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Molecular structure, FT-IR, NMR ($^{13}C/^{1}H$), UV–Vis spectroscopy and DFT calculations on (2Z, 5Z)-3-N(4-methoxy phenyl)-2-N'(4- methoxy phenyl imino)-5-((E)-3-(2-nitrophenyl)allylidene) thiazolidin-4-one

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Table S1: Atomic coordinates (xyz) of the optimized structure for MNTZ

Atoms	B3LYP			PBEPBE		
	x	*y*	*z*	*x*	*y*	*z*
S1	0.016787	0.671831	-0.088855	0.017602	0.672093	-0.098385
O1	-8.081380	-2.451031	0.874117	-8.160143	-2.403057	0.896011
O2	-5.959632	-2.525009	1.351256	-6.006085	-2.552478	1.300060
O3	0.461762	-3.172567	-0.227766	0.433301	-3.188622	-0.227557
O4	6.598275	-4.144933	-0.222611	6.575618	-4.222344	-0.189248
O5	2.920892	6.427342	-0.048464	3.033968	6.430556	-0.028586
N1	-6.941099	-1.988391	0.834102	-6.997036	-1.973577	0.820507
N2	1.797914	-1.280775	-0.124967	1.796443	-1.290473	-0.127952
N3	2.780203	0.847304	-0.144174	2.797654	0.840831	-0.165733
C1	-6.754504	-0.700361	0.142266	-6.792217	-0.678029	0.135771
C2	-7.900736	0.084170	0.005610	-7.937599	0.117211	-0.010767
C3	-7.815669	1.339350	-0.583432	-7.840288	1.385255	-0.584252
C4	-6.579684	1.791681	-1.052668	-6.589107	1.842666	-1.030211
C5	-5.449465	0.992310	-0.933899	-5.459616	1.034298	-0.905015
C6	-5.485430	-0.277517	-0.319724	-5.506962	-0.252360	-0.306945
C7	-4.268455	-1.091579	-0.259234	-4.297839	-1.070065	-0.245067
C8	-3.011472	-0.587814	-0.219777	-3.023630	-0.570428	-0.220316
C9	-1.841109	-1.422295	-0.214573	-1.863654	-1.409146	-0.215626
C10	-0.556904	-0.996422	-0.169030	-0.561501	-0.989769	-0.173982
C11	0.573017	-1.961046	-0.175815	0.556084	-1.966963	-0.177987
C12	1.745738	0.116989	-0.112907	1.749189	0.108970	-0.121089
C13	3.045723	-1.993545	-0.128200	3.038096	-2.011892	-0.123830
C14	3.326007	-2.897684	-1.158434	3.258129	-3.020273	-1.079990
C15	4.520272	-3.603176	-1.155992	4.450448	-3.740318	-1.068411
C16	5.455161	-3.408327	-0.128457	5.442861	-3.459606	-0.107499
C17	5.175245	-2.501252	0.900902	5.222715	-2.448486	0.847036
C18	3.967444	-1.803224	0.897783	4.018413	-1.733822	0.837161
C19	2.739662	2.251547	-0.084886	2.775998	2.240457	-0.092951
C20	2.100631	2.955334	0.944194	2.042072	2.962168	0.872201
C21	2.139181	4.351887	0.994121	2.103414	4.362000	0.930401
C22	2.823257	5.065364	0.005693	2.904309	5.066918	0.014224
C23	3.482417	4.366543	-1.018386	3.660511	4.352706	-0.939783
C24	3.452883	2.981782	-1.053743	3.609070	2.963364	-0.980578
C25	7.579217	-3.998109	0.793001	7.602972	-3.976767	0.768590
C26	2.276558	7.185041	0.962324	2.284581	7.187878	0.917430
H2	-8.839532	-0.306255	0.376720	-8.887733	-0.283332	0.346519
H3	-8.704132	1.954214	-0.680615	-8.732069	2.008679	-0.687482
H4	-6.499724	2.763501	-1.530080	-6.498075	2.827664	-1.497076
H5	-4.511037	1.334615	-1.355638	-4.506373	1.379164	-1.313840
H7	-4.390734	-2.167851	-0.234772	-4.425674	-2.153907	-0.201952
H8	-2.861073	0.488732	-0.164975	-2.865765	0.514815	-0.171534
H9	-1.972740	-2.501667	-0.252557	-1.996574	-2.497448	-0.248959
H14	2.603351	-3.054941	-1.950406	2.488960	-3.245520	-1.820404
H15	4.753604	-4.312173	-1.942761	4.639180	-4.529791	-1.799888
H17	5.879820	-2.331889	1.705726	5.974678	-2.211521	1.601912
H18	3.750916	-1.099960	1.693481	3.847731	-0.947953	1.575265
H20	1.590413	2.410315	1.731813	1.444170	2.422877	1.612281
H21	1.640647	4.862777	1.809061	1.532588	4.886763	1.699249
H23	4.019153	4.935397	-1.770378	4.289549	4.916228	-1.633846
H24	3.973485	2.439065	-1.835862	4.201892	2.405047	-1.709800
H25a	7.961880	-2.970724	0.840743	7.991935	-2.944073	0.695814
H25b	8.393585	-4.671940	0.523731	8.409078	-4.684670	0.531694
H25c	7.187190	-4.281488	1.777939	7.250979	-4.158012	1.801139
H26a	1.192225	7.013841	0.968796	1.196627	7.023002	0.804046
H26b	2.472355	8.231918	0.725886	2.514645	8.241943	0.709139
H26c	2.679399	6.959958	1.958420	2.577238	6.950823	1.957617

