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Electronic Supplementary Information

On the Lewis acidic character of bis(salicylaldiminato)zinc(II) Schiff-base complexes: a computational and experimental investigation on a series of compounds varying the bridging diimine

Giuseppe Forte,*[,a] Ivan Pietro Oliveri,[b] Giuseppe Consiglio,[b] Salvatore Failla[b] and Santo Di Bella*[,b]

[a] *Dipartimento di Scienze del Farmaco, Università di Catania, I-95125 Catania, Italy. E-mail:gforte@unict.it*
[b] *Dipartimento di Scienze Chimiche, Università di Catania, I-95125 Catania, Italy. E-mail:sdibella@unict.it*

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I. Calculated atomic charges on relevant atoms and dipole moment for monomers, dimers, and adducts

Table S1 Calculated atomic charges (*e*) on relevant atoms and dipole moment (μ, Debye) for $Zn(sal)_2$ and ZnL monomers [a]

	$Zn(sal)_2$	Zn(salen)	**1**	**2**	**3**	**4**	**5**	**6**
Zn	0.91	1.09	1.08	1.29	1.28	1.25	1.28	1.21
O	-0.60	-0.68	-0.68	-0.64	-0.67	-0.66	-0.66	-0.64
O′	-0.63	-0.66	-0.67	-0.70	-0.67	-0.66	-0.68	-0.64
N	-0.29	-0.56	-0.56	-0.64	-0.50	-0.60	-0.59	-0.53
N′	-0.29	-0.51	-0.55	-0.71	-0.50	-0.60	-0.85	-0.53
μ	4.04	5.35	5.43	2.62	4.98	3.74	3.34	3.41

[a] See Scheme 1 for atom labelling.

Table S2 Calculated atomic charges (*e*) on relevant atoms and dipole moment (μ, Debye) for ZnL dimers [a]

	$[Zn(salen)]_2$	**1D**	**2D**	**3D**	**4D**	**5D**	**6D**
Zn	1.12	1.02	1.16	1.23	1.22	1.29	1.19
O	-0.69	-0.68	-0.64	-0.72	-0.70	-0.70	-0.68
O′	-0.72	-0.62	-0.67	-0.68	-0.70	-0.72	-0.70
N	-0.35	-0.38	-0.51	-0.55	-0.67	-0.93	-0.65
N′	-0.35	-0.37	-0.41	-0.40	-0.46	-0.45	-0.40
μ	0.000	0.000	3.71	0.000	0.000	0.000	0.000

[a] See Table 2 for atom labelling.

Table S3 Calculated atomic charges (*e*) on relevant atoms and dipole moment (μ, Debye) for **1**-**6**·py adducts [a]

	1·py	**2·py**	**3·py**	**4·py**	**5·py**	**6·py**
Zn	0.91	1.16	1.12	1.07	1.26	1.12
O	-0.59	-0.63	-0.65	-0.64	-0.68	-0.65
O′	-0.60	-0.67	-0.65	-0.63	-0.67	-0.66
N	-0.26	-0.62	-0.36	-0.46	-0.57	-0.47
N′	-0.33	-0.74	-0.35	-0.52	-0.85	-0.50
N_{py}	-0.37	-0.23	-0.37	-0.30	-0.34	-0.24
μ	5.96	4.62	7.66	4.38	4.88	3.66

[a] See Table 5 for atom labelling.

II. Charge decomposition analysis and frontier MOs for $Zn(sal)_2$ and Zn(salen)

In order to better understanding the origin of the different atomic charge, in terms of MOs, on the Zn atom in $Zn(sal)_2$ and Zn(salen) a charge decomposition analysis, CDA, was performed. From the CDA it can see that the net charge transfer from L^{2-} to Zn^{2+} is higher for $Zn(Sal)_2$ with respect Zn(Salen). In particular, a charge transfer of 0.244 *e* is found for Zn(Salen) while 0.293 *e* is obtained for $Zn(Sal)_2$. Note that the charge transfer does not correspond exactly to the calculated atomic charge because the CDA method, besides charge transfer between fragments, includes the electronic polarization of fragments.

A detailed analysis reveals that the main contribution to such transfer is due to the HOMO-39, HOMO-33 and HOMO-15 in Zn(Salen), while the HOMO-40 HOMO-34 HOMO-15 and HOMO-9 are mainly involved in $Zn(Sal)_2$ (Fig. S1). In Table S1 is reported the contribution of the two fragments, *i.e.*, the Zn^{2+} and L^{2-}, to the molecular orbitals mentioned above. The composition of such MOs in terms of atomic orbitals is reported in Table S2. As far as the Zn(Salen) is concerned it results that L^{2-} gives a predominant contribution by means of p-type orbitals in molecular orbitals lower in energy (HOMO-39 and HOMO-33), while the s-type percentage is higher in H-15. The p-type contribution arises from heteroatoms, nitrogen in particular, lying along the direction of zinc, the latter of which is involved by means of 4s, and $3dx^2$-y^2 and dz^2 orbitals. At variance of Zn(Salen), in $Zn(Sal)_2$ the contribution of p-type atomic orbitals of the ligand increases with the decreasing of the MOs energy while the zinc contributes with the same type of d orbitals described for Zn(Salen).

