
D(11-1-3-7)	0.1	0.1	D(11-1-3-7)	0.1	0.1
D(1-2-4-6)	0.0	0.0	D(1-2-4-6)	-0.1	-0.1
D(1-2-4-13)	179.9	180.0	D(1-2-4-13)	179.6	179.6
D(12-2-4-6)	-179.9	-180.0	D(12-2-4-6)	-179.9	-179.9
D(12-2-4-13)	0.0	0.0	D(12-2-4-13)	-0.2	-0.2
D(1-3-5-6)	-0.2	-0.1	D(1-3-5-6)	-0.4	-0.3
D(1-3-5-10)	-179.9	-179.8	D(1-3-5-10)	179.8	179.8
D(7-3-5-6)	179.7	179.8	D(7-3-5-6)	179.6	179.6
D(7-3-5-10)	0.0	0.1	D(7-3-5-10)	-0.3	-0.3
D(1-3-7-8)	179.8	179.8	D(1-3-7-8)	179.9	179.9
D(1-3-7-14)	-0.1	-0.2	D(1-3-7-14)	0.0	0.0
D(5-3-7-8)	-0.1	-0.1	D(5-3-7-8)	0.0	0.0
D(5-3-7-14)	-180.0	180.0	D(5-3-7-14)	-179.9	-179.9
D(2-4-6-5)	-0.1	0.0	D(2-4-6-5)	-0.1	-0.1
D(2-4-6-21)	179.7	179.8	D(2-4-6-21)	179.4	179.4
D(13-4-6-5)	180.0	-180.0	D(13-4-6-5)	-179.9	-179.8
D(13-4-6-21)	-0.2	-0.1	D(13-4-6-21)	-0.3	-0.3
D(3-5-6-4)	0.2	0.1	D(3-5-6-4)	0.4	0.3
D(3-5-6-21)	-179.7	-179.8	D(3-5-6-21)	-179.1	-179.2
D(10-5-6-4)	179.9	179.8	D(10-5-6-4)	-179.8	-179.8
D(10-5-6-21)	0.1	-0.1	D(10-5-6-21)	0.7	0.7
D(3-5-10-9)	0.1	0.0	D(3-5-10-9)	0.5	0.4
D(3-5-10-16)	-179.4	-179.7	D(3-5-10-16)	-179.0	-179.2
D(6-5-10-9)	-179.6	-179.7	D(6-5-10-9)	-179.4	-179.5
D(6-5-10-16)	0.8	0.6	D(6-5-10-16)	1.2	0.9
D(4-6-21-19)	179.7	-180.0	D(4-6-21-19)	179.4	179.5
D(4-6-21-23)	-3.4	-3.0	D(5-6-21-19)	-1.1	-1.1
D(5-6-21-19)	-0.5	-0.1	D(3-7-8-9)	0.2	0.2
D(5-6-21-23)	176.4	176.9	D(3-7-8-15)	-179.8	-179.8
D(3-7-8-9)	0.1	0.0	D(14-7-8-9)	-179.9	-179.9
D(3-7-8-15)	-179.9	-179.9	D(14-7-8-15)	0.1	0.1
D(14-7-8-9)	-180.0	180.0	D(7-8-9-10)	-0.1	0.0
D(14-7-8-15)	0.0	0.1	D(7-8-9-24)	-180.0	-179.9
D(7-8-9-10)	-0.1	0.0	D(15-8-9-10)	179.9	179.9
D(7-8-9-24)	-179.9	-179.7	D(15-8-9-24)	0.0	0.1