Table S2: Optimized bond lengths computed at B3LYP and PBE functionals with 6-31g(d,p) basis set

Bond length (Å)	X-ray[11]	6-31G(d,p)		Bond length (Å)	X-ray[11]	6-31G(d,p)	
		B3LYP	PBE			B3LYP	PBE
S1–C10	1.753 (3)	1.766	1.761	N2–C11	1.384 (3)	1.402	1.414
S1–C12	1.777 (2)	1.816	1.821	N2–C12	1.388 (3)	1.399	1.400
O1–N1	1.225 (3)	1.231	1.242	N2–C13	1.440 (3)	1.437	1.436
O2–N1	1.232 (3)	1.232	1.244	N3–C12	1.267 (3)	1.267	1.279
O3–C11	1.206 (3)	1.218	1.229	N3–C19	1.426 (4)	1.406	1.402
O4–C16	1.365 (3)	1.363	1.368	C6–C7	1.465 (3)	1.465	1.461
O4–C25	1.431 (3)	1.420	1.426	C7–C8	1.341 (3)	1.355	1.369
O5–C22	1.374 (4)	1.366	1.370	C8–C9	1.438 (3)	1.437	1.431
O5–C26	1.385 (5)	1.418	1.425	C9–C10	1.336 (4)	1.354	1.369
N1–C1	1.448 (3)	1.474	1.480	C10–C11	1.491 (4)	1.486	1.484

Table S3: Optimized bond angles computed at B3LYP and PBE levels with 6-31g(d,p) basis set

Bond angles (°)	X-ray[11]	6-31G(d,p)		Bond angles (°)	X-ray[11]	6-31G(d,p)	
		B3LYP	PBE			B3LYP	PBE
S1–C10–C9	126.1 (2)	127.36	127.10	N2–C13–C14	120.5 (2)	119.74	119.56
S1–C10–C11	111.0 (2)	111.50	111.94	N2–C13–C18	119.0 (2)	120.36	120.49
S1–C12–N2	110.7 (2)	109.93	109.95	N3–C19–C20	121.4 (3)	123.08	123.66
S1–C12–N3	125.0 (2)	126.99	127.07	N3–C19–C24	120.3 (3)	118.33	117.92
O1–N1–O2	122.5 (2)	124.08	124.17	C1–C6–C7	123.4 (2)	124.42	124.49
O1–N1–C1	118.4 (2)	117.44	117.42	C5–C6–C7	120.9 (2)	119.78	119.83
O2–N1–C1	119.2 (2)	118.47	118.40	C6–C7–C8	123.9 (3)	124.41	124.53
O3–C11–C10	125.5 (2)	125.22	125.40	C7–C8–C9	122.5 (3)	122.66	122.72
O3–C11–N2	124.6 (2)	124.34	124.39	C8–C9–C10	124.8 (3)	126.15	126.27
O4–C16–C15	116.1 (2)	115.67	115.54	C9–C10–C11	122.9 (2)	121.13	120.96
O4–C16–C17	124.0 (2)	124.64	124.78	C10–S1–C12	91.4 (1)	91.15	91.16
O5–C22–C21	124.2 (3)	124.87	124.96	C11–N2–C12	116.9 (2)	116.91	116.67
O5–C22–C23	115.8 (3)	115.69	115.58	C11–N2–C13	120.9 (2)	121.19	121.22
N1–C1–C2	116.1 (2)	115.67	115.59	C12–N2–C13	122.1 (2)	121.87	122.09
N1–C1–C6	121.6 (2)	121.86	122.03	C12–N3–C19	116.1 (2)	123.45	123.83
N2–C11–C10	109.9 (2)	110.44	110.21	C16–O4–C25	116.7 (2)	118.30	117.41
N2–C12–N3	124.3 (2)	123.06	122.91	C22–O5–C26	118.8 (3)	118.15	117.28