Table S4 Relevant MOs involved in the charge transfer between L^{2-} and Zn^{2+} fragments

Zn(Salen)

MO	% L^{2-}	% Zn^{2+}
H-39	95.55	4.45
H-33	89.00	11.00
H-15	88.08	11.92

$Zn(Sal)_2$

MO	% L^{2-}	% Zn^{2+}
H-40	95.42	4.58
H-34	92.75	7.25
H-15	95.17	4.83
H-9	88.31	11.69

Table S5 Atomic orbital composition of relevant MOs involved in the charge transfer between L^{2-} and Zn^{2+} fragments

Zn(Salen)

MO	%s	%p	%d
H-39 (L^{2-})	41.15	58.85	0.00
H-39 (Zn^{2+})	31.91	0.00	68.09
H-33 (L^{2-})	41.32	58.68	0.00
H-33 (Zn^{2+})	27.20	0.36	72.44
H-15 (L^{2-})	67.87	32.13	0.00
H-15 (Zn^{2+})	72.57	0.65	26.78

$Zn(Sal)_2$

MO	%s	%p	%d
H-40 (L^{2-})	50.86	49.14	0.00
H-40 (Zn^{2+})	97.60	2.40	0.00
H-34 (L^{2-})	50.57	59.43	0.00
H-34 (Zn^{2+})	55.17	0.00	44.83
H-15 (L^{2-})	30.85	66.65	0.00
H-15 (Zn^{2+})	67.08	0.00	32.92
H-9 (L^{2-})	15.46	84.54	0.00
H-9 (Zn^{2+})	12.90	0.62	86.48

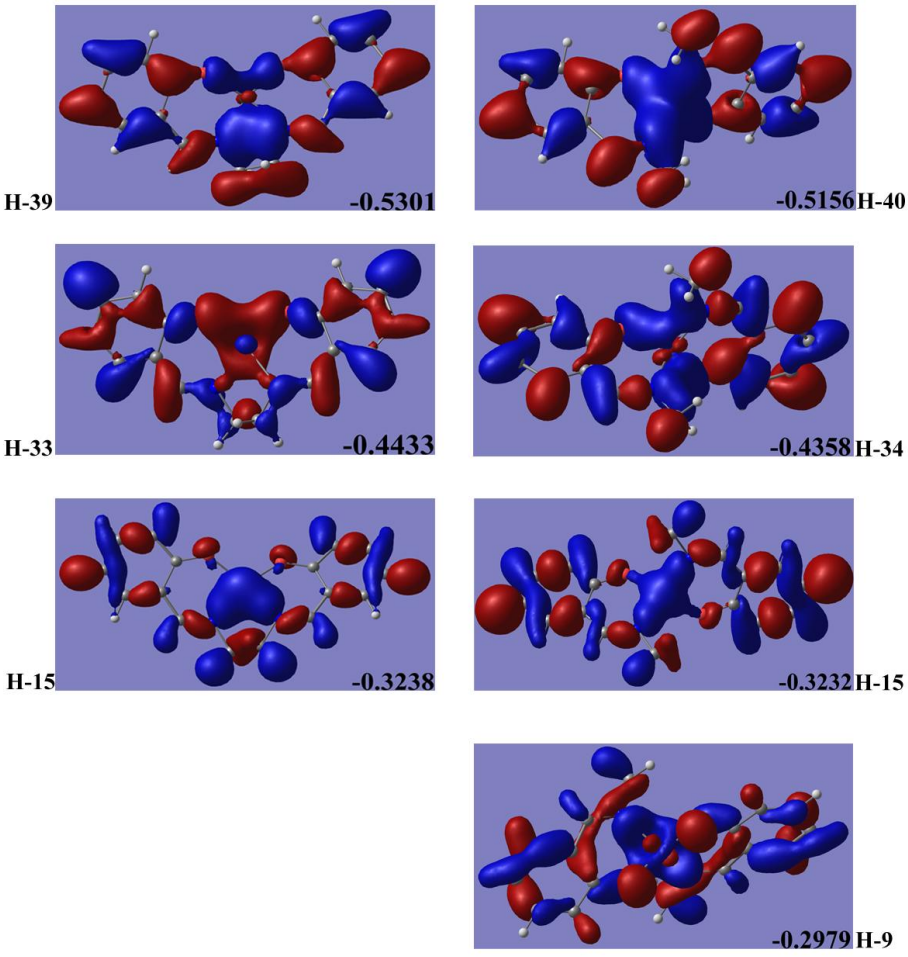


Fig. S1 Main MOs involved in the charge transfer from L^{2-} to Zn^{2+} for Zn(salen) (left) and $Zn(sal)_2$

