N-H···O Hydrogen Bonding to the Alkoxy Oxygen of a Carboxylic Ester Group: Crystal Structures of Methyl 2,6-Diaminobenzoate and Its Derivatives.

Songjie Yang, A. Christopher Garner and John D. Wallis.
School of Science and Technology, Nottingham Trent University, Clifton Lane, Nottingham NG11 8NS, UK.

Supplementary Information.

1. **Synthesis of compounds.**
2. **Details of X-ray crystallography**
3. **Details of searches of the Cambridge Structural Database.**

Experimental.

General. Solution NMR spectra were measured on a Jeol ECLIPSE 400 spectrometer at 400 MHz for ^{1}H and at 100.6 MHz for ^{13}C using $CDCl_3$ as solvent and tetramethylsilane (TMS) as standard unless otherwise stated, and measured in p.p.m. downfield from TMS with coupling constants reported in Hz. IR spectra were recorded on a Perkin Elmer Spectrum 100 FT-IR Spectrometer using Attenuated Total Reflection sampling on solids or oils and are reported in cm^{-1}. Accurate mass spectra were recorded on a Waters Xevo QTOF G2 XS spectrometer, equipped with a Waters Acquity UPLC system and fitted with electrospray source operated in + ve mode.

Methyl 2,6-diaminobenzoate 11.

A solution of methyl 2,6-dinitrobenzoate[S1] (100 mg, 0.44 mmol) in a mixture of THF (10 ml) and methanol (10 ml) was degassed and then nitrogen gas bubbled through for 5 min. The solution was added to a Miniclave containing 10% Pd/C catalyst (*ca*. 5 mg) and toluene (2 ml) under a nitrogen atmosphere and the cell sealed and pressurized with hydrogen to 5.0 bar. The reaction mixture was stirred for 1 h. The hydrogen replaced with nitrogen under stirring, and the mixture filtered carefully through a bed of Celite. Careful evaporation of the stirred solution under nitrogen gave diamine **11** in quantitative yield as a green oil, which darkened on exposure to air. ^{1}H NMR (400 MHz $CDCl_3$): 6.94 (1H, t, J = 8.1 Hz, 4-*H*), 5.94 (1H, d, J = 8.1 Hz, 3-,5-*H*), 5.44 (4H, br, 2 x NH_2), 3.89 (3H, s, CO_2CH_3); ^{13}C NMR (100 MHz $CDCl_3$): 169.2 (*C*=O), 151.3 (2,6-*C*), 134.0 (4-*C*), 104.7 (3-,5-*C*), 97.7 (1-*C*), 51.4 (CO_2CH_3); ν_{max}/cm^{-1}: 3461, 3347, 2947, 1657, 1595, 1571, 1457, 1353, 1299, 1243, 1189, 1139, 1101, 1049, 952, 833, 803, 771, 705. On standing for a few days under nitrogen, a few crystals formed under the stirrer bar, m.p. 79-81 °C (lit. 78-80 °C).

Methyl 2,6-diaminobenzoate *bis* HBF_4 salt, 12.

Methyl 2,6-dinitrobenzoate (200 mg, 0.88 mmol) dissolved in a 1:1 mixture of methanol and THF (20 ml) was reduced to methyl 2,6-diaminobenzoate as above. The filtered solution was acidified under nitrogen with excess 54% tetrafluoroboric acid in ether and left stirring for 1 h. Removal of most of the solvent under vacuum and addition of ether (30 ml) led to formation of a white precipitate. The mixture was stirred for 1 h under nitrogen and then filtered to give **12** (290 mg, 95%) as a cream solid, m.p. 210-212 °C dec. ^{1}H NMR (400 MHz, DMSO-d_6): 9.06 (6H, br, 2 x NH_3), 7.26 (1H, t, J = 8.1 Hz, 4-*H*), 6.70 (2H, d, J = 8.1 Hz, 3-,5-*H*), 3.80

(3H, s, CO_2CH_3); ^{13}C NMR (100 MHz, DMSO-d_6): 166.5 (*C*=O), 142.2 (2-,6-*C*), 133.8 (4-*C*), 115.3 (3-,5 -*C*), 105.0 (1-*C*), 54.8 (CO_2CH_3); ν_{max}/cm^{-1}: 3193, 1739, 1575, 1502, 1474, 1433, 1303, 1267, 1252, 1197, 990, 837, 792, 770,749.