Table S4: Optimized dihedral angles computed at B3LYP and PBE functionals with 6-31g(d,p) basis set

Dihedral angles (°)	X-ray[11]	6-31G(d,p)		Dihedral angles (°)	X-ray[11]	6-31G(d,p)	
		B3LYP	PBE			B3LYP	PBE
S1–C10–C9–C8	−2.1 (4)	0.65	0.72	N3–C12–S1–C10	178.8 (2)	176.13	175.56
S1–C10–C11–O3	−179.3 (2)	–179.88	–179.86	N3–C12–N2–C11	−177.1 (2)	–175.91	–175.31
S1–C10–C11–N2	2.3 (3)	–0.38	–0.37	N3–C12–N2–C13	−0.3 (4)	2.16	2.94
S1–C12–N2–C11	2.8 (3)	2.71	2.79	N3–C19–C20–C21	179.3 (3)	177.02	177.30
S1–C12–N2–C13	179.61 (18)	–179.22	–178.97	N3–C19–C24–C23	−179.8 (3)	–177.96	–178.43
S1–C12–N3–C19	−0.6 (4)	3.95	5.55	C1–C6–C7–C8	−154.6 (3)	–154.48	–156.42
O1–N1–C1–C2	33.4 (4)	21.18	18.01	C5–C6–C7–C8	26.8 (4)	28.98	27.09
O1–N1–C1–C6	−148.8 (3)	–160.41	–163.85	C6–C7–C8–C9	176.5 (2)	–177.45	–177.32
O2–N1–C1–C2	−145.6 (2)	–157.77	–160.90	C7–C8–C9–C10	−179.7 (3)	–179.61	–179.09
O2–N1–C1–C6	32.1 (4)	20.64	17.24	C8–C9–C10–C11	175.8 (2)	–179.68	–179.82
O3–C11–C10–C9	2.5 (4)	0.40	0.60	C9–C10–S1–C12	177.4 (3)	–178.75	–178.91
O3–C11–N2–C12	178.3 (2)	177.96	177.88	C10–C11–N2–C12	−3.3 (3)	–1.55	–1.62
O4–C16–C15–C14	−178.1 (3)	–179.69	–179.78	C10–C11–N2–C13	179.8 (2)	–179.64	–179.87
O4–C16–C17–C18	178.5 (3)	–179.79	–179.77	C11–N2–C13–C14	83.3 (3)	55.36	49.26
O5–C22–C21–C20	−179.3 (3)	179.69	179.56	C11–N2–C13–C18	−95.1 (3)	–123.71	–129.66
O5–C22–C23–C24	178.5 (3)	179.65	179.66	C12–S1–C10–C11	−0.7 (2)	1.56	1.59
N1–C1–C2–C3	178.8 (2)	177.36	176.89	C12–N2–C13–C14	−93.4 (3)	–122.63	–128.90
N1–C1–C6–C5	−179.8 (2)	–178.45	–177.86	C12–N2–C13–C18	88.2 (3)	58.29	52.17
N1–C1–C6–C7	1.6 (4)	4.88	5.51	C12–N3–C19–C20	81.2 (3)	54.91	47.61
N2–C11–C10–C9	−175.9 (2)	179.90	–179.91	C12–N3–C19–C24	−99.1 (3)	–129.63	–136.85
N2–C12–S1–C10	−1.1 (2)	–2.37	–2.43	C25–O4–C16–C15	170.5 (3)	–179.58	–179.66
N2–C12–N3–C19	179.3 (2)	–177.68	–176.70	C25–O4–C16–C17	−9.4 (4)	0.43	0.34
N2–C13–C14–C15	−178.6 (3)	–179.04	–178.90	C26–O5–C22–C21	−4.4 (4)	–0.47	–0.88
N2–C13–C18–C17	179.1 (2)	179.56	179.34	C26–O5–C22–C23	172.6 (3)	–179.88	179.90

Table S5: Experimental and calculated wavenumbers obtained at B3LYP and PBE functionals with 6–31g(d,p) basis set