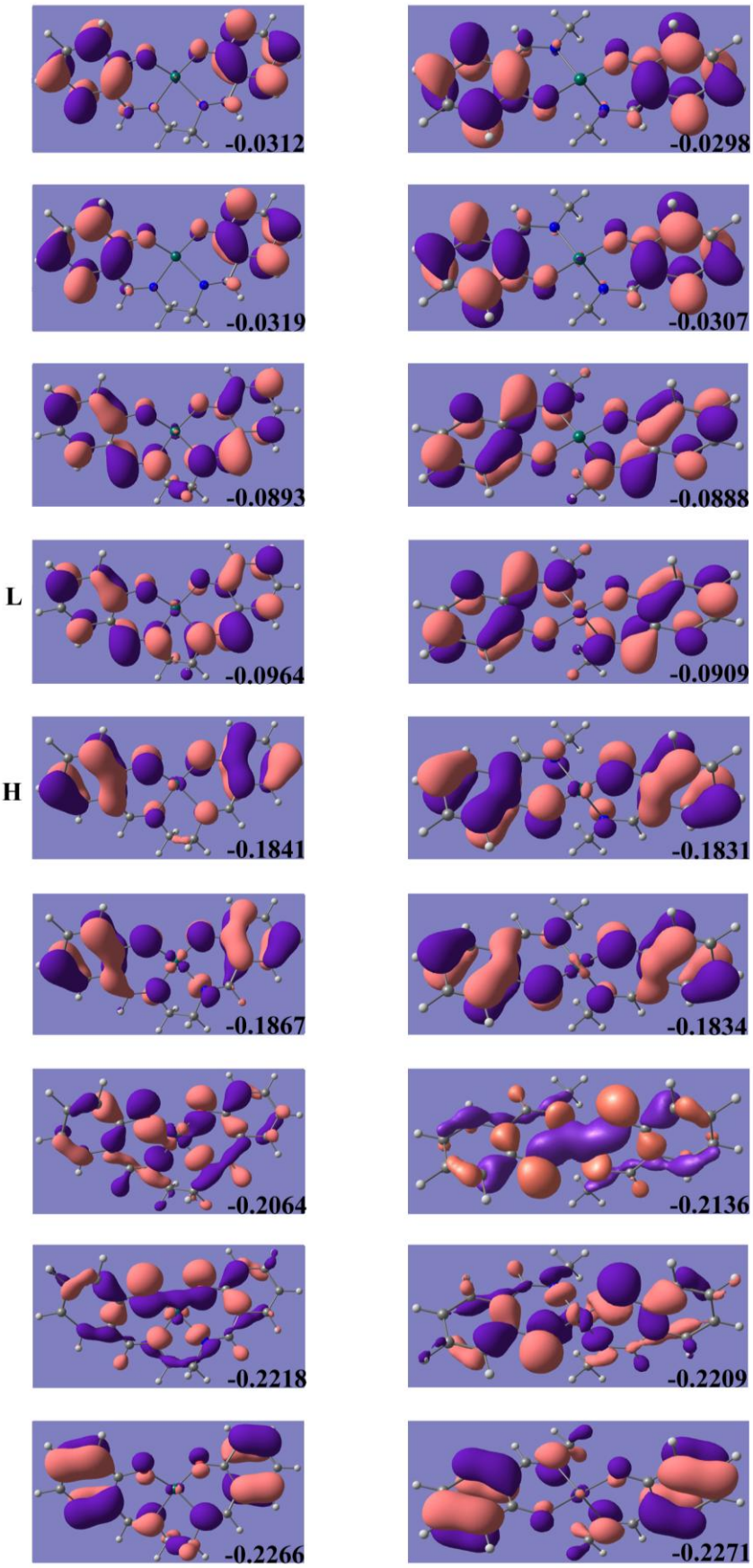
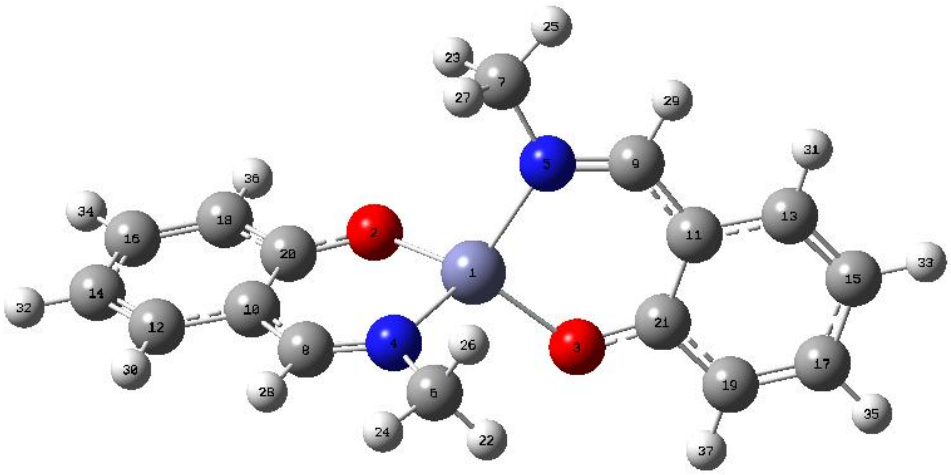


Fig. S2 Frontier MOs and energies (a.u.) for optimized structures of Zn(salen) (left) and $Zn(sal)_2$ (right).

III. Optimised molecular structure for $Zn(sal)_2$ and ZnL complexes

$Zn(sal)_2$



Cartesian Coordinates

		X	Y	Z
1	Zn	0.000	0.000	0.086
2	O	-0.583	-1.634	-0.808
3	O	0.583	1.634	-0.808
4	N	1.550	-0.839	1.075
5	N	-1.550	0.839	1.075
6	C	2.421	-0.021	1.913
7	C	-2.421	0.021	1.913
8	C	1.843	-2.102	0.913
9	C	-1.843	2.102	0.913
10	C	1.156	-3.078	0.113
11	C	-1.156	3.078	0.113
12	C	1.690	-4.398	0.139
13	C	-1.690	4.398	0.139
14	C	1.133	-5.433	-0.591
15	C	-1.133	5.433	-0.591
16	C	0.000	-5.163	-1.391
17	C	0.000	5.163	-1.391
18	C	-0.549	-3.893	-1.450
19	C	0.549	3.893	-1.450
20	C	-0.006	-2.801	-0.707
21	C	0.006	2.801	-0.707
22	H	2.820	0.818	1.322
23	H	-2.820	-0.818	1.322
24	H	3.262	-0.606	2.325
25	H	-3.262	0.606	2.325
26	H	1.844	0.409	2.748
27	H	-1.844	-0.409	2.748
28	H	2.732	-2.485	1.448
29	H	-2.732	2.485	1.448
30	H	2.571	-4.582	0.763
31	H	-2.571	4.582	0.763
32	H	1.562	-6.435	-0.552