D(15-8-9-10)	179.9	179.9	D(8-9-10-5)	-0.3	-0.3
D(15-8-9-24)	0.1	0.2	D(8-9-10-16)	179.1	179.3
D(8-9-10-5)	-0.1	0.0	D(24-9-10-5)	179.6	179.6
D(8-9-10-16)	179.5	179.7	D(24-9-10-16)	-1.0	-0.8
D(24-9-10-5)	179.8	179.7	D(5-10-16-17)	179.2	179.3
D(24-9-10-16)	-0.7	-0.6	D(5-10-16-19)	-2.7	-2.2
D(5-10-16-17)	-176.8	-176.4	D(9-10-16-17)	-0.2	-0.3
D(5-10-16-19)	-1.4	-0.8	D(9-10-16-19)	177.9	178.2
D(9-10-16-17)	3.6	3.9	D(10-16-17-18)	0.8	0.9
D(9-10-16-19)	179.0	179.5	D(10-16-17-20)	-176.4	-176.4
D(10-16-17-18)	-3.5	-3.0	D(19-16-17-18)	-177.4	-177.7
D(10-16-17-20)	178.1	178.3	D(19-16-17-20)	5.3	5.0
D(19-16-17-18)	-179.4	-179.1	D(10-16-19-21)	2.6	2.0
D(19-16-17-20)	2.2	2.3	D(10-16-19-22)	-175.7	-175.8
D(10-16-19-21)	1.1	0.6	D(17-16-19-21)	-179.1	-179.3
D(10-16-19-22)	-179.7	-179.5	D(17-16-19-22)	2.7	2.9
D(17-16-19-21)	177.2	177.0	D(16-17-20-22)	-10.8	-10.5
D(17-16-19-22)	-3.5	-3.2	D(16-17-20-37)	-138.7	-138.6
D(16-17-20-22)	-0.3	-0.8	D(16-17-20-42)	105.2	105.3
D(16-17-20-37)	-127.1	-127.9	D(18-17-20-22)	171.9	172.1
D(16-17-20-42)	118.1	117.4	D(18-17-20-37)	44.1	44.1
D(18-17-20-22)	-178.7	-179.4	D(18-17-20-42)	-72.1	-72.1
D(18-17-20-37)	54.5	53.5	D(16-19-21-6)	-0.5	-0.3
D(18-17-20-42)	-60.3	-61.2	D(22-19-21-6)	177.5	177.2
D(16-19-21-6)	-0.1	-0.1	D(16-19-22-20)	-9.3	-9.3
D(16-19-21-23)	-177.2	-177.4	D(16-19-22-23)	107.0	106.7
D(22-19-21-6)	-179.2	-180.0	D(16-19-22-25)	-136.3	-136.6
D(22-19-21-23)	3.7	2.7	D(21-19-22-20)	172.4	172.9
D(16-19-22-20)	3.2	2.6	D(21-19-22-23)	-71.3	-71.1
D(16-19-22-25)	-179.5	179.9	D(21-19-22-25)	45.4	45.6
D(21-19-22-20)	-177.6	-177.5	D(17-20-22-19)	11.8	11.7
D(21-19-22-25)	-0.3	-0.2	D(17-20-22-23)	-101.6	-102.0
D(17-20-22-19)	-1.7	-1.0	D(17-20-22-25)	140.9	141.1
D(17-20-22-25)	-178.6	-177.9	D(37-20-22-19)	137.3	137.4
D(37-20-22-19)	120.7	121.8	D(37-20-22-23)	23.9	23.8
D(37-20-22-25)	-56.2	-55.1	D(37-20-22-25)	-93.6	-93.2
D(42-20-22-19)	-114.2	-113.8	D(42-20-22-19)	-100.6	-101.0
D(42-20-22-25)	68.9	69.3	D(42-20-22-23)	146.0	145.4
D(17-20-37-38)	59.0	60.9	D(42-20-22-25)	28.5	28.5
D(17-20-37-43)	-60.3	-58.4	D(17-20-37-38)	57.7	59.2
D(17-20-37-44)	-177.8	-175.6	D(17-20-37-43)	-62.8	-61.3
D(22-20-37-38)	-59.0	-58.0	D(17-20-37-44)	179.5	-178.4
D(22-20-37-43)	-178.4	-177.4	D(22-20-37-38)	-63.5	-62.4
D(22-20-37-44)	64.2	65.5	D(22-20-37-43)	176.0	177.1
D(42-20-37-38)	172.7	174.6	D(22-20-37-44)	58.3	60.0
D(42-20-37-43)	53.4	55.3	D(42-20-37-38)	172.7	174.4