	Exp.	B3LYP/6-31G(d,p)			PBE/6-31G(d,p)			Vibrational Assignments from B3LYP/6-31G(d,p) PED (≥(10)%)
Mode	FT-IR	Unscaled	Scaled	Int	Unscaled	scaled	Int	
162		3246.7	3120.1	1.90	3172.9	3128.5	2.61	ν_{CH} R1 (86)
161		3232.8	3106.7	5.54	3168.6	3124.2	0.60	ν_{CH} R2 (92)
160		3228.8	3102.9	3.95	3165.3	3120.9	3.86	ν_{CH} R2 (90)
159		3223.3	3097.6	9.16	3153.8	3109.7	8.87	ν_{CH} R3 (99)
158		3222.2	3096.5	6.36	3151.5	3107.4	9.12	ν_{CH} (88)
157		3219.2	3093.6	9.27	3151.1	3107	8.65	ν_{CH} R1 (84)
156		3217.1	3091.6	12.71	3150.4	3106.3	4.88	ν_{CH} R2 (91)
155		3217.0	3091.6	4.51	3149.7	3105.6	16.65	ν_{CH} R2 (90)
154		3212.0	3086.7	9.53	3146.8	3102.8	9.84	ν_{CH} R2 (89)
153		3211.9	3086.6	8.67	3142.3	3098.3	3.66	ν_{CH} R1 (92)
152		3202.3	3077.4	2.56	3136.5	3092.5	3.07	ν_{CH} R3 (93)
151		3199.2	3074.5	14.55	3130.7	3086.9	11.14	ν_{CH} R3 (94)
150		3195.2	3070.6	2.31	3128.2	3084.4	1.86	ν_{CH} R1 (91)
149		3182.2	3058.1	1.97	3107.8	3064.3	1.11	ν_{CH} (92)
148		3163.3	3039.9	5.35	3091.5	3048.2	23.86	ν_{CH} (87)
147		3151.9	3029	29.51	3090.2	3046.9	25.11	ν_{CH3} (99)
146	3008.8	3148.6	3025.8	30.94	3084	3040.8	5.18	ν_{CH3} (100)
145		3080.8	2960.7	37.90	3013.5	2971.3	33.56	ν_{CH3} (99)
144	2951.1	3074.1	2954.2	40.97	3008.8	2966.6	35.30	ν_{CH3} (100)
143	2929.7	3018.1	2900.4	65.21	2947.1	2905.8	78.39	ν_{CH3} (99)
142		3013.4	2895.9	62.60	2943.9	2902.7	74.64	ν_{CH3} (100)
141	1713.0	1795.6	1725.5	120.31	1734.9	1710.6	114.73	$\nu_{C=O}$ (79)
140	1654.2	1725.1	1657.8	865.85	1665.4	1642.1	569.07	$\nu_{C=N}$ (74)
139	1637.0	1674.0	1608.7	66.40	1624.9	1602.2	98.27	ν_{CC} R1 (68)
138	1608.0	1670.2	1605.1	65.84	1619.9	1597.3	11.78	ν_{CC} R2 (69)
137		1665.6	1600.7	23.05	1616.9	1594.3	35.92	ν_{CC} R3 (81)
136		1657.6	1592.9	133.76	1597.1	1574.8	127.83	$\nu_{C=C}$ (58)
135	1587.0	1647.6	1583.4	53.92	1591.4	1569.2	22.78	$\nu_{C=C}$ (69)
134		1636.9	1573.1	20.03	1588	1565.7	51.72	ν_{CC} R2 (63)
133	1566.1	1629.6	1566	133.88	1573.4	1551.4	116.23	$\nu_{as\ NO2}$ (58)
132		1619.8	1556.7	2.58	1571.1	1549.1	2.32	ν_{CC} R3 (66) + δ_{HCC} (10)
131	1513.7	1605.5	1542.9	60.83	1551	1529.3	99.09	ν_{CC} R1 (52) + δ_{HCC} (12)
130	1498.7	1559.5	1498.6	248.61	1510.6	1489.5	240.58	ν_{C-O} R2 (44) + δ_{CCC} (14)
129		1551.6	1491.1	208.84	1502.8	1481.8	192.01	ν_{C-O} R3 (61) + δ_{CCC} (12)
128	1461.1	1519.6	1460.3	45.52	1468.7	1448.1	50.00	δ_{HCH} (75) + τ_{HCOC} (16)
127		1519.1	1459.9	78.93	1468.2	1447.7	97.37	δ_{HCH} (75) + τ_{HCOC} (16)
126		1514.1	1455	18.83	1465.1	1444.6	35.38	δ_{HCC} (40)
125		1505.4	1446.7	5.74	1451.9	1431.6	5.93	δ_{HCH} (74) + τ_{HCOC} (25)
124		1504.4	1445.8	5.15	1451.8	1431.5	6.69	δ_{HCH} (75) + τ_{HCOC} (24)
123		1489.3	1431.3	33.08	1436.4	1416.3	7.15	δ_{HCH} (84)
122		1488.3	1430.3	27.20	1436.1	1416	43.38	δ_{HCH} (82)
121	1439.8	1481.2	1423.4	7.26	1434.1	1414	22.87	ν_{CC} R1 (26) + δ_{HCC} (48)
120		1465.9	1408.8	0.57	1428.2	1408.2	9.63	ν_{CC} R2 (47) + δ_{HCC} (18)
119		1461.3	1404.3	6.46	1426.5	1406.5	0.99	ν_{CC} R3 (48) + δ_{HCC} (24)
118	1374.4	1393.1	1338.8	208.70	1371.9	1352.7	35.30	$\nu_{s\ NO2}$ (61)
117	1345.4	1381.0	1327.2	421.52	1370.2	1351	9.54	ν_{N-C} (42) + δ_{CNC} (10)
116		1374.2	1320.6	31.66	1347	1328.1	37.48	ν_{CC} R1 (32) + δ_{HCC} (15)
115		1360.5	1307.4	157.86	1335.9	1317.2	202.29	ν_{CC} R2 (55)
114		1349.4	1296.7	31.18	1322.8	1304.2	396.79	δ_{HCC} R1 (49)
113	1295.9	1348.2	1295.6	84.99	1306.3	1288	15.72	ν_{CC} R3 (57)