33	H	-1.562	6.435	-0.552
34	H	-0.451	-5.969	-1.978
35	H	0.451	5.969	-1.978
36	H	-1.422	-3.679	-2.071
37	H	1.422	3.679	-2.071

Structural parameters

R(1-3)	1.952
R(1-2)	1.952
R(1-5)	2.021
R(1-4)	2.021
R(2-20)	1.306
R(3-21)	1.306
R(4-8)	1.306
R(4-6)	1.459
R(5-7)	1.459
R(5-9)	1.306
R(6-22)	1.102
R(6-24)	1.104
R(6-26)	1.102
R(7-25)	1.104
R(7-27)	1.102
R(7-23)	1.102
R(8-10)	1.437
R(8-28)	1.106
R(9-11)	1.437
R(9-29)	1.106
R(10-12)	1.424
R(10-20)	1.449
R(11-13)	1.424
R(11-21)	1.449
R(12-14)	1.383
R(12-30)	1.095
R(13-15)	1.383
R(13-31)	1.095
R(14-16)	1.414
R(14-32)	1.091
R(15-17)	1.414
R(15-33)	1.091
R(16-18)	1.385
R(16-34)	1.094
R(17-19)	1.385
R(17-35)	1.094
R(18-20)	1.428
R(18-36)	1.092
R(19-21)	1.428
R(19-37)	1.092
A(3-1-2)	125.46
A(3-1-5)	96.08
A(3-1-4)	110.03
A(1-3-21)	125.50
A(2-1-5)	110.03
A(2-1-4)	96.08
A(1-2-20)	125.50
A(5-1-4)	121.42
A(1-5-7)	120.40

A(1-5-9)	120.82
A(1-4-8)	120.82
A(1-4-6)	120.40
A(2-20-10)	124.68
A(2-20-18)	118.40
A(3-21-11)	124.68
A(3-21-19)	118.40
A(8-4-6)	118.65
A(4-8-10)	128.22
A(4-8-28)	117.04
A(4-6-22)	109.55
A(4-6-24)	111.85
A(4-6-26)	110.00
A(7-5-9)	118.65
A(5-7-25)	111.85
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A(5-9-29)	117.04
A(22-6-24)	109.13
A(22-6-26)	107.36
A(24-6-26)	108.85
A(25-7-27)	108.85
A(25-7-23)	109.13
A(27-7-23)	107.36
A(10-8-28)	114.74
A(8-10-12)	116.10
A(8-10-20)	124.65
A(11-9-29)	114.74
A(9-11-13)	116.10
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A(12-10-20)	119.25
A(10-12-14)	122.19
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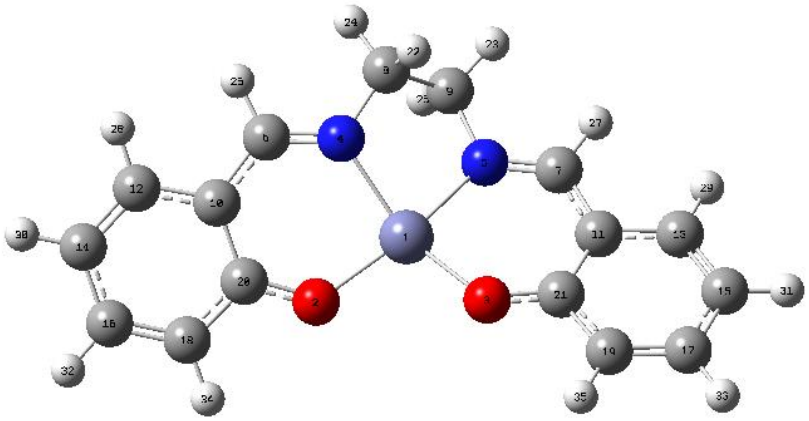
A(16-14-32)	120.66
A(14-16-18)	121.08
A(14-16-34)	119.59
A(17-15-33)	120.66
A(15-17-19)	121.08
A(15-17-35)	119.59
A(18-16-34)	119.33
A(16-18-20)	121.95
A(16-18-36)	121.33
A(19-17-35)	119.33
A(17-19-21)	121.95
A(17-19-37)	121.33
A(20-18-36)	116.73
A(21-19-37)	116.73

Zn(salen)



