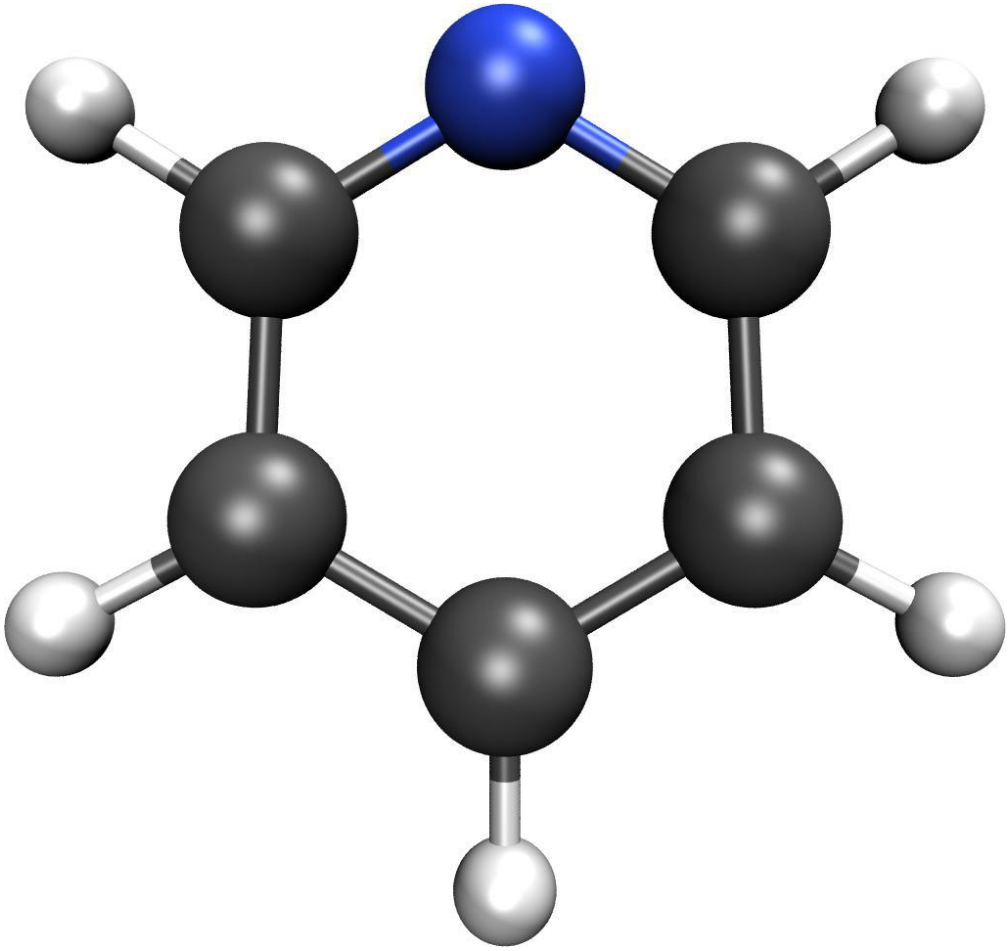
THE Zysman-Colman GROUP

Calculation Report

Pyridine

Optimisation, Frequencies, Excited States ()



Summary of Results

Pyridine - Optimisation, Frequencies, Excited States ()

Metadata

Username:	osl
Date:	24/06/2022 12:28:25
Duration:	58 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Optimisation, Frequencies, Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)
No. merged calculations:	3

Calculation 1

Username:	osl
Date:	24/06/2022 12:20:46
Duration:	33 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Optimisation, Frequencies
Orbital spin:	restricted
Multiplicity:	1 (singlet)

Calculation 2

Username:	osl
Date:	24/06/2022 12:24:30
Duration:	13 s
Success:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

Calculation 3

Username:	osl
Date:	24/06/2022 12:28:25
Duration:	10 s
Success:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	9
Final energy:	-6748.4564 eV
Final energy:	-651,127 $kJmol^{-1}$

Geometry

Formula:	C_5NH_5
Molar mass:	79.0999 $gmol^{-1}$
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.88 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