112		1339.4	1287.1	62.47	1295.9	1277.8	51.55	δ_{HCC} R2 (22) + δ_{HCC} (27)
111		1338.3	1286.2	19.87	1290.2	1272.1	50.55	δ_{HCC} R2 (20) + δ_{HCC} (28)
110	1268.8	1327.7	1275.9	5.33	1280.4	1262.5	60.15	δ_{HCC} R3 (74)
109		1307.5	1256.5	42.99	1275.8	1257.9	155.30	ν_{CC} R1 (12) + δ_{HCC} (47)
108		1303.7	1252.9	219.42	1267.2	1249.5	103.94	ν_{N3C19} (41) + ν_{CC} (10)
107	1243.5	1298.2	1247.6	497.80	1264.8	1247.1	566.32	$\nu_{O\text{-}C}$ (40)
106		1289.6	1239.3	151.96	1254.4	1236.8	172.32	$\nu_{C\text{-}O}$ (33) + δ_{HCC} (20)
105		1286.2	1236	102.56	1244.4	1227	29.91	δ_{HCC} (41)
104	1183.5	1245.3	1196.7	2.05	1219.1	1202	7.16	δ_{HCC} (34)
103		1215.2	1167.8	85.81	1185.2	1168.6	135.13	ν_{NC} (10) + δ_{HCC} (18) + τ_{HCOC} (11)
102	1166.6	1212.3	1165.1	10.15	1174.4	1158	21.64	δ_{HCH} (10) + τ_{HCOC} (62)
101		1211.3	1164.1	87.97	1171.8	1155.4	10.89	τ_{HCOC} (40)
100		1201.9	1155	58.33	1168.6	1152.3	1.44	δ_{HCC} (32)
99	1148.3	1196.3	1149.7	44.02	1159.6	1143.4	110.11	δ_{HCC} (66)
98		1191.1	1144.6	77.40	1155.6	1139.4	240.57	δ_{HCC} (58)
97		1185.5	1139.3	227.32	1151.5	1135.4	26.34	δ_{HCC} (11)
96		1178.7	1132.7	0.59	1136.1	1120.2	0.62	δ_{HCH} (25) + τ_{HCOC} (74)
95		1178.5	1132.6	0.69	1135.6	1119.7	1.81	δ_{HCH} (25) + τ_{HCOC} (74)
94		1168.5	1122.9	116.57	1134.2	1118.3	84.42	ν_{NC} (30)
93		1162.7	1117.4	5.53	1127.8	1112	14.27	ν_{NC} (21) + δ_{HCC} R1 (16)
92	1100.4	1139.5	1095.1	7.87	1107	1091.5	5.81	δ_{HCC} R2 (62)
91		1133.1	1088.9	16.28	1098.9	1083.5	17.21	δ_{HCC} R3 (87)
90	1058.2	1095.7	1053	11.15	1059.4	1044.6	17.83	ν_{NC} (10) + δ_{HCC} (14) + δ_{CCC} (47)
89		1078.3	1036.2	20.56	1050.2	1035.5	17.34	$\nu_{O\text{-}CH3}$ (51)
88	1035.3	1077.1	1035.1	71.17	1047.9	1033.2	68.60	$\nu_{O\text{-}CH3}$ (73)
87		1074.6	1032.7	5.04	1046.3	1031.6	40.54	ν_{CC} (53) + δ_{HCC} (11)
86	1026.1	1069.2	1027.5	63.56	1043.6	1029	62.06	$\nu_{C10\text{-}C11}$ (30) + ν_{OC} (12)