Cartesian Coordinates

		X	Y	Z
1	Zn	0.000	0.000	0.066
2	O	0.522	-1.475	1.224
3	O	-0.522	1.475	1.224
4	N	-0.403	-1.275	-1.506
5	N	0.403	1.275	-1.506
6	C	-0.294	-2.573	-1.450
7	C	0.294	2.573	-1.450
8	C	-0.516	-0.578	-2.780
9	C	0.516	0.578	-2.780
10	C	0.000	-3.341	-0.275
11	C	0.000	3.341	-0.275
12	C	-0.054	-4.758	-0.404
13	C	0.054	4.758	-0.404
14	C	0.258	-5.603	0.645
15	C	-0.258	5.603	0.645
16	C	0.663	-5.035	1.875
17	C	-0.663	5.035	1.875
18	C	0.749	-3.663	2.037
19	C	-0.749	3.663	2.037
20	C	0.416	-2.755	0.986
21	C	-0.416	2.755	0.986
22	H	-1.529	-0.148	-2.872
23	H	0.344	1.251	-3.640
24	H	-0.344	-1.251	-3.640
25	H	1.529	0.148	-2.872
26	H	-0.412	-3.152	-2.386
27	H	0.412	3.152	-2.386
28	H	-0.359	-5.174	-1.370
29	H	0.359	5.174	-1.370
30	H	0.201	-6.686	0.525
31	H	-0.201	6.686	0.525
32	H	0.917	-5.690	2.714
33	H	-0.917	5.690	2.714
34	H	1.066	-3.221	2.984
35	H	-1.066	3.221	2.984

Structural parameters

R(1-5)	2.063
R(1-4)	2.063
R(1-3)	1.947
R(1-2)	1.947
R(2-20)	1.307
R(3-21)	1.307
R(4-8)	1.457
R(4-6)	1.304
R(5-7)	1.304
R(5-9)	1.457
R(6-10)	1.435
R(6-26)	1.107
R(7-11)	1.435
R(7-27)	1.107
R(8-9)	1.550
R(8-24)	1.105
R(8-22)	1.105
R(9-25)	1.105
R(9-23)	1.105
R(10-20)	1.451
R(10-12)	1.423
R(11-21)	1.451
R(11-13)	1.423
R(12-14)	1.383
R(12-28)	1.095
R(13-15)	1.383
R(13-29)	1.095
R(14-16)	1.414
R(14-30)	1.091
R(15-17)	1.414
R(15-31)	1.091
R(16-18)	1.385
R(16-32)	1.094
R(17-19)	1.385
R(17-33)	1.094
R(18-20)	1.428
R(18-34)	1.092
R(19-21)	1.428
R(19-35)	1.092
A(5-1-4)	80.78
A(5-1-3)	92.16
A(5-1-2)	150.33
A(1-5-7)	124.48
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A(4-1-3)	150.33
A(4-1-2)	92.16
A(1-4-8)	112.71
A(1-4-6)	124.48
A(3-1-2)	106.96
A(1-3-21)	127.73
A(1-2-20)	127.73
A(2-20-10)	125.29
A(2-20-18)	118.00
A(3-21-11)	125.29
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A(8-4-6)	121.33
A(4-8-9)	107.78
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A(7-5-9)	121.33
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A(5-7-27)	118.40
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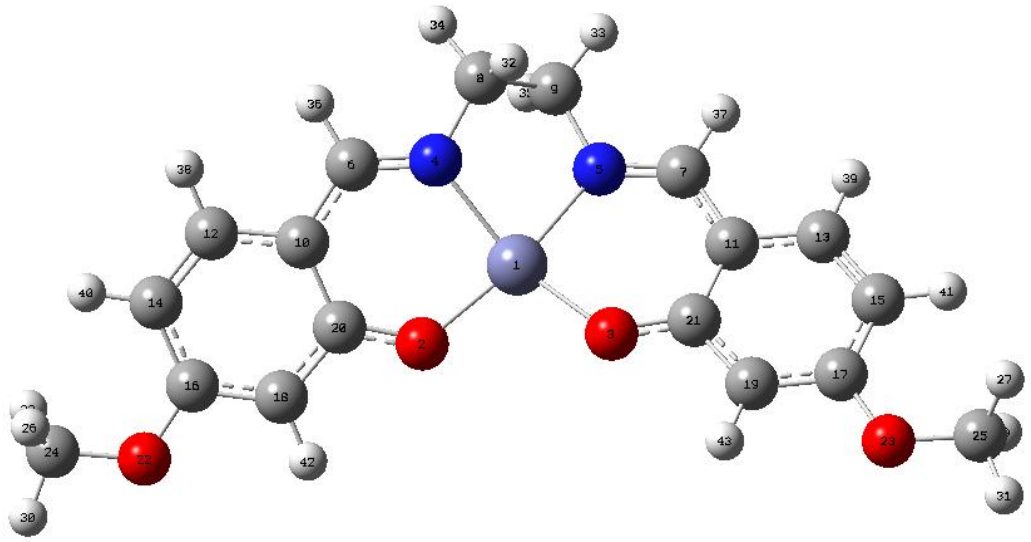
A(17-19-35)	121.36
A(20-18-34)	116.65
A(21-19-35)	116.65