Methyl 2,6-diaminobenzoate *bis* BPh_3 complex 13.

Methyl 2,6-dinitrobenzoate (100 mg, 0.44 mmol) dissolved in a 1:1 mixture of methanol and THF (20 ml) was reduced to methyl 2,6-diaminobenzoate as above. The reaction mixture was filtered carefully through a bed of Celite and acidified under nitrogen with excess HCl in ether. The solvent was removed, the residue dissolved in acetonitrile (5 ml), and treated with sodium tetraphenylborate (171 mg, 0.50 mmol) in acetonitrile (5 ml), and stirred. The solution was left to evaporate under a slow nitrogen stream for several days to give mainly oily brown material, but also serendipitously a few crystals of the bis BPh_3 complex **13** were isolated. Attempts to deliberately make this complex from diamine **11** and BPh_3 were unsuccessful.

Methyl 2-amino-6-(tosylamino)benzoate 14

Methyl 2,6-dinitrobenzoate (200 mg, 0.88 mmol) dissolved in a 1:1 mixture of methanol and THF (20 ml) was reduced to methyl 2,6-diaminobenzoate as above. The reaction mixture was filtered carefully through a bed of Celite. After removal of solvent under vacuum, dry THF (20 m), triethylamine (6 ml) and tosyl chloride (180 mg, 0.94 mmol) were added under nitrogen, and the resulting solution was stirred overnight. After evaporation of solvent, the residue was purified by column chromatography eluting with chloroform/ethyl acetate (20:1) to give monotosyl compound **14** (190 mg, 67.1%) as a white powder, m.p. 151-153 °C, R_f (silica, chloroform: ethyl acetate 20:1) 0.47; δ_H (400 MHz, $CDCl_3$): 10.25 (1H, s, N*H*S), 7.69 (2H, d, J = 7.9 Hz, 2',6'-*H*), 7.21 (2H, d, J = 8.0 Hz, 3',5'-*H*), 7.08 (1H, t, J = 8.2 Hz, 4-*H*), 6.89 (1H, d, J = 8.2 Hz, 3-*H*), 6.32 (1H, d, J = 8.2 Hz, 5-*H*), 5.35 (2H, s, NH_2), 3.88 (3H, s, OCH_3), 2.36 (3H, s, CH_3); δ_C (100 MHz, $CDCl_3$): 168.6 (*C*=O), 150.6 (6-*C*), 143.7 (1'-*C*), 140.6 (2-*C*), 136.3 (4'-*C*), 134.0 (4-*C*), 129.5 (2',6'-*C*), 127.3 (3',5'-*C*), 112.5 (3-*C*), 108.5 (5-*C*), 101.1 (1-*C*), 52.3 (OCH_3), 21.5 (CH_3); ν_{max}/cm^{-1}: 3493, 3386, 3070, 3032, 2965, 1661, 1610, 1566, 1470, 1426, 1400, 1370, 1329, 1269, 1241, 1183, 1159, 1122, 1060, 1019, 949, 898, 807, 708. *HRMS* (ESI) calcd for $C_{15}H_{16}N_2O_4S_1$ ($[M+H]^+$): 321.0909, found: 321.1133. Traces of the ditosyl compound **15** ran ahead of the main fraction.

Methyl 2,6-di(tosylamino)benzoate 15.