85	1009.7	1029.2	989	1.98	997.5	983.5	1.34	δ_{CCC} R2 (67)
84		1024.8	984.9	1.16	991.8	977.9	0.67	δ_{HCC} R3(11) + δ_{CCC} (64)
83	968.2	1006.8	967.5	24.71	963.1	949.6	37.62	τ_{HCCC} (76)
82		1001.4	962.3	12.34	956.9	943.5	7.36	τ_{HCCC} (70)
81	954.2	979.1	940.9	1.92	936.7	923.5	2.01	τ_{HCCC} (87)
80	921.6	963.3	925.7	0.18	921.2	908.3	0.27	τ_{HCCC} (77) + τ_{CCCC} (20)
79		954.2	917	0.99	908.7	895.9	1.29	τ_{HCCC} (77) + τ_{CCCC} (12)
78		940.1	903.5	0.66	893.5	881	0.23	τ_{HCCC} (66) + τ_{CCCC} (15)
77		933.4	897	5.05	890.5	878	11.24	τ_{HCCC} (68)
76		933.0	896.6	3.09	885.9	873.5	2.20	τ_{HCCC} (69)
75	877.8	907.1	871.8	1.15	868.6	856.4	1.61	τ_{HCCC} (61)
74	859.0	882.5	848.1	47.11	855.9	844	29.15	δ_{NCN} (11)
73	841	876.1	842	14.48	849.3	837.4	5.51	δ_{ONO} (18) + δ_{CCC} (10)
72		871.3	837.3	6.22	843.8	832	30.55	τ_{HCCC} (75)
71	833.1	867.5	833.7	25.67	833.4	821.7	1.15	ν_{NC} (20) + τ_{HCCC} (12)
70		850.2	817.1	58.93	820.5	809	77.22	τ_{HCCC} (48)
69		847.8	814.7	17.82	815.2	803.7	30.72	τ_{HCCC} (58) + γ_{OCCC} (11)
68		846.8	813.8	38.62	811.2	799.8	29.13	δ_{ONO} (19) + τ_{HCCC} (12)
67	795.2	818.6	786.7	16.00	787.2	776.2	21.13	τ_{HCCC} (67)
66		815.6	783.8	3.13	779.2	768.3	26.76	τ_{HCCC} (75)
65		810.4	778.8	20.55	774.3	763.5	5.78	δ_{CCO} (12) + τ_{HCCC} (42)
64		802.3	771	9.62	769.5	758.7	11.68	τ_{HCCC} (51) + γ_{NCCC} (33)
63	750.3	787.7	757	8.79	765.2	754.5	7.10	$\nu_{C\text{-}O}$ (17) + δ_{CCC} (13)
62	733.5	760.8	731.1	24.12	734	723.7	5.21	τ_{HCCC} (33) + γ_{OCON} (30)
61		752.4	723.1	9.69	729.5	719.3	27.93	τ_{HCCC} (20)
60	707.9	736.1	707.4	20.47	703.3	693.5	13.76	γ_{ONCC} (71)
59	696.9	725.3	697	2.51	698.8	689	3.35	τ_{CCCC} (57)
58		715.2	687.3	9.03	689.7	680	4.84	τ_{CCCC} (22) + γ_{OCCC} (12)
57	683	710.4	682.7	12.53	683.5	673.9	11.97	τ_{CCCC} (46)
56		694.2	667.1	1.82	671.3	662	0.78	δ_{CCC} (23) + τ_{CCCC} (14)