D(42-20-37-44)	-64.1	-61.9	D(42-20-37-43)	52.2	54.0
D(19-22-25-26)	173.1	175.9	D(42-20-37-44)	-65.4	-63.2
D(19-22-25-36)	-7.6	-5.0	D(19-22-25-26)	51.0	50.9
D(20-22-25-26)	-10.4	-7.5	D(19-22-25-36)	-132.7	-132.5
D(20-22-25-36)	168.9	171.6	D(20-22-25-26)	-70.9	-71.4
D(22-25-26-27)	-42.2	-36.4	D(20-22-25-36)	105.3	105.1
D(22-25-26-28)	141.3	147.3	D(23-22-25-26)	168.4	-0.3
D(36-25-26-27)	138.5	144.4	D(23-22-25-36)	-15.3	179.0
D(36-25-26-28)	-38.0	-31.9	D(22-25-26-27)	-0.9	11.4
D(25-26-27-29)	0.6	0.4	D(22-25-26-28)	178.4	-169.3
D(25-26-27-31)	-177.3	-177.1	D(36-25-26-27)	-177.1	-176.7
D(28-26-27-29)	177.1	176.7	D(36-25-26-28)	2.3	2.6
D(28-26-27-31)	-0.8	-0.8	D(25-26-27-29)	-1.2	-1.4
D(25-26-28-30)	-1.3	-1.4	D(25-26-27-31)	179.1	179.0
D(25-26-28-32)	178.7	178.4	D(28-26-27-29)	179.4	179.3
D(27-26-28-30)	-177.9	-177.9	D(28-26-27-31)	-0.3	-0.3
D(27-26-28-32)	2.1	1.9	D(25-26-28-30)	0.7	0.8
D(26-27-31-33)	178.8	178.7	D(25-26-28-32)	-179.4	-179.4
D(26-27-31-35)	-0.7	-0.7	D(27-26-28-30)	-179.8	-179.9
D(29-27-31-33)	0.9	1.1	D(27-26-28-32)	0.0	0.0
D(29-27-31-35)	-178.7	-178.3	D(26-27-31-33)	179.9	180.0
D(26-28-32-34)	179.0	179.0	D(26-27-31-35)	0.4	0.4
D(26-28-32-35)	-1.7	-1.5	D(29-27-31-33)	0.2	0.4
D(30-28-32-34)	-1.0	-1.2	D(29-27-31-35)	-179.3	-179.2
D(30-28-32-35)	178.3	178.3	D(26-28-32-34)	-179.7	-179.7
D(27-31-35-32)	1.1	1.1	D(26-28-32-35)	0.2	0.3
D(27-31-35-45)	-179.2	-179.2	D(30-28-32-34)	0.1	0.1
D(33-31-35-32)	-178.4	-178.3	D(30-28-32-35)	-180.0	-179.9
D(33-31-35-45)	1.2	1.4	D(27-31-35-32)	-0.2	-0.2
D(28-32-35-31)	0.1	-0.1	D(27-31-35-45)	179.8	179.8
D(28-32-35-45)	-179.6	-179.6	D(33-31-35-32)	-179.7	-179.8
D(34-32-35-31)	179.4	179.4	D(33-31-35-45)	0.2	0.2
D(34-32-35-45)	-0.2	-0.2	D(28-32-35-31)	-0.1	-0.1
D(31-35-46-48)	-123.4	-123.5	D(28-32-35-45)	179.9	179.9
D(31-35-46-49)	1.3	1.4	D(34-32-35-31)	179.8	179.9
D(32-35-46-48)	55.5	55.5	D(34-32-35-45)	-0.1	-0.1
D(32-35-46-49)	-179.8	-179.7	D(31-35-45-46)	-179.3	-179.4
D(20-37-38-39)	-15.8	-16.1	D(32-35-45-46)	0.7	0.5
D(20-37-38-40)	165.8	165.3	D(20-37-38-39)	-0.2	-1.8
D(43-37-38-39)	105.2	104.5	D(20-37-38-40)	179.9	178.5
D(43-37-38-40)	-73.2	-74.1	D(43-37-38-39)	121.7	120.0
D(44-37-38-39)	-140.0	-140.5	D(43-37-38-40)	-58.2	-59.7
D(44-37-38-40)	41.6	40.9	D(44-37-38-39)	-123.3	-125.3
D(37-38-40-41)	177.5	177.7	D(44-37-38-40)	56.8	54.9
D(39-38-40-41)	-1.0	-1.0	D(37-38-40-41)	179.5	179.4
			D(39-38-40-41)	-0.4	-0.3

D(35-45-46-47)	-61.6	-61.7
D(35-45-46-48)	60.9	61.0
D(35-45-46-49)	179.7	179.6

Table S16. Calculated optimized geometries of bond lengths (Å) for 2d A and 2d B (C₂₅H₂₀N₂O₆)

2d A			2d B		
Bond Lengths	HF	B3LYP	Bond Lengths	HF	B3LYP
R(1-2)	1.358	1.375	R(1-2)	1.360	1.376
R(1-3)	1.420	1.420	R(1-3)	1.419	1.420
R(1-11)	1.075	1.084	R(1-11)	1.075	1.084
R(2-4)	1.412	1.410	R(2-4)	1.412	1.409
R(2-12)	1.075	1.084	R(2-12)	1.076	1.084
R(3-5)	1.404	1.425	R(3-5)	1.404	1.425
R(3-7)	1.418	1.419	R(3-7)	1.419	1.419
R(4-6)	1.361	1.380	R(4-6)	1.362	1.382
R(4-13)	1.075	1.084	R(4-13)	1.074	1.083
R(5-6)	1.418	1.423	R(5-6)	1.422	1.426
R(5-10)	1.424	1.426	R(5-10)	1.422	1.423
R(6-21)	1.393	1.396	R(6-21)	1.403	1.404
R(7-8)	1.356	1.374	R(7-8)	1.357	1.374
R(7-14)	1.075	1.084	R(7-14)	1.075	1.084
R(8-9)	1.415	1.412	R(8-9)	1.415	1.412
R(8-15)	1.075	1.084	R(8-15)	1.075	1.084
R(9-10)	1.361	1.380	R(9-10)	1.361	1.381
R(9-24)	1.068	1.079	R(9-24)	1.068	1.078
R(10-16)	1.416	1.418	R(10-16)	1.417	1.421
R(16-17)	1.391	1.405	R(16-17)	1.383	1.401
R(16-19)	1.380	1.393	R(16-19)	1.386	1.399
R(17-18)	1.183	1.208	R(17-18)	1.184	1.208
R(17-20)	1.523	1.535	R(17-20)	1.515	1.522
R(19-21)	1.331	1.342	R(19-21)	1.252	1.275
R(19-22)	1.370	1.384	R(19-22)	1.515	1.519
R(20-22)	1.513	1.516	R(20-22)	1.534	1.538
R(20-36)	1.535	1.539	R(20-36)	1.524	1.528
R(20-41)	1.085	1.096	R(20-41)	1.085	1.097
R(21-23)	0.999	1.025	R(22-23)	1.080	1.091
R(22-25)	1.439	1.437	R(22-25)	1.538	1.550
R(25-26)	1.503	1.499	R(25-26)	1.494	1.485
R(25-35)	1.216	1.252	R(25-35)	1.190	1.218
R(26-27)	1.379	1.395	R(26-27)	1.384	1.400
R(26-28)	1.395	1.403	R(26-28)	1.396	1.404
R(27-29)	1.073	1.082	R(27-29)	1.073	1.082
R(27-31)	1.390	1.394	R(27-31)	1.385	1.387
R(28-30)	1.071	1.081	R(28-30)	1.069	1.079
R(28-32)	1.380	1.391	R(28-32)	1.381	1.392
R(31-33)	1.075	1.084	R(31-33)	1.075	1.083
R(31-34)	1.376	1.390	R(31-34)	1.379	1.395
R(32-34)	1.403	1.414	R(32-34)	1.401	1.414
R(32-49)	1.344	1.363	R(32-49)	1.346	1.364