Complex 1



Cartesian Coordinates

		X	Y	Z
1	Zn	0.000	0.000	0.397
2	O	-0.455	-1.497	-0.762
3	O	0.455	1.497	-0.762
4	N	0.479	-1.248	1.967
5	N	-0.479	1.248	1.967
6	C	0.425	-2.551	1.912
7	C	-0.425	2.551	1.912
8	C	0.550	-0.547	3.241
9	C	-0.550	0.547	3.241
10	C	0.162	-3.330	0.741
11	C	-0.162	3.330	0.741
12	C	0.274	-4.739	0.866
13	C	-0.274	4.739	0.866
14	C	0.000	-5.612	-0.173
15	C	0.000	5.612	-0.173
16	C	-0.433	-5.064	-1.409
17	C	0.433	5.064	-1.409
18	C	-0.579	-3.688	-1.568
19	C	0.579	3.688	-1.568
20	C	-0.287	-2.772	-0.527
21	C	0.287	2.772	-0.527
22	O	-0.739	-5.823	-2.504
23	O	0.739	5.823	-2.504
24	C	-0.604	-7.241	-2.405
25	C	0.604	7.241	-2.405
26	H	0.438	-7.535	-2.191
27	H	1.272	7.659	-1.632
28	H	-1.272	-7.659	-1.632
29	H	-0.438	7.535	-2.191
30	H	-0.896	-7.634	-3.387
31	H	0.896	7.634	-3.387
32	H	1.535	-0.055	3.335

33	H	-0.418	1.229	4.101
34	H	0.418	-1.229	4.101
35	H	-1.535	0.055	3.335
36	H	0.571	-3.123	2.849
37	H	-0.571	3.123	2.849
38	H	0.598	-5.146	1.829
39	H	-0.598	5.146	1.829
40	H	0.109	-6.686	-0.030
41	H	-0.109	6.686	-0.030
42	H	-0.919	-3.288	-2.525
43	H	0.919	3.288	-2.525

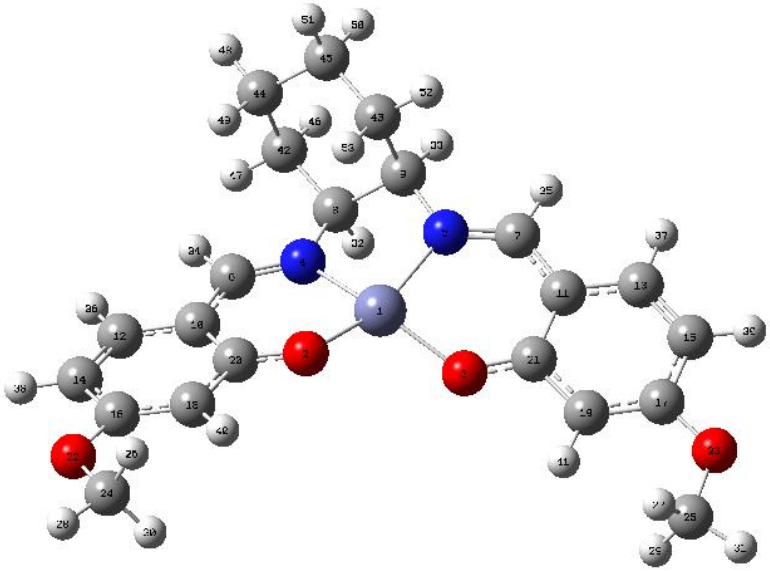
Structural parameters

R(1-2)	1.947
R(1-5)	2.062
R(1-4)	2.062
R(1-3)	1.947
R(2-20)	1.307
R(3-21)	1.307
R(4-8)	1.456
R(4-6)	1.306
R(5-7)	1.306
R(5-9)	1.456
R(6-10)	1.431
R(6-36)	1.107
R(7-11)	1.431
R(7-37)	1.107
R(8-9)	1.551
R(8-34)	1.106
R(8-32)	1.105
R(9-35)	1.105
R(9-33)	1.106
R(10-20)	1.457
R(10-12)	1.419
R(11-21)	1.457
R(11-13)	1.419
R(12-14)	1.384
R(12-38)	1.095
R(13-15)	1.384
R(13-39)	1.095
R(14-16)	1.420
R(14-40)	1.089
R(15-17)	1.420
R(15-41)	1.089
R(16-18)	1.393
R(16-22)	1.367
R(17-19)	1.393
R(17-23)	1.367
R(18-20)	1.417
R(18-42)	1.091
R(19-21)	1.417
R(19-43)	1.091
R(22-24)	1.429
R(23-25)	1.429
R(24-30)	1.097
R(24-26)	1.104
R(24-28)	1.104
R(25-31)	1.097

R(25-29)	1.104
R(25-27)	1.104
A(2-1-5)	149.78
A(2-1-4)	92.44
A(2-1-3)	106.94
A(1-2-20)	127.76
A(5-1-4)	80.80
A(5-1-3)	92.44
A(1-5-7)	124.20
A(1-5-9)	112.74
A(4-1-3)	149.78
A(1-4-8)	112.74
A(1-4-6)	124.20
A(1-3-21)	127.76
A(2-20-10)	124.79
A(2-20-18)	118.13
A(3-21-11)	124.79
A(3-21-19)	118.13
A(8-4-6)	121.30
A(4-8-9)	107.77
A(4-8-34)	112.18
A(4-8-32)	109.37
A(4-6-10)	125.87
A(4-6-36)	118.31
A(7-5-9)	121.30
A(5-7-11)	125.87
A(5-7-37)	118.31
A(5-9-8)	107.77
A(5-9-35)	109.37
A(5-9-33)	112.18
A(10-6-36)	115.80
A(6-10-20)	124.05
A(6-10-12)	117.05
A(11-7-37)	115.80
A(7-11-21)	124.05
A(7-11-13)	117.05
A(9-8-34)	110.54
A(9-8-32)	108.58
A(8-9-35)	108.58
A(8-9-33)	110.54
A(34-8-32)	108.35
A(35-9-33)	108.35
A(20-10-12)	118.79
A(10-20-18)	117.07
A(10-12-14)	123.00
A(10-12-38)	117.99
A(21-11-13)	118.79
A(11-21-19)	117.07
A(11-13-15)	123.00
A(11-13-39)	117.99
A(14-12-38)	119.01
A(12-14-16)	118.05
A(12-14-40)	120.24
A(15-13-39)	119.01
A(13-15-17)	118.05
A(13-15-41)	120.24
A(16-14-40)	121.71
A(14-16-18)	120.87
A(14-16-22)	123.44
A(17-15-41)	121.71
A(15-17-19)	120.87