HOMO & LUMO

$E_{HOMO,LUMO}$:	6.71 eV
E_{HOMO}:	-7.17 eV
E_{LUMO}:	-0.47 eV

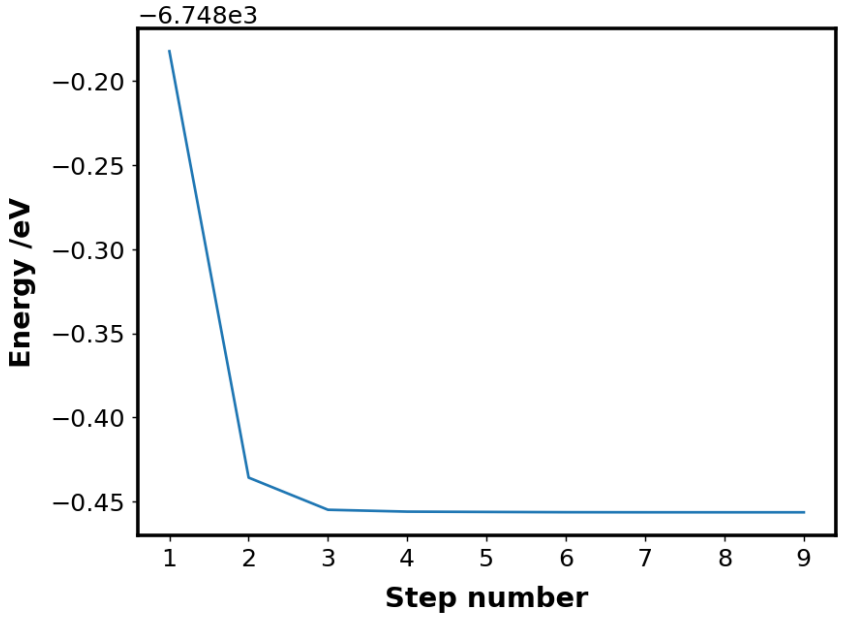
Permanent Dipole Moment

Total:	2.20 D
X axis angle:	89.98 °
XY plane angle:	0.01 °

Vibrational Frequencies

Negative frequencies:	0

SCF Energies



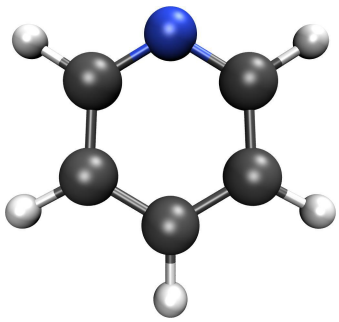
SCF Energies

No. of steps: 9

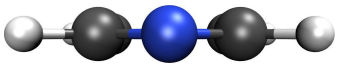
Final energy: -6748.4564 eV

Final energy: -651,127 kJmol^{-1}

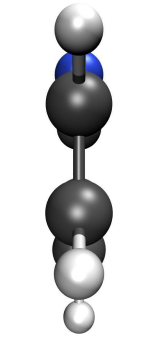
Geometry



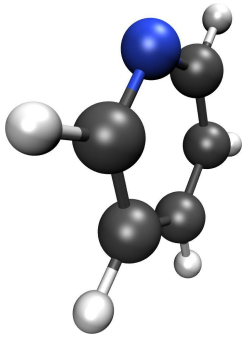
X/Y plane



X/Z plane



Z/Y plane



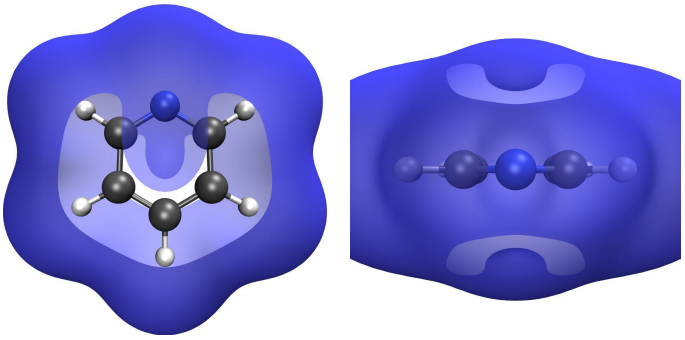
45° to axes

Aligned structure

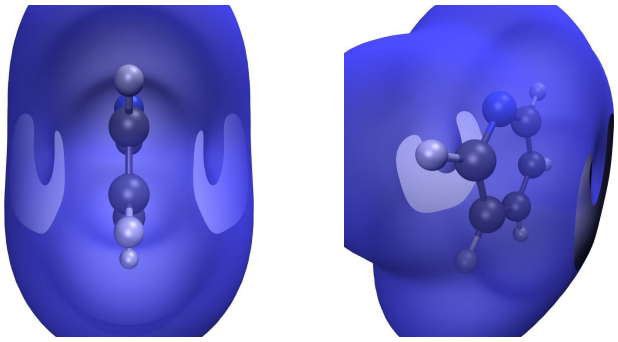
Geometry

Formula:	C_5NH_5
Molar mass:	79.0999 gmol^{-1}
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.88 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