R(34-44)	1.353	1.368	R(34-44)	1.350	1.363
R(36-37)	1.506	1.511	R(36-37)	1.507	1.512
R(36-42)	1.087	1.096	R(36-42)	1.084	1.094
R(36-43)	1.082	1.091	R(36-43)	1.086	1.094
R(37-38)	1.184	1.206	R(37-38)	1.185	1.207
R(37-39)	1.326	1.354	R(37-39)	1.323	1.351
R(39-40)	0.946	0.969	R(39-40)	0.947	0.969
R(44-45)	1.410	1.435	R(44-45)	1.411	1.437
R(45-46)	1.083	1.091	R(45-46)	1.082	1.090
R(45-47)	1.087	1.095	R(45-47)	1.086	1.095
R(45-48)	1.081	1.089	R(45-48)	1.081	1.089
R(49-50)	1.401	1.424	R(49-50)	1.402	1.425
R(50-51)	1.086	1.095	R(50-51)	1.086	1.095
R(50-52)	1.080	1.089	R(50-52)	1.080	1.089
R(50-53)	1.086	1.095	R(50-53)	1.086	1.094

Table S17. Calculated optimized geometries of bond angles (°) for 2d A and 2d B (C₂₅H₂₀N₂O₆)

2d A			2d B		
Bond Angles	HF	B3LYP	Bond Angles	HF	B3LYP
A(2-1-3)	120.3	120.5	A(2-1-3)	120.4	120.7
A(2-1-11)	120.7	120.6	A(2-1-11)	120.6	120.5
A(1-2-4)	121.1	121.1	A(1-2-4)	121.0	121.0
A(1-2-12)	120.1	120.0	A(1-2-12)	119.9	119.8
A(3-1-11)	119.0	118.9	A(3-1-11)	119.0	118.8
A(1-3-5)	119.0	118.7	A(1-3-5)	118.6	118.3
A(1-3-7)	122.4	122.8	A(1-3-7)	122.8	123.1
A(4-2-12)	118.8	118.9	A(4-2-12)	119.1	119.2
A(2-4-6)	119.5	119.6	A(2-4-6)	120.0	120.2
A(2-4-13)	120.3	120.5	A(2-4-13)	120.8	121.1
A(5-3-7)	118.6	118.4	A(5-3-7)	118.7	118.5
A(3-5-6)	119.2	119.2	A(3-5-6)	120.0	120.0
A(3-5-10)	120.0	119.7	A(3-5-10)	119.7	119.4
A(3-7-8)	120.0	120.4	A(3-7-8)	120.1	120.4
A(3-7-14)	119.2	119.0	A(3-7-14)	119.2	119.0
A(6-4-13)	120.3	119.9	A(6-4-13)	119.2	118.8
A(4-6-5)	120.9	120.9	A(4-6-5)	120.1	119.9
A(4-6-21)	121.4	121.5	A(4-6-21)	119.7	119.6
A(6-5-10)	120.8	121.1	A(6-5-10)	120.4	120.6
A(5-6-21)	117.7	117.6	A(5-6-21)	120.2	120.5
A(5-10-9)	120.3	120.5	A(5-10-9)	120.8	121.0
A(5-10-16)	116.1	116.4	A(5-10-16)	114.8	115.1
A(6-21-19)	123.6	123.3	A(6-21-19)	118.1	117.9
A(6-21-23)	121.4	124.0	A(8-7-14)	120.7	120.6
A(8-7-14)	120.8	120.6	A(7-8-9)	121.8	121.7
A(7-8-9)	121.9	121.7	A(7-8-15)	120.0	119.9
A(7-8-15)	120.0	119.9	A(9-8-15)	118.2	118.4
A(9-8-15)	118.2	118.4	A(8-9-10)	118.9	118.9
A(8-9-10)	119.2	119.2	A(8-9-24)	120.1	120.7
A(8-9-24)	120.0	120.7	A(10-9-24)	121.0	120.3
A(10-9-24)	120.8	120.1	A(9-10-16)	124.4	123.9
A(9-10-16)	123.6	123.1	A(10-16-17)	127.6	127.7
A(10-16-17)	127.7	128.4	A(10-16-19)	120.1	120.1
A(10-16-19)	122.8	122.2	A(17-16-19)	112.3	112.2
A(17-16-19)	109.4	109.3	A(16-17-18)	126.2	125.9
A(16-17-18)	125.9	125.9	A(16-17-20)	108.1	107.7
A(16-17-20)	108.0	107.4	A(16-19-21)	126.3	125.8
A(16-19-21)	119.0	119.4	A(16-19-22)	109.2	109.3
A(16-19-22)	112.6	112.9	A(18-17-20)	125.7	126.3
A(18-17-20)	126.1	126.6	A(17-20-22)	104.8	105.4
A(17-20-22)	102.7	103.5	A(17-20-36)	112.9	112.9
A(17-20-36)	111.0	110.9	A(17-20-41)	105.0	105.4