Methyl 2,6-dinitrobenzoate (100 mg, 0.44 mmol) dissolved in a 1:1 mixture of methanol and THF (20 ml) was reduced to methyl 2,6-diaminobenzoate as above. After removal of solvent under vacuum, dry THF (10 ml, triethylamine (2 ml) and tosyl chloride (180 mg, 0.94 mmol) were added under nitrogen, and the resulting solution was stirred overnight. After evaporation of solvent, the residue was purified by column chromatography eluting with chloroform/ethyl acetate (20:1) to give ditosyl derivative **15** (71 mg, 33.9 %) as a white powder, m.p. 142-144 ^{o}C, R_f (silica, chloroform: ethyl acetate 20:1) 0.54; δ_H (400 MHz, $CDCl_3$): 9.21 (2H, s, 2×N*H*), 7.57 (4H, d, J = 8.2 Hz, 2×2',6'-*H*), 7.34 (3H, s, 3,4,5-*H*), 7.20 (4H, d, J = 8.2 Hz, 2×3',5'-*H*), 3.81 (3H, s, OCH_3), 2.38 (6H, s, 2×CH_3); δ_C (100 MHz, $CDCl_3$): 166.6 (*C*=O), 144.3 (2×4'-*C*), 139.5 (2,6-*C*), 135.7 (2×1'-*C*), 134.0 (4-*C*), 129.7 (2×3',5'-*C*), 127.1 (2×2',6'-*C*), 117.5 (3,5-*C*), 109.3 (1-*C*), 53.3 (OCH_3), 21.6 (2×CH_3); ν_{max}/cm^{-1}: 3316, 3040, 2963, 2922, 1685, 1597, 1579, 1459, 1381, 1320, 1288, 1239, 1154, 1120, 1087, 1070, 1036, 945, 855, 809, 701; *HRMS* (ESI) calcd for $C_{22}H_{22}N_2O_6S_2$ ($[M+H]^+$): 475.0997, found: 475.1084.. Traces of the monotosyl compound **14** ran behind the main fraction.

Methyl 8-Dimethylaminonaphthalene-1-carboxylate 7.[S2]

^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (1H, dd, J = 7.8, 1.4 Hz, Ar-H_1), 7.65 (1H, d, J = 8.2 Hz, Ar-H_1), 7.43-7.49 (3H, m, Ar-H_3), 7.39 (1H, d, J = 7.3 Hz, Ar-H_1), 3.90 (3H, s, OCH_3), 2.6 (6H, s, $N(CH_3)_2$); ^{13}C NMR (100 MHz, $CDCl_3$): 172.0 (*C*=O), 150.5.2 (8-*C*), 134.8, 130.9, 129.3, 128.0, 126.6, 125.2, 125.1, 125.0, 119.3 (Ar -C_9), 51.9 (OCH_3), 46.0 (N-$(CH_3)_2$); ν_{max}/cm^{-1}: 3049, 2980, 2944, 2862, 2829, 2786, 1718, 1505, 1467, 1452, 1434, 1376, 1341, 1271, 1195, 1151, 1144, 1083, 1045, 1029, 1012, 947, 894, 832, 809, 774, 733, 720, 665, 637.

X-ray Crystallography.

General.

Low temperature (100-150 K) X-ray diffraction data (Mo Kα) were measured on an Rigaku Oxford Diffraction Xcalibur diffractometer equipped with a Sapphire detector and an 700 series Cryostream low temperature system using the CrysAlis-Pro software package.[S3]

Structures were solved and refined using the SHELXS and SHELXL suite of programs[S4] using

Table S1. Crystal Data.

	11	**12**	**13**	**14**
Formula	$C_8H_{10}N_2O_2$	$C_8H_{12}N_2O_2$. 2BF_4	$C_8H_{10}N_2O_2$. 2$C_{18}H_{15}B$. 2CH_3CN	$C_{15}H_{16}N_2O_4S$
Formula weight	166.18	341.8	732.51	320.36
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/c$	$P2_1$/n	P-1	$P2_1/c$
a[Å]	5.4015(6)	7.1001(4)	11.5169(8)	9.7212(3)
b[Å]	11.0987(11)	10.8475(7)	12.9904(10)	35.4733(12)
c[Å]	13.6141(17)	16.4165(11)	15.2893(9)	26.2238(10)
α[°]	90	90	67.212(6)	90
β [°]	97.202(12)	94.379(6)	77.440(5)	97.360(3)
γ[°]	90	90	77.991(6)	90
V [Å^3]	809.72(16)	1260.68(14)	2038.8(3)	8968.6(5)
Z	4	4	2	24
ρ [g cm^{-3}]	1.363	1.191	1.193	1.424
T [K]	100(2)	100(2)	150(2)	150(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073
μ (mm^{-1})	0.100	0.200	0.072	0.236
unique refl.	1884	2966	8170	24833
Refl, I > 2σI	1556	2368	4549	14496
R_1	0.0453	0.0438	0.0721	0.0625
wR_2	0.1101	0.0881	0.180	0.1580
$\Delta\rho$(r)[e Å^{-3}]	0.344/ -0.220	0.296/ -0.254	0.274/ -0.258	0.392/ -0.362
Crystallisation solvent.	CH_3OH/THF	CH_3CN	CH_3CN	$(CH_3)_2CO$