A(15-17-23)	123.44
A(18-16-22)	115.69
A(16-18-20)	122.20
A(16-18-42)	119.67
A(16-22-24)	118.34
A(19-17-23)	115.69
A(17-19-21)	122.20
A(17-19-43)	119.67
A(17-23-25)	118.34
A(20-18-42)	118.13
A(21-19-43)	118.13
A(22-24-30)	105.52
A(22-24-26)	111.54
A(22-24-28)	111.52
A(23-25-31)	105.52
A(23-25-29)	111.54
A(23-25-27)	111.52
A(30-24-26)	109.29
A(30-24-28)	109.29
A(26-24-28)	109.57
A(31-25-29)	109.29
A(31-25-27)	109.29
A(29-25-27)	109.57

Complex 2



Cartesian Coordinates

		X	Y	Z
1	Zn	0.117	0.069	-0.037
2	O	-1.235	-1.229	0.455
3	O	1.683	-1.091	-0.147
4	N	-1.277	1.410	-0.686
5	N	1.254	1.726	0.090
6	C	-2.539	1.120	-0.871
7	C	2.562	1.756	0.074
8	C	-0.696	2.728	-0.980

9	C	0.460	2.945	0.053
10	C	-3.163	-0.128	-0.559
11	C	3.419	0.616	0.042
12	C	-4.544	-0.264	-0.880
13	C	4.824	0.847	0.089
14	C	-5.264	-1.403	-0.604
15	C	5.746	-0.173	0.044
16	C	-4.602	-2.487	0.036
17	C	5.276	-1.511	-0.063
18	C	-3.257	-2.400	0.378
19	C	3.915	-1.788	-0.126
20	C	-2.484	-1.235	0.096
21	C	2.934	-0.752	-0.076
22	O	-5.389	-3.576	0.270
23	O	6.259	-2.457	-0.099
24	C	-4.786	-4.705	0.906
25	C	5.858	-3.824	-0.208
26	H	-4.411	-4.447	1.911
27	H	5.240	-4.131	0.653
28	H	-5.581	-5.455	0.992
29	H	5.297	-4.006	-1.141
30	H	-3.957	-5.111	0.301
31	H	6.788	-4.405	-0.218
32	H	-0.218	2.659	-1.977
33	H	1.074	3.802	-0.291
34	H	-3.213	1.885	-1.295
35	H	3.064	2.742	0.075
36	H	-5.043	0.580	-1.368
37	H	5.172	1.882	0.168
38	H	-6.320	-1.505	-0.854
39	H	6.821	0.006	0.085
40	H	-2.724	-3.213	0.870
41	H	3.528	-2.803	-0.213
42	C	-1.656	3.929	-0.973
43	C	-0.111	3.255	1.450
44	C	-2.206	4.249	0.426
45	C	-1.064	4.458	1.429
46	H	-1.090	4.800	-1.350
47	H	-2.474	3.775	-1.696
48	H	-2.844	5.147	0.377
49	H	-2.852	3.425	0.775
50	H	-0.498	5.369	1.157
51	H	-1.468	4.633	2.440
52	H	0.726	3.422	2.148
53	H	-0.645	2.355	1.805

Structural parameters

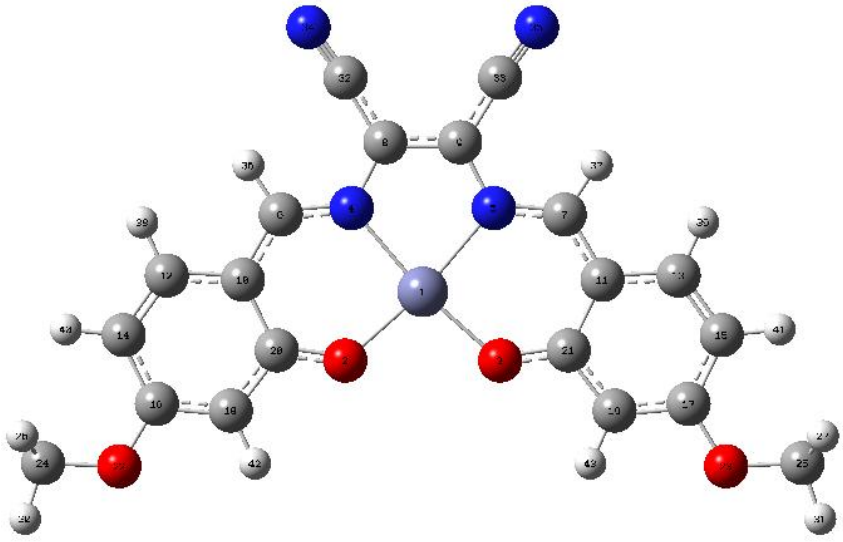
R(1-2)	1.937
R(1-4)	2.040
R(1-5)	2.014
R(1-3)	1.952
R(2-20)	1.300
R(3-21)	1.298
R(4-6)	1.307
R(4-8)	1.471
R(5-9)	1.455
R(5-7)	1.308