A(17-20-41)	105.1	105.0	A(21-19-22)	124.5	124.9
A(21-19-22)	128.3	127.8	A(19-22-20)	103.3	103.7
A(19-21-23)	114.9	112.7	A(19-22-23)	106.9	107.1
A(19-22-20)	107.3	106.8	A(19-22-25)	112.3	112.4
A(19-22-25)	121.2	120.3	A(22-20-36)	117.6	117.8
A(22-20-36)	117.9	117.8	A(22-20-41)	108.1	107.2
A(22-20-41)	113.0	112.4	A(20-22-23)	110.5	110.7
A(20-22-25)	131.5	132.8	A(20-22-25)	113.2	112.5
A(36-20-41)	106.5	106.5	A(36-20-41)	107.7	107.5
A(20-36-37)	114.4	114.1	A(20-36-37)	114.3	114.4
A(20-36-42)	109.4	109.1	A(20-36-42)	109.8	109.5
A(20-36-43)	110.6	110.8	A(20-36-43)	110.6	110.8
A(21-23-35)	127.6	131.4	A(23-22-25)	110.4	110.0
A(22-25-26)	120.4	121.7	A(22-25-26)	119.7	119.5
A(22-25-35)	121.6	120.6	A(22-25-35)	119.0	118.8
A(26-25-35)	118.0	117.7	A(26-25-35)	121.2	121.7
A(25-26-27)	122.7	123.7	A(25-26-27)	117.9	118.2
A(25-26-28)	117.5	117.1	A(25-26-28)	122.4	122.6
A(25-35-23)	105.8	106.9	A(27-26-28)	119.7	119.3
A(27-26-28)	119.7	119.1	A(26-27-29)	119.7	119.1
A(26-27-29)	120.9	120.8	A(26-27-31)	119.7	120.0
A(26-27-31)	119.6	119.9	A(26-28-30)	119.8	119.7
A(26-28-30)	118.3	117.7	A(26-28-32)	120.7	120.9
A(26-28-32)	120.8	121.2	A(29-27-31)	120.6	121.0
A(29-27-31)	119.4	119.2	A(27-31-33)	120.9	121.2
A(27-31-33)	120.8	121.0	A(27-31-34)	120.9	121.2
A(27-31-34)	121.0	121.2	A(30-28-32)	119.4	119.3
A(30-28-32)	121.0	121.2	A(28-32-34)	119.3	119.4
A(28-32-34)	119.3	119.3	A(28-32-49)	124.4	124.1
A(28-32-49)	124.5	124.3	A(33-31-34)	118.2	117.6
A(33-31-34)	118.2	117.8	A(31-34-32)	119.8	119.3
A(31-34-32)	119.6	119.2	A(31-34-44)	119.3	117.6
A(31-34-44)	119.5	118.5	A(34-32-49)	116.3	116.5
A(34-32-49)	116.2	116.4	A(32-34-44)	120.8	123.0
A(32-34-44)	120.8	122.2	A(32-49-50)	119.9	118.6
A(32-49-50)	119.8	118.4	A(34-44-45)	116.7	118.5
A(34-44-45)	116.6	117.1	A(37-36-42)	107.4	107.4
A(37-36-42)	106.5	106.9	A(37-36-43)	107.9	108.3
A(37-36-43)	108.8	109.1	A(36-37-38)	125.4	126.0
A(36-37-38)	125.7	126.1	A(36-37-39)	111.8	111.4
A(36-37-39)	111.8	111.3	A(42-36-43)	106.5	106.0
A(42-36-43)	106.8	106.6	A(38-37-39)	122.8	122.6
A(38-37-39)	122.5	122.6	A(37-39-40)	109.1	107.5
A(37-39-40)	108.8	107.2	A(44-45-46)	111.1	111.5
A(44-45-46)	111.1	111.4	A(44-45-47)	110.4	110.2
A(44-45-47)	110.5	110.3	A(44-45-48)	106.4	105.5