SCF Density



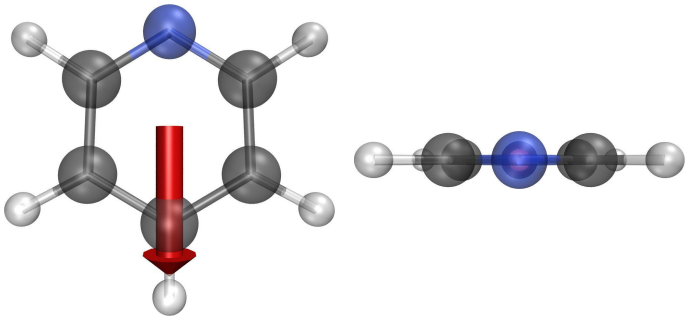
X/Y plane | X/Z plane



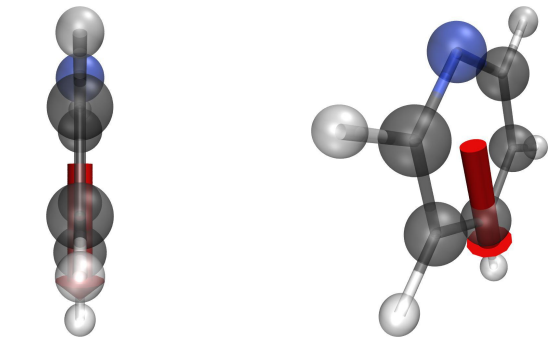
Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

Permanent Dipole Moment



X/Y plane | X/Z plane



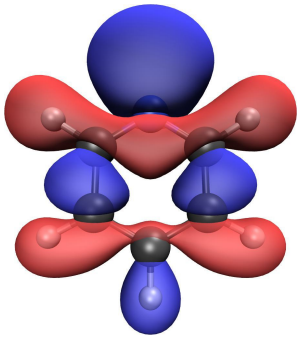
Z/Y plane | 45° to axes

Aligned structure (dipole moment in red)

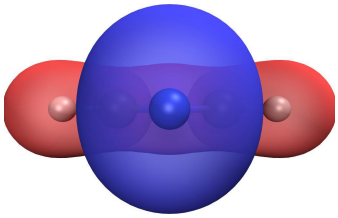
Dipole Moment

Origin X:	0.00 D
Origin Y:	0.00 D
Origin Z:	0.00 D
Vector X:	-0.00 D
Vector Y:	-2.20 D
Vector Z:	-0.00 D
Total:	2.20 D
X axis angle:	89.98 °
XY plane angle:	0.01 °