the XSEED interface.^{S5} Molecular illustrations were made with Mercury.^{S6} Data are deposited at the Cambridge Crystallographic Data Centre with code numbers CCDC 1994134-1994137.

Table S2. Hydrogen bonding in **12.**

H-bond	N-H	H---O	N---O	<le H/°	sym. op.
N1 H11 O1	0.85(2)	2.48(2)	2.730(2)	97.8(16)	
N1 H12 O1	0.95(2)	2.49(2)	2.729(2)	93.9(16)	
N2 H22 O2	0.91(2)	2.24(2)	2.7057(19)	111.3(17)	
N2 H21 O2	0.91(2)	2.82(2)	2.7057(19)	74.4(17)	

N2 H22 F1	0.91(2)	2.21(2)	2.8372(19)	125.3(18)	4_565
N1 H13 F1	0.89(2)	2.38(2)	3.063(2)	133.7(18)	
N2 H23 F2	0.93(2)	1.94(2)	2.8696(18)	175(2)	2_544
N1 H12 F2	0.93(2)	2.56(2)	2.953(18)	105(2)	
N1 H11 F3	0.85(2)	1.99(2)	2.8263(19)	169(2)	1_455
N2 H23 F3	0.93(2)	2.63(2)	3.1705(19)	117.8(16)	2_544
N1 H11 F4	0.85(2)	2.61(2)	3.210(2) 1	28.8(17)	1_455
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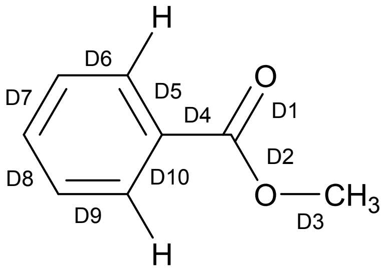
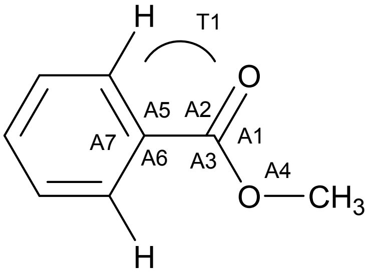
N1 H12 F5	0.96(2)	2.54(2)	3.1009(19)	117.4(16)	3_665
N1 H13 F5	0.89(2)	2.04(2)	2.784(2)	141.0(19)	1_455
N2 H21 F5	0.94(2)	2.09(2)	2.9939(19)	160(2)	4_465
N2 H21 F6	0.94(2)	2.45(2)	3.1999(19)	136.8(18)	4_465
C8 H83 F6	0.96(2)	2.54(2)	3.443(2)	156.9(16)	3_665
N2 H22 F7	0.91(2)	2.36(2)	3.1167(19)	140.0(19)	4_565
N1 H12 F8	0.96(2)	1.87(2)	2.8196(19)	174(2)	3_665
N2 H23 F8	0.92(2)	2.50(2)	2.843(19)	103(2)	4_565

CSD searches.

Searches were carried out with Cambridge Structural Database, version 5.40, Nov. 2018.[S7]

1. Methyl benzoates.





Search conditions: no errors, no disorder, no polymers, no ions, only organic molecules, single crystal X-ray data, 3D coordinates available, $R \leq 7.0\%$, $90 < T < 120$ K. No constraint on phenyl substitution, but no fused rings.

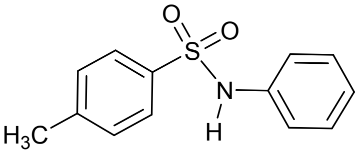
147 hits, 203 molecules.