A(44-45-48)	106.5	105.8	A(46-45-47)	109.8	110.0
A(46-45-47)	109.8	110.0	A(46-45-48)	109.6	110.2
A(46-45-48)	109.5	109.9	A(47-45-48)	109.4	109.4
A(47-45-48)	109.4	109.4	A(49-50-51)	111.2	111.2
A(49-50-51)	111.2	111.2	A(49-50-52)	106.1	105.7
A(49-50-52)	106.1	105.7	A(49-50-53)	111.5	111.5
A(49-50-53)	111.4	111.4	A(51-50-52)	109.2	109.4
A(51-50-52)	109.2	109.4	A(51-50-53)	109.5	109.6
A(51-50-53)	109.5	109.5	A(52-50-53)	109.3	109.5
A(52-50-53)	109.3	109.5			

Table S18. Calculated optimized geometries of Dihedral angles (°) for 2d A and 2d B (C₂₅H₂₀N₂O₆)

2d A			2d B		
Dihedral Angles	HF	B3LYP	Dihedral Angles	HF	B3LYP
D(3-1-2-4)	0.0	0.0	D(3-1-2-4)	0.3	0.1
D(3-1-2-12)	180.0	179.9	D(3-1-2-12)	-179.8	-179.8
D(11-1-2-4)	-179.9	-179.9	D(11-1-2-4)	-179.8	-179.9
D(11-1-2-12)	0.0	0.0	D(11-1-2-12)	0.1	0.1
D(2-1-3-5)	0.1	0.1	D(2-1-3-5)	0.0	0.0
D(2-1-3-7)	-179.8	-179.8	D(2-1-3-7)	180.0	179.9
D(11-1-3-5)	-180.0	180.0	D(11-1-3-5)	-179.9	-179.9
D(11-1-3-7)	0.1	0.1	D(11-1-3-7)	0.0	0.0
D(1-2-4-6)	0.0	0.0	D(1-2-4-6)	-0.2	-0.1
D(1-2-4-13)	179.9	180.0	D(1-2-4-13)	180.0	-179.7
D(12-2-4-6)	-180.0	-180.0	D(12-2-4-6)	179.9	179.9
D(12-2-4-13)	0.0	0.0	D(12-2-4-13)	0.0	0.2
D(1-3-5-6)	-0.2	-0.1	D(1-3-5-6)	-0.4	-0.2
D(1-3-5-10)	-179.9	-179.8	D(1-3-5-10)	179.5	179.7
D(7-3-5-6)	179.7	179.8	D(7-3-5-6)	179.6	179.9
D(7-3-5-10)	-0.1	0.1	D(7-3-5-10)	-0.4	-0.2
D(1-3-7-8)	179.8	179.8	D(1-3-7-8)	-179.9	-179.9
D(1-3-7-14)	-0.1	-0.2	D(1-3-7-14)	0.1	0.1
D(5-3-7-8)	-0.1	-0.1	D(5-3-7-8)	0.0	0.0
D(5-3-7-14)	-180.0	180.0	D(5-3-7-14)	-180.0	180.0
D(2-4-6-5)	-0.1	-0.1	D(2-4-6-5)	-0.2	-0.1
D(2-4-6-21)	179.7	179.8	D(2-4-6-21)	179.3	179.7
D(13-4-6-5)	180.0	-180.0	D(13-4-6-5)	179.6	179.5
D(13-4-6-21)	-0.2	-0.1	D(13-4-6-21)	-0.8	-0.6
D(3-5-6-4)	0.2	0.1	D(3-5-6-4)	0.6	0.3
D(3-5-6-21)	-179.7	-179.8	D(3-5-6-21)	-179.0	-179.6
D(10-5-6-4)	180.0	179.8	D(10-5-6-4)	-179.4	-179.6
D(10-5-6-21)	0.1	-0.1	D(10-5-6-21)	1.1	0.5
D(3-5-10-9)	0.1	0.0	D(3-5-10-9)	0.6	0.4
D(3-5-10-16)	-179.4	-179.8	D(3-5-10-16)	-178.9	-179.1
D(6-5-10-9)	-179.6	-179.7	D(6-5-10-9)	-179.5	-179.7
D(6-5-10-16)	0.8	0.5	D(6-5-10-16)	1.1	0.8
D(4-6-21-19)	179.7	-179.8	D(4-6-21-19)	178.9	179.1
D(4-6-21-23)	-3.1	-3.1	D(5-6-21-19)	-1.6	-1.0
D(5-6-21-19)	-0.4	0.0	D(3-7-8-9)	0.2	0.1
D(5-6-21-23)	176.8	176.8	D(3-7-8-15)	-179.9	-179.9
D(3-7-8-9)	0.1	0.0	D(14-7-8-9)	-179.8	-179.9
D(3-7-8-15)	-179.9	-179.9	D(14-7-8-15)	0.1	0.1
D(14-7-8-9)	-180.0	180.0	D(7-8-9-10)	0.0	0.0
D(14-7-8-15)	0.0	0.0	D(7-8-9-24)	179.9	-179.9
D(7-8-9-10)	-0.1	0.0	D(15-8-9-10)	-180.0	-180.0
D(7-8-9-24)	-179.9	-179.7	D(15-8-9-24)	0.0	0.2