55	647.1	665.3	639.4	11.48	646.8	637.7	10.12	δ_{CCC} (44)
54		659.3	633.6	9.19	640.1	631.1	7.42	δ_{CCC} (27)
53		650.6	625.2	2.63	627.3	618.5	1.63	δ_{CCC} (62)
52		625.1	600.7	2.51	603.6	595.2	1.15	δ_{CCC} (12)
51	591.0	611.5	587.7	6.67	593.2	584.9	7.70	ν_{SC} (10) + δ_{CNC} (11)
50		589.4	566.4	4.57	565.1	557.2	26.21	τ_{CNCN} (47) + γ_{CCCN} (20)
49	560.7	578.6	556	24.15	557.8	549.9	5.04	δ_{CNO} (19)
48		567.0	544.8	34.51	548	540.3	30.02	δ_{CNO} (17)
47		564.1	542.1	31.48	544.5	536.9	33.64	δ_{CCN} (20) + γ_{OCCC} (18)
46	531.1	541.6	520.5	22.07	520.1	512.8	22.97	τ_{HCCC} (20) + γ_{OCCC} (22)
45	514.1	534.6	513.8	2.02	515.3	508.1	3.45	τ_{CCCC} (16)
44		524.8	504.3	5.50	508.7	501.6	5.98	δ_{CCC} (15) + γ_{OCCC} (32)
43		517.4	497.2	11.51	502.5	495.4	11.37	ν_{SC} (17) + δ_{CCS} (28)
42	469.1	486.6	467.6	5.32	473.1	466.5	6.04	τ_{CCOC} (32)
41		474.5	456	6.57	457.9	451.5	4.65	τ_{CCCC} (31)
40	446.9	464.7	446.5	4.81	448.7	442.4	3.07	ν_{SC} (10) + δ_{CCN} (21)
39		450.9	433.3	4.69	436.8	430.6	3.39	δ_{CCS} (16) + τ_{CCCC} (12)
38		437.5	420.5	2.58	421.8	415.9	3.95	τ_{CCCN} (13) + τ_{CCCC} (14)
37		428.0	411.3	0.32	412.9	407.1	7.93	τ_{HCCC} (11) + τ_{CCCC} (67)
36		425.9	409.3	6.41	412.2	406.4	3.74	τ_{CCCC} (50)
35	397.6	422.4	405.9	9.16	409	403.3	1.80	δ_{CNO} (10)
34		404.6	388.8	0.36	391	385.5	1.43	ν_{NC} (14)
33		393.5	378.2	0.41	380.7	375.4	0.43	τ_{CCCC} (11) + γ_{CCCN} (10)
32		381.1	366.2	0.71	366.9	361.7	0.28	δ_{CNC} (38)
31		359.0	345	10.18	348.7	343.8	9.90	ν_{NC} (10) + δ_{CCC} (23)
30		347.7	334.2	2.55	333.8	329.2	2.62	δ_{CCS} (12) + τ_{CCCC} (17)
29		304.3	292.4	0.35	298.7	294.5	1.04	δ_{CCN} (17) + τ_{CCCC} (22)
28		299.1	287.4	5.24	292.4	288.3	1.13	δ_{CCN} (41) + τ_{CCCC} (15)
27		291.4	280.1	4.72	283.5	279.5	5.11	τ_{CCCC} (12) + τ_{HCOC} (23)
26		266.7	256.3	2.72	263.3	259.7	2.45	τ_{HCOC} (33)
25		257.1	247.1	3.68	254.7	251.1	1.36	δ_{COC} (23) + τ_{HCOC} (28)
24		249.9	240.2	0.96	248.9	245.5	2.32	δ_{COC} (37) + τ_{HCOC} (35)
23		243.9	234.4	1.71	234.5	231.3	3.56	τ_{HCOC} (21) + τ_{CCCC} (14)
22		237.0	227.7	1.76	231.3	228	5.65	τ_{HCOC} (18)
21		227.3	218.4	6.40	223.4	220.3	4.96	τ_{HCOC} (15)
20		180.8	173.7	1.24	178.2	175.7	1.60	τ_{CCCC} (36) + γ_{NCCC} (14)
19		169.6	162.9	1.83	166	163.7	2.41	τ_{CCCC} (18)
18		162.7	156.3	0.12	162.5	160.2	0.06	τ_{COCC} (10)
17		145.0	139.3	2.15	142.1	140.1	3.23	τ_{CCCC} (17)
16		133.6	128.4	3.23	134.9	133.1	2.38	τ_{CCCN} (15)
15		125.5	120.6	0.83	126.9	125.1	1.72	τ_{CCCC} (10) + γ_{CCCN} (10)
14		112.8	108.4	5.20	112.7	111.1	4.86	δ_{CCC} (18) + τ_{COCC} (14)
13		93.1	89.5	1.08	96	94.7	1.03	τ_{COCC} (44)
12		88.7	85.3	1.78	91.2	89.9	0.33	τ_{COCC} (45)
11		76.8	73.8	0.61	82.1	81	0.92	τ_{CCCN} (41)
10		64.7	62.2	0.15	63.8	62.9	0.46	τ_{ONCC} (22)
9		62.7	60.2	0.62	62.2	61.4	0.79	τ_{CNCN} (13) + τ_{CCCC} (42)
8		45.7	43.9	0.36	45.2	44.6	0.55	τ_{ONCC} (31)
7		43.9	42.2	0.41	42.3	41.7	0.81	τ_{ONCC} (22) + τ_{CNCC} (21)
6		33.8	32.5	1.24	39.8	39.2	0.85	τ_{CNCC} (68)
5		29.5	28.3	0.60	29.8	29.4	0.52	τ_{CNCC} (20) + τ_{CNCN} (33)
4		24.6	23.7	0.46	25.4	25.1	0.58	τ_{CNCC} (55)
3		18.5	17.7	1.51	18.8	18.5	1.44	δ_{CNC} (12) + τ_{CCCC} (41)
2		16.1	15.4	0.51	16.9	16.7	0.30	δ_{CNC} (30) + τ_{CCCC} (15)
1		14.7	14.1	0.84	15.6	15.4	0.85	τ_{CCCC} (57)