Table S3. Geometric parameters for methyl benzoates, as defined above**.**

Name	Count	Minimum	Maximum	Mean	Std. Dev
DIST1	203	1.193	1.236	1.209	0.006
DIST2	203	1.292	1.373	1.340	0.008
DIST3	203	1.419	1.771	1.449	0.024
DIST4	203	1.447	1.511	1.487	0.008
DIST5	203	1.373	1.411	1.393	0.005
DIST6	203	1.358	1.399	1.383	0.007
DIST7	203	1.367	1.43	1.398	0.009
DIST8	203	1.358	1.425	1.396	0.009
DIST9	203	1.346	1.404	1.386	0.007
DIST10	203	1.373	1.412	1.393	0.006
ANG1	203	121.746	125.722	123.412	0.597
ANG2	203	120.862	126.832	124.292	0.637
ANG3	203	110.501	116.009	112.289	0.633
ANG4	203	84.996	117.977	115.379	2.247
ANG5	203	116.534	120.613	118.327	0.683
ANG6	203	120.419	125.105	122.128	0.643

ANG7	203	117.763	121.856	119.525	0.622
TOR1	203	0.197	27.326	6.071	5.026

2. Nitrogen bonding geometry of benzenesulfonylaniline derivatives.



Search conditions: no errors, no disorder, no polymers, no ions, only organic molecules, single crystal X-ray data, 3D coordinates available, R ≤ 7.5%, 80 < T < 150 K. No constraint on phenyl substitution, but no fused rings.

41 hits, 50 molecules:

(a) 28 with pyramidal N bonding geometry.
(b) 15 with "planar" N bonding geometry (However, H atoms often fixed with wrong geometry)
(c) 7 with intermediate N bonding geometry. (IDAFIF, QERLAD, SECPAT, TIHZEQ, TSBZON01, UCUFOO, YOHCAA, H atom positions refined and usually N-H involved in hydrogen bonding.

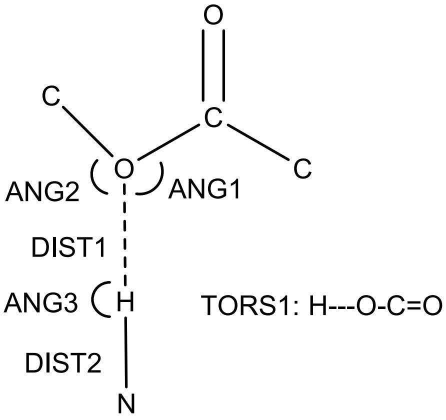
Table S4. Table of sum of angles at the sulfonamide nitrogen atom, as defined above.

Entry	Index	Σangles	
1	ABAWOS	342.587	
2	CEMCOP	349.132	
3	DAVLUK	342.106	
4	DEFZOG	343.776	
5	DEFZUM	337.148	
6	DEFZUM	348.293	
7	DEHNIQ	360	*
8	EQANUH	359.999	*
9	EQEJIV	360	*
10	EXUJIS	346.686	
11	EXUJIS	340.918	
12	FAXBUB06	360	*
13	FOXXEX	339.101	
14	GAGDID	359.999	*
15	GEXRIN	348.784	

16	GEXRIN	349.988	
17	GIMTEE	359.872	*
18	GIMTEE	359.819	*
19	GOFREA	346.404	
20	HOMWEN	355.467	**
21	ICINIT	360	*
22	IDAFIF	356.451	**
23	IMOMAA	359.999	*
24	IMOMAA	360.001	*
25	JISZOB	348.05	
26	JISZOB	349.764	
27	KUCJOJ	360	*
28	KUCKAW	360	*
29	PAHPAQ	349.257	
30	PILGOH	345.027	
31	PILGOH	348.005	
32	PIXYAY	343.938	
33	POGLED	351.832	
34	QERLAD	356.256	**
35	SECPAT	341.16	
36	SECPAT	354.559	**
37	SULNUJ	360	*
38	TIBBUE	341.088	
39	TIHZEQ	350.553	
40	TIHZOA	346.436	
41	TIHZUG	340.574	
42	TSBZON01	354.159	**
43	UCUFOO	348.957	
44	UCUFOO	354.539	**
45	VIGPEH	338.886	
46	WEDMEA	341.845	
47	WEFHAR01	344.013	
48	YEXREZ	360	*
49	YEXRID	360	*
50	YOHCAA	351.696	

*planar; **sum of angles close to planar (Σangles: 354-359°).