D(15-8-9-10)	179.9	179.9	D(8-9-10-5)	-0.3	-0.3
D(15-8-9-24)	0.1	0.2	D(8-9-10-16)	179.1	179.2
D(8-9-10-5)	-0.1	0.0	D(24-9-10-5)	179.7	179.6
D(8-9-10-16)	179.5	179.7	D(24-9-10-16)	-0.9	-0.9
D(24-9-10-5)	179.8	179.7	D(5-10-16-17)	177.7	-179.9
D(24-9-10-16)	-0.7	-0.5	D(5-10-16-19)	-2.7	-1.5
D(5-10-16-17)	-177.0	-176.4	D(9-10-16-17)	-1.7	0.6
D(5-10-16-19)	-1.5	-1.0	D(9-10-16-19)	177.9	179.0
D(9-10-16-17)	3.4	3.9	D(10-16-17-18)	4.1	3.7
D(9-10-16-19)	178.9	179.3	D(10-16-17-20)	-173.4	-174.1
D(10-16-17-18)	-3.5	-3.2	D(19-16-17-18)	-175.6	-174.8
D(10-16-17-20)	178.1	178.1	D(19-16-17-20)	6.9	7.4
D(19-16-17-18)	-179.5	-179.1	D(10-16-19-21)	2.4	1.1
D(19-16-17-20)	2.1	2.2	D(10-16-19-22)	-176.4	-177.8
D(10-16-19-21)	1.3	0.9	D(17-16-19-21)	-177.9	179.7
D(10-16-19-22)	-179.6	-179.2	D(17-16-19-22)	3.3	0.9
D(17-16-19-21)	177.5	177.1	D(16-17-20-22)	-13.9	-12.3
D(17-16-19-22)	-3.3	-3.0	D(16-17-20-36)	-143.1	-142.2
D(16-17-20-22)	-0.3	-0.7	D(16-17-20-41)	99.8	100.8
D(16-17-20-36)	-127.2	-127.9	D(18-17-20-22)	168.6	169.9
D(16-17-20-41)	118.0	117.4	D(18-17-20-36)	39.4	40.1
D(18-17-20-22)	-178.7	-179.4	D(18-17-20-41)	-77.7	-77.0
D(18-17-20-36)	54.4	53.4	D(16-19-21-6)	-0.2	0.2
D(18-17-20-41)	-60.4	-61.4	D(22-19-21-6)	178.5	178.9
D(16-19-21-6)	-0.3	-0.4	D(16-19-22-20)	-11.7	-8.5
D(16-19-21-23)	-177.6	-177.5	D(16-19-22-23)	104.8	108.7
D(22-19-21-6)	-179.3	179.8	D(16-19-22-25)	-134.0	-130.3
D(22-19-21-23)	3.4	2.7	D(21-19-22-20)	169.5	172.6
D(16-19-22-20)	3.1	2.5	D(21-19-22-23)	-74.0	-70.2
D(16-19-22-25)	-179.2	179.9	D(21-19-22-25)	47.2	50.8
D(21-19-22-20)	-177.9	-177.7	D(17-20-22-19)	15.0	12.3
D(21-19-22-25)	-0.1	-0.3	D(17-20-22-23)	-99.0	-102.4
D(17-20-22-19)	-1.6	-1.0	D(17-20-22-25)	136.7	134.1
D(17-20-22-25)	-179.0	-178.0	D(36-20-22-19)	141.3	139.2
D(36-20-22-19)	120.8	121.8	D(36-20-22-23)	27.3	24.5
D(36-20-22-25)	-56.6	-55.2	D(36-20-22-25)	-97.0	-99.1
D(41-20-22-19)	-114.2	-113.8	D(41-20-22-19)	-96.6	-99.6
D(41-20-22-25)	68.4	69.2	D(41-20-22-23)	149.4	145.7
D(17-20-36-37)	58.8	60.4	D(41-20-22-25)	25.1	22.2
D(17-20-36-42)	-60.6	-59.1	D(17-20-36-37)	59.9	63.0
D(17-20-36-43)	-178.0	-176.1	D(17-20-36-42)	-60.8	-57.7
D(22-20-36-37)	-59.2	-58.6	D(17-20-36-43)	-178.0	-174.2
D(22-20-36-42)	-178.6	-178.0	D(22-20-36-37)	-62.3	-60.2
D(22-20-36-43)	64.0	64.9	D(22-20-36-42)	177.0	179.1
D(41-20-36-37)	172.7	174.2	D(22-20-36-43)	59.8	62.6
D(41-20-36-42)	53.3	54.7	D(41-20-36-37)	175.4	178.8