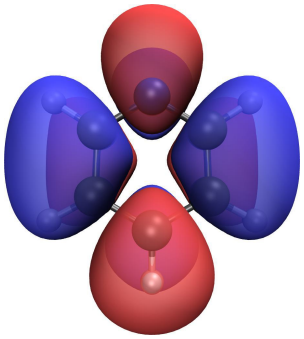
HOMO & LUMO



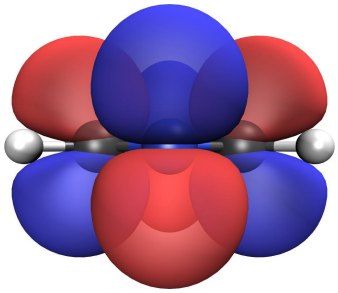
X/Y plane



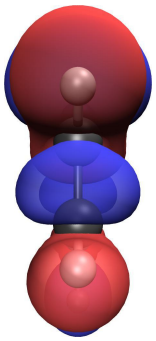
X/Z plane



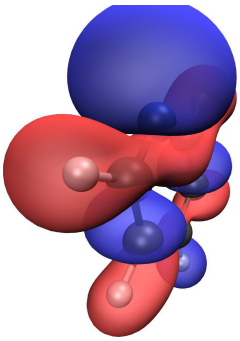
X/Y plane



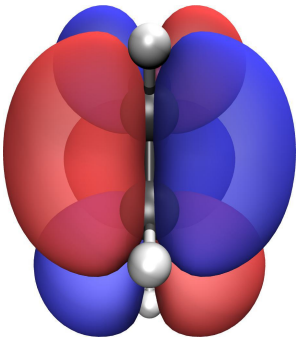
X/Z plane



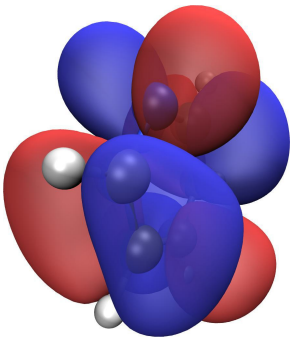
Z/Y plane



45° to axes



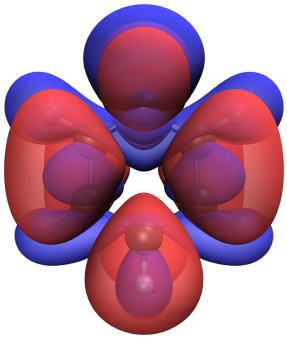
Z/Y plane



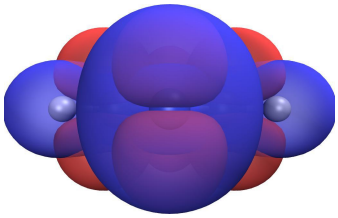
45° to axes

HOMO density (isovalue: 0.02)

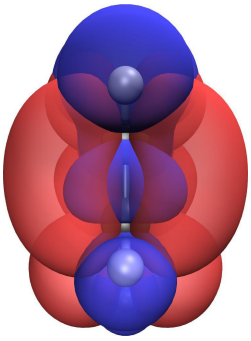
LUMO density (isovalue: 0.02)