3. Intermolecular N-H—OR v C=O



Search conditions: no errors, no disorder, no polymers, no ions, only organic molecules, single crystal X-ray data, 3D coordinates available, R ≤ 7.5%, no limits on temperature of measurement. N-H···O distance ≤ 2.3 Å.

17 hits.

Table S5. Selected geometry for intermolecular N-H···O(R)C(=O)C interactions.

Index	NAME	DIST1	DIST2	ANG1	ANG2	ANG3	TOR1	TEMP /K
1	CERSUP	2.289	0.866	114.226	124.585	166.925	156.282	100
2	GUFTAE	2.255	0.88	118.072	123.553	167.2	179.325	173
3	JONQOU	2.275	0.89	145.036	95.18	157.08	144.987	100
4	LIZDAA	2.214	0.951	127.879	112.049	160.98	158.504	RT
5	MAVTAE	2.033	0.959	126.96	114.482	164.137	176.43	RT
6	MAVTEI	1.958	0.96	126.872	112.037	168.045	163.174	RT
7	MAVTOS	2.187	0.873	120.571	123.351	146.435	175.618	173
8	MAVTUY	2.087	0.932	122.931	121.563	157.733	176.846	173
9	MAVVEK	2.122	0.96	124.383	118.151	165.351	174.985	RT
10	MAVVOU	1.923	0.961	126.96	111.893	169.758	153.353	RT
11	MAYCIB	2.132	0.918	116.535	126.824	165.999	-179.406	173
12	NEMNOK	2.138	0.879	121.451	121.309	170.702	175.769	100
13	PERYER	2.175	0.849	106.499	116.683	162.637	-125.665	100
14	QARHUN	2.222	0.959	142.111	102.3	140.629	165.759	RT
15	VIWGOY	2.25	1.061	123.587	117.664	160.717	169.154	RT
16	VIZZOV	2.243	0.86	148.258	94.569	166.044	160.439	RT
17	ZIFHAA	2.296	0.824	140.923	101.753	169.999	164.622	RT

Entries 5-10 contain a N-H making two hydrogen bonds to a α-hydroxyester.

Search under the same restrictions for N-H···O=C(C)(OR) gave 2042 hits.

4.Intramolecular N-H—OR v C=O

Search conditions: no errors, no disorder, no polymers, no ions, only organic molecules, single crystal X-ray data, 3D coordinates available, R ≤ 7.5%, no limits on temperature of measurement. N-H···O distance ≤ 2.3 Å.

Restricted angle at hydrogen (N-H···O) to 120-180^{o}.

57 hits, 61 molecules.

(Without angular restriction: 168 hits).

Table S6. Selected geometry for intramolecular N-H···O(R)C(=O)C interactions.