D(41-20-36-43)	-64.1	-62.4	D(41-20-36-42)	54.7	58.1
D(19-22-25-26)	173.3	176.2	D(41-20-36-43)	-62.6	-58.5
D(19-22-25-35)	-7.3	-4.8	D(19-22-25-26)	-94.0	-90.8
D(20-22-25-26)	-9.6	-7.2	D(19-22-25-35)	88.8	91.6
D(20-22-25-35)	169.8	171.8	D(20-22-25-26)	149.5	152.5
D(22-25-26-27)	-45.0	-36.4	D(20-22-25-35)	-27.7	-25.1
D(22-25-26-28)	138.1	146.9	D(22-25-26-27)	-163.2	-167.6
D(35-25-26-27)	135.5	144.6	D(22-25-26-28)	16.4	11.7
D(35-25-26-28)	-41.4	-32.1	D(23-25-26-27)	-151.7	-154.6
D(25-26-27-29)	0.9	0.4	D(23-25-26-28)	27.9	24.7
D(25-26-27-31)	-177.1	-176.7	D(35-25-26-27)	14.0	9.9
D(28-26-27-29)	177.7	177.0	D(35-25-26-28)	-166.4	-170.7
D(28-26-27-31)	-0.3	-0.1	D(25-26-27-29)	-0.6	-0.7
D(25-26-28-30)	-1.2	-1.5	D(25-26-27-31)	179.1	179.4
D(25-26-28-32)	178.6	178.5	D(28-26-27-29)	179.8	179.9
D(27-26-28-30)	-178.2	-178.3	D(28-26-27-31)	-0.5	0.1
D(27-26-28-32)	1.6	1.7	D(25-26-28-30)	2.9	3.1
D(26-27-31-33)	179.7	179.0	D(25-26-28-32)	-179.6	-179.4
D(26-27-31-34)	-0.9	-1.0	D(27-26-28-30)	-177.6	-177.6
D(29-27-31-33)	1.7	1.9	D(27-26-28-32)	-0.1	0.0
D(29-27-31-34)	-178.9	-178.2	D(26-27-31-33)	-178.8	-179.5
D(26-28-32-34)	-1.8	-2.2	D(26-27-31-34)	0.7	0.4
D(26-28-32-49)	178.6	177.4	D(29-27-31-33)	1.0	0.6
D(30-28-32-34)	178.1	177.8	D(29-27-31-34)	-179.6	-179.4
D(30-28-32-49)	-1.6	-2.7	D(26-28-32-34)	0.4	-0.5
D(27-31-34-32)	0.7	0.5	D(26-28-32-49)	-179.5	178.6
D(27-31-34-44)	-176.8	-175.9	D(30-28-32-34)	177.9	177.1
D(33-31-34-32)	-179.8	-179.5	D(30-28-32-49)	-1.9	-3.9
D(33-31-34-44)	2.7	4.1	D(27-31-34-32)	-0.4	-0.9
D(28-32-34-31)	0.6	1.1	D(27-31-34-44)	-177.7	-177.1
D(28-32-34-44)	178.1	177.3	D(33-31-34-32)	179.1	179.1
D(49-32-34-31)	-179.8	-178.5	D(33-31-34-44)	1.7	2.9
D(49-32-34-44)	-2.2	-2.3	D(28-32-34-31)	-0.2	0.9
D(28-32-49-50)	-2.9	-1.1	D(28-32-34-44)	177.2	176.9
D(34-32-49-50)	177.5	178.5	D(49-32-34-31)	179.7	-178.2
D(31-34-44-45)	-105.4	-117.8	D(49-32-34-44)	-3.0	-2.2
D(32-34-44-45)	77.1	65.9	D(28-32-49-50)	-4.3	-1.7
D(20-36-37-38)	-15.0	-14.3	D(34-32-49-50)	175.8	177.4
D(20-36-37-39)	166.6	167.0	D(31-34-44-45)	-105.9	-125.0
D(42-36-37-38)	106.0	106.4	D(32-34-44-45)	76.8	58.9
D(42-36-37-39)	-72.4	-72.3	D(20-36-37-38)	3.8	2.3
D(43-36-37-38)	-139.2	-138.7	D(20-36-37-39)	-176.6	-177.9
D(43-36-37-39)	42.4	42.6	D(42-36-37-38)	125.9	124.2
D(36-37-39-40)	177.3	177.6	D(42-36-37-39)	-54.5	-56.0
D(38-37-39-40)	-1.2	-1.1	D(43-36-37-38)	-119.7	-121.7
D(34-44-45-46)	-61.2	-63.5	D(43-36-37-39)	59.9	58.0

D(34-44-45-47)	60.9	58.9	D(36-37-39-40)	179.3	179.3
D(34-44-45-48)	179.6	177.1	D(38-37-39-40)	-1.1	-0.9
D(32-49-50-51)	-59.7	-60.3	D(34-44-45-46)	-61.4	-69.5
D(32-49-50-52)	-178.4	-179.0	D(34-44-45-47)	60.8	53.0
D(32-49-50-53)	62.7	62.1	D(34-44-45-48)	179.4	170.9
			D(32-49-50-51)	-59.5	-60.7
			D(32-49-50-52)	-178.1	-179.2
			D(32-49-50-53)	63.0	61.9