ν: Stretching, **δ:** Bending, **τ:** Torsion, **γ:** Out-of-plane,

Table S6: Experimental and calculated ^{1}H and ^{13}C isotropic chemical shifts (ppm) for MNTZ using the B3LYP/6–31G(d,p) level of theory

Atoms	^{1}H chemical shifts		Atoms	^{13}C chemical shifts	
	Experimental	Calculated		Experimental	Calculated
H2	8.00	8.40	C1	148.13	144.74
H3	7.43	7.39	C2	122.34	123.28
H4	7.54	7.57	C3	122.34	124.75
H5	7.64	7.67	C4	129.20	129.92
H7	7.67	7.70	C5	122.34	125.12
H8	6.71	6.95	C6	133.36	131.33
H9	7.54	7.55	C7	141.80	136.88
H14	7.35	7.42	C8	125.20	123.59
H15	6.90	7.00	C9	129.60	127.03
H17	6.90	6.80	C10	128.50	128.98
H18	7.35	7.41	C11	165.87	159.32
H20	7.04	7.03	C12	150.72	146.01
H21	6.90	6. 94	C13	122.34	124.78
H23	6.90	6.76	C14	122.34	124.08
H24	7.04	6.82	C15	114.86	112.71
H25a	3.81	3.61	C16	159.90	153.42
H25b	3.85	3.97	C17	114.57	105.44
H25c	3.81	3.61	C18	122.34	125.30
H26a	3.81	3.58	C19	135.79	136.47
H26b	3.85	3.95	C20	114.86	114.88
H26c	3.81	3.60	C21	114.57	105.48
			C22	157.20	151.14
			C23	114.86	114.03
			C24	122.34	120.43
			C25	55.65	53.01
			C26	55.57	52.85

Table S7: The thermodynamic parameters of MNTZ calculated using B3LYP and PBE functionals with 6-31g(d,p) basis set in the ground state at 298.15 K

Thermodynamic parameters	6-31G(d,p)	
	B3LYP	PBE
Zero-point vibrational energy (Kcal.mol^{-1})	266.941	259.507
Rotational constant (GHZ)	0.111	0.111
	0.048	0.048
	0.035	0.034
Rotational temperature (Kelvin)	0.005	0.005
	0.002	0.002
	0.002	0.002
Energy (Kcal.mol^{-1})		
Total	286.474	279.483
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	284.697	277.706
Molecular capacity at constant volume (cal .mol^{-1} K^{-1})		
Total	117.661	121.162
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	111.699	115.201
Entropy (cal.mol^{-1} K^{-1})		
Total	210.554	212.237
Translational	44.438	44.438
Rotational	38.688	38.708
Vibrational	127.428	129.091
Zero point correction (Hartree/Particle)	0.425	0.414
Thermal correction to Energy	0.457	0.445
Thermal correction to Enthalpy	0.457	0.446
Thermal correction to Gibbs Free Energy	0.357	0.346

Table S8: The calculated thermodynamic parameters of MNTZ using B3LYP/6-31g(d,p) and PBE/6-31g(d,p) levels at different temperatures

T (K)	**B3LYP/6-31G(d,p)**			**PBE/6-31G(d,p)**		
	S(J/mol.K)	Cp(J/mol.K)	ΔH(kJ/mol)	S(J/mol.K)	Cp(J/mol.K)	ΔH(kJ/mol)
100	526.08	220.18	13.92	520.47	219.42	13.73
200	724.85	368.74	43.30	718.64	370.83	43.19
298.15	900.00	517.98	86.84	894.95	521.51	87.02
300	903.21	520.73	87.80	898.18	524.27	87.99
400	1072.57	659.85	147.01	1068.61	663.65	147.56
500	1232.68	775.41	218.97	1229.54	778.92	219.9
600	1382.54	867.85	301.31	1380.01	870.87	302.57
700	1522.08	941.77	391.93	1519.97	944.27	393.46
800	1651.88	1001.66	489.20	1650.07	1003.68	490.95
900	1772.79	1050.87	591.90	1771.2	1052.5	593.84
1000	1885.70	1091.81	699.10	1884.26	1093.1	701.18