Index	NAME	DIST1	DIST2	ANG1	ANG3	ANG4	TOR1
1	ACEVAI	2.179	0.815	123.418	94.003	129.734	116.453
2	ACEVAI	2.181	0.812	120.314	93.954	131.169	114.354
3	AWAQIZ	2.218	0.86	99.293	134.716	127.944	150.109
4	AZASER10	2.263	0.861	149.144	77.201	120.496	120.369
5	BIMFOS10	2.26	0.86	106.883	135.377	124.668	177.796
6	CEWDIU	2.252	0.848	106.968	135.836	121.919	171.973
7	CITPIF	2.243	0.88	151.433	100.817	120.452	-8.781
8	DAZVUY	2.211	0.88	105.769	138.313	123.024	175.056
9	DUGXAE	2.296	0.9	121.403	98.091	123.968	109.41
10	ESEGAL	2.252	0.868	149.876	88.562	136.54	136.12
11	FEFVUK	2.067	0.874	109.897	133.425	125.126	179.661
12	FIMPID	2.213	0.86	110.509	89.88	123.222	93.417
13	FOMFUJ	2.13	0.864	104.427	137.869	134.788	179.294
14	FOMGAQ	2.3	0.858	104.073	139.6	125.17	172.809
15	GARWII	1.991	0.884	106.158	139.144	129.578	174.757
16	GAVJIX	2.294	0.86	106.655	135.742	120.785	178.996
17	GIRGAR	2.064	0.86	110.799	97.013	138.08	89.168
18	HAMLIQ	2.028	0.856	105.289	137.293	131.889	177.084
19	HOMQUX	2.014	0.884	107.7	135.787	131.922	177.882
20	HOMREI	2.054	0.883	107.563	136.053	129.099	175.891
21	HUXZUX	2.055	0.865	106.724	134.47	127.551	166.588
22	HUXZUX	2.085	0.842	107.711	134.645	125.731	179.689
23	IFEGUW	2.248	0.88	78.003	108.31	132.88	115.45
24	ISITAF	2.196	0.875	101.904	129.174	128.588	145.1
25	KAXPAD	1.969	0.859	105.178	131.944	131.528	160.395
26	KIDCOS	2.166	0.855	110.142	132.918	120.296	178.338
27	LAXSAF	2.275	0.831	136.429	98.278	123.884	154.479
28	LEKQEX	2.121	0.916	108.403	132.949	121.316	173.89
29	LEPDEQ	2.247	0.88	101.5	96.879	130.951	-94.896
30	LEVWEO	2.175	0.952	109.122	134.452	123.393	177.382
31	MIVPEM	2.048	0.879	124.573	95.808	129.972	122.664

32	MOZYUV	2.104	0.859	99.89	130.599	124.959	144.769
33	NEJTUU	2.25	0.861	107.906	134.133	120.674	165.579
34	OFEXAY	2.296	0.881	101.993	128.227	121.792	154.326
35	OJOSEM	2.256	0.782	93.149	128.156	137.721	139.108
36	PABXOF	2.069	0.949	107.321	134.892	125.704	176.986
37	PEHQOI	2.269	0.903	102.27	142.596	143.997	175.526
38	PILYOB	2.08	0.86	107.298	134.886	127.601	179.093
39	QUZWOY	2.01	0.88	117.265	100.071	132.066	119.011
40	QUZWOY	2.037	0.881	122.655	99.386	131.237	-123.85
41	RATHUQ	2.102	0.813	106.54	137.816	131.353	174.815
42	ROZXIP	2.293	0.86	93.854	127.54	122.614	144.559
43	SALQAZ	2.028	0.996	106.127	135.398	126.047	161.78
44	SOJJEG	2.148	1.08	125.364	94.572	121.671	115.74
45	SOVBUA	2.228	0.865	105.496	137.867	122.081	179.709
46	TAQYOA	2.259	0.86	106.875	134.761	123.714	172.823
47	TEZCEH	2.28	0.887	86.184	126.736	128.764	124.636
48	TIBNIE	2.251	0.802	116.203	82.334	135.952	92.09
49	TIBPEC	2.299	0.865	132.153	77.973	133.376	95.824
50	TIHVAI	2.223	0.861	106.784	136.43	124.23	178.556
51	VOHXAS	2.27	0.861	107.782	135.319	121.015	176.235
52	WOSBOX	2.153	0.86	105.832	87.145	140.481	-87.932
53	XIQMUI	1.948	0.845	97.052	123.729	132.177	140.419
54	XIQMUI	1.892	0.845	107.742	131.961	134.371	173.541
55	XIQNET	1.984	0.908	104.185	136.195	129.309	158.036
56	XIQNOD	1.936	0.92	108.351	132.126	129.672	173.93
57	XOGHOR	2.21	0.855	105.423	137.153	128.782	171.833
58	XORZAH	2.235	0.795	107.657	136.178	120.003	176.202
59	XOXCUK	2.058	0.88	109.855	132.791	125.498	179.432
60	YIBROQ	2.174	0.889	126.368	96.935	120.871	120.001
61	ZITLAR	2.191	0.86	100.614	130.096	126.681	147.398

Search under the same restrictions for N-H···O=C(C)(OR) gave 1108 hits (or 1385 without any angular restriction at H).

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