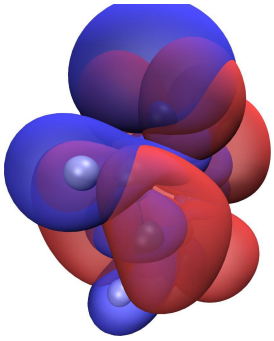
X/Y plane



X/Z plane

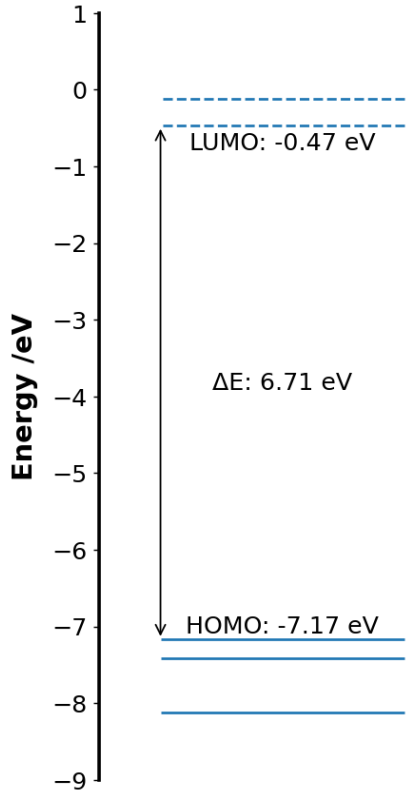


Z/Y plane

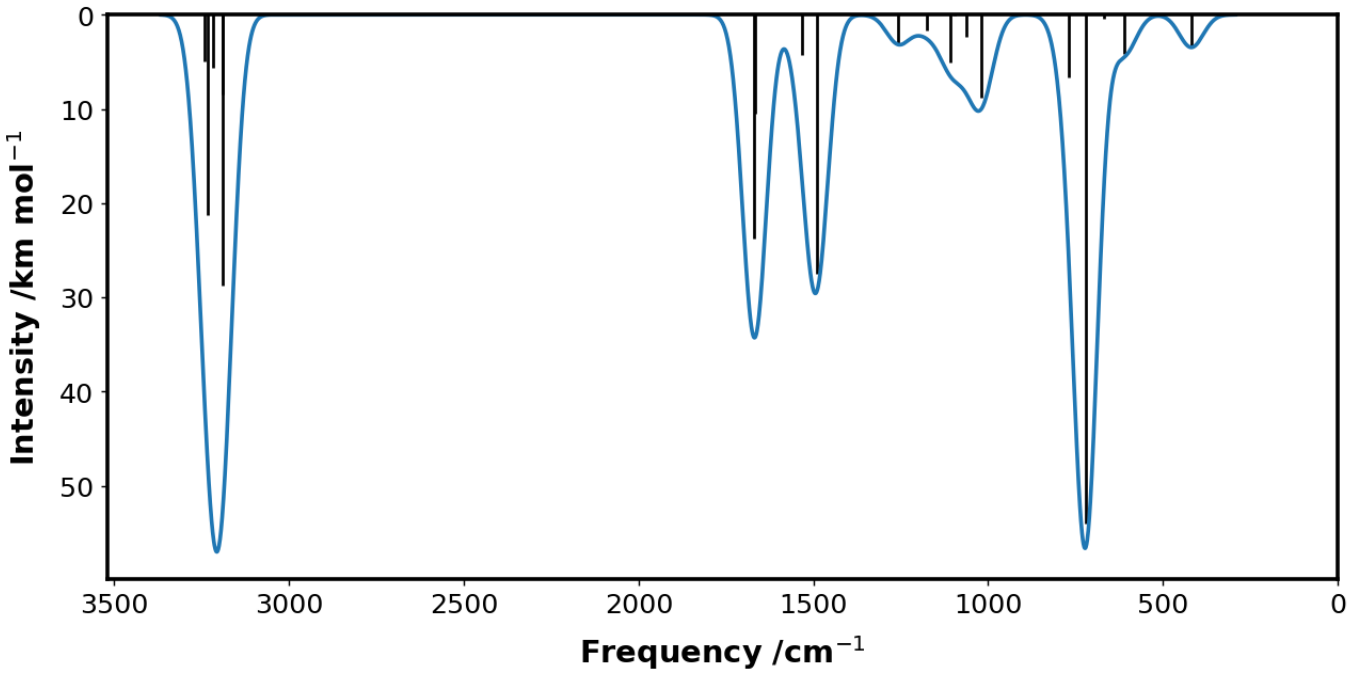


45° to axes

HOMO (blue) & LUMO (red) density (isovalue: 0.02)



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: 418, 722, 1028, 1253, 1494, 1668, 3206.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	383.7300	0.0000
2	A	418.8300	3.4700
3	A	610.8100	4.1300
4	A	669.5500	0.4300
5	A	720.8700	53.9400
6	A	769.0500	6.6100
7	A	903.1900	0.0000
8	A	964.8600	0.0000
9	A	1006.5300	0.0000
10	A	1019.4400	8.7800
11	A	1019.6600	0.0100
12	A	1063.0900	2.3400
13	A	1094.9400	0.0300
14	A	1107.3800	5.0600
15	A	1176.8300	1.7100
16	A	1256.6600	3.0700
17	A	1347.6300	0.0200
18	A	1387.9500	0.0000
19	A	1491.3400	27.4400
20	A	1533.3700	4.3300
21	A	1666.2100	10.5600
22	A	1669.7000	23.7500
23	A	3189.0900	28.7200
24	A	3191.5700	8.4800
25	A	3216.3200	5.6200
26	A	3232.9100	21.2400
27	A	3240.5600	4.9800

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
37	LUMO+15	A	15.0342
36	LUMO+14	A	14.5841
35	LUMO+13	A	12.7701
34	LUMO+12	A	12.6778
33	LUMO+11	A	9.0193
32	LUMO+10	A	8.9991
31	LUMO+9	A	8.2736
30	LUMO+8	A	6.8258
29	LUMO+7	A	5.1991
28	LUMO+6	A	5.1849
27	LUMO+5	A	4.5869
26	LUMO+4	A	4.2866
25	LUMO+3	A	4.1186
24	LUMO+2	A	2.8373
23	LUMO+1	A	-0.1198
22	**LUMO**	**A**	**-0.4664**
21	**HOMO**	**A**	**-7.1729**
20	HOMO-1	A	-7.4192
19	HOMO-2	A	-8.1232
18	HOMO-3	A	-10.1396
17	HOMO-4	A	-11.1930
16	HOMO-5	A	-11.2837
15	HOMO-6	A	-11.9543
14	HOMO-7	A	-13.1334
13	HOMO-8	A	-13.4087
12	HOMO-9	A	-14.7906
11	HOMO-10	A	-17.5660
10	HOMO-11	A	-17.6204
9	HOMO-12	A	-21.3179
8	HOMO-13	A	-22.5352
7	HOMO-14	A	-26.3512
6	HOMO-15	A	-278.7372

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.1374880	0.6846500	-0.0000203
C	-1.1954410	-0.7066373	0.0000749
C	-0.0004716	-1.4179164	0.0000717
C	1.1949723	-0.7074353	-0.0001501
C	1.1379485	0.6838900	0.0000885
N	0.0004626	1.3802168	0.0001982
H	-2.0551243	1.2706886	-0.0005978
H	-2.1544681	-1.2150527	0.0001467
H	-0.0008321	-2.5041577	0.0003545
H	2.1536570	-1.2164949	-0.0006432
H	2.0559747	1.2693189	0.0002970

About

Silico Calculation Report

Part of the silico software package

Version 1.0.0-pre.32

11 February 2022

Silico makes use of a number of 3rd party libraries and programs; please cite these appropriately in your works:

Extraction and processing of results: **cclib**[1]
Rendering of 3D images: **VMD**[2], **Tachyon**[3]
Rendering of graphs: **Matplotlib**[4]
Calculation of CIE colour coordinates: **Colour Science**[5]
Generation of reports: **Mako**[6], **Weasyprint**[7]
Scientific constants: **SciPy**[8]
Conversion of file formats: **Pybel**[9], **Openbabel**[10]
Calculation of spin-orbit coupling: **PySOC**[11]
Rendering of 2D structures: **RDKit**[12]
Saving of state during submission: **Dill**[13,14]

Bibliography

[1] N. M. O'boyle, A. L. Tenderholt and K. M. Langner, *Journal of Computational Chemistry,* 2008, **29,** 839--845

[2] W. Humphrey, A. Dalke and K. Schulten, *Journal of Molecular Graphics,* 1996, **14,** 33--38

[3] J. Stone, Masters Thesis, Computer Science Department, University of Missouri-Rolla, 1998

[4] J. D. Hunter, *Computing in Science & Engineering,* 2007, **9,** 90--95

[5] T. Mansencal, M. Mauderer, M. Parsons, N. Shaw, K. Wheatley, S. Cooper, J. D. Vandenberg, L. Canavan, K. Crowson, O. Lev, K. Leinweber, S. Sharma, T. J. Sobotka, D. Moritz, M. Pppp, C. Rane, P. Eswaramoorthy, J. Mertic, B. Pearlstine, M. Leonhardt, O. Niemitalo, M. Szymanski and M. Schambach, Colour 0.3.15, Zenodo, 2020

[6] M. Bayer, https://www.makotemplates.org, (accessed May 2020)

[7] K. Community, https://weasyprint.org, (accessed May 2020)

[8] P. Virtanen, R. Gommers, T. E. Oliphant, M. Haberland, T. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, K. Jarrod Millman, N. Mayorov, A. R. J. Nelson, E. Jones, R. Kern, E. Larson, C. Carey, İ. Polat, Y. Feng, E. W. Moore, J. Vand erPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt and S. 1. 0. Contributors, *Nature Methods,* 2020, **17,** 261--272

[9] N. M. O'Boyle, C. Morley and G. R. Hutchison, *Chemistry Central Journal,* 2008, **2,** 5

[10] N. M. O'Boyle, M. Banck, C. A. James, C. Morley, T. Vandermeersch and G. R. Hutchison, *Journal of Cheminformatics,* 2011, **3,** 33

[11] X. Gao, S. Bai, D. Fazzi, T. Niehaus, M. Barbatti and W. Thiel, *Journal of Chemical Theory and Computation,* 2017, **13,** 515--524

[12] G. Landrum, https://www.rdkit.org/, (accessed February 2022)

[13] M. McKerns, L. Strand, T. Sullivan, A. Fang and M. Aivazis, *Proceedings of the 10th Python in Science Conference,* 2011,

[14] M. McKerns and M. Aivazis, https://uqfoundation.github.io/project/pathos, (accessed February 2022)

[15] K. Shizu and H. Kaji, *The Journal of Physical Chemistry A,* 2021, **125,** 9000--9010