R(6-10)	1.430
R(6-34)	1.104
R(7-11)	1.427
R(7-35)	1.107
R(8-9)	1.566
R(8-42)	1.537
R(8-32)	1.108
R(9-43)	1.541
R(9-33)	1.109
R(10-12)	1.425
R(10-20)	1.454
R(11-13)	1.424
R(11-21)	1.456
R(12-14)	1.376
R(12-36)	1.095
R(13-15)	1.376
R(13-37)	1.095
R(14-16)	1.422
R(14-38)	1.090
R(15-17)	1.422
R(15-39)	1.090
R(16-18)	1.390
R(16-22)	1.364
R(17-19)	1.390
R(17-23)	1.365
R(18-20)	1.426
R(18-40)	1.090
R(19-21)	1.427
R(19-41)	1.090
R(22-24)	1.429
R(23-25)	1.429
R(24-28)	1.097
R(24-26)	1.104
R(24-30)	1.103
R(25-31)	1.097
R(25-29)	1.104
R(25-27)	1.104
R(42-44)	1.536
R(42-46)	1.105
R(42-47)	1.103
R(43-45)	1.535
R(43-52)	1.102
R(43-53)	1.105
R(44-45)	1.535
R(44-48)	1.102
R(44-49)	1.104
R(45-50)	1.106
R(45-51)	1.102
A(2-1-4)	92.56
A(2-1-5)	158.34
A(2-1-3)	100.13
A(1-2-20)	127.07
A(4-1-5)	82.24
A(4-1-3)	157.02
A(1-4-6)	123.97
A(1-4-8)	112.52
A(5-1-3)	92.26
A(1-5-9)	112.31
A(1-5-7)	125.61

A(1-3-21)	127.96
A(2-20-10)	124.75
A(2-20-18)	117.98
A(3-21-11)	124.80
A(3-21-19)	118.10
A(6-4-8)	123.46
A(4-6-10)	125.71
A(4-6-34)	119.36
A(4-8-9)	106.49
A(4-8-42)	116.91
A(4-8-32)	107.15
A(9-5-7)	121.76
A(5-9-8)	107.68
A(5-9-43)	110.35
A(5-9-33)	110.68
A(5-7-11)	125.67
A(5-7-35)	118.28
A(10-6-34)	114.93
A(6-10-12)	117.23
A(6-10-20)	123.97
A(11-7-35)	116.04
A(7-11-13)	117.54
A(7-11-21)	123.51
A(9-8-42)	110.48
A(9-8-32)	106.47
A(8-9-43)	110.64
A(8-9-33)	108.12
A(42-8-32)	108.82
A(8-42-44)	112.98
A(8-42-46)	107.11
A(8-42-47)	110.54
A(43-9-33)	109.34
A(9-43-45)	112.06
A(9-43-52)	108.89
A(9-43-53)	107.88
A(12-10-20)	118.77
A(10-12-14)	122.75
A(10-12-36)	117.93
A(10-20-18)	117.26
A(13-11-21)	118.92
A(11-13-15)	122.67
A(11-13-37)	117.97
A(11-21-19)	117.10
A(14-12-36)	119.32
A(12-14-16)	118.56
A(12-14-38)	122.51
A(15-13-37)	119.37
A(13-15-17)	118.57
A(13-15-39)	122.52
A(16-14-38)	118.93
A(14-16-18)	120.88
A(14-16-22)	114.63
A(17-15-39)	118.91
A(15-17-19)	120.96
A(15-17-23)	114.58
A(18-16-22)	124.48
A(16-18-20)	121.77
A(16-18-40)	122.47
A(16-22-24)	117.60

A(19-17-23)	124.46
A(17-19-21)	121.78
A(17-19-41)	122.45
A(17-23-25)	117.59
A(20-18-40)	115.76
A(21-19-41)	115.77
A(22-24-28)	105.65
A(22-24-26)	111.41
A(22-24-30)	111.36
A(23-25-31)	105.66
A(23-25-29)	111.37
A(23-25-27)	111.36
A(28-24-26)	109.56
A(28-24-30)	109.57
A(26-24-30)	109.23
A(31-25-29)	109.58
A(31-25-27)	109.58
A(29-25-27)	109.22
A(44-42-46)	109.25
A(44-42-47)	111.15
A(42-44-45)	110.95
A(42-44-48)	109.67
A(42-44-49)	109.99
A(46-42-47)	105.45
A(45-43-52)	111.13
A(45-43-53)	110.00
A(43-45-44)	111.34
A(43-45-50)	109.35
A(43-45-51)	109.86
A(52-43-53)	106.67
A(45-44-48)	110.39
A(45-44-49)	109.27
A(44-45-50)	109.35
A(44-45-51)	110.39
A(48-44-49)	106.48
A(50-45-51)	106.42

Complex 3



Cartesian coordinate

		X	Y	Z
1	Zn	0.000	0.040	-0.001
2	O	-1.449	-1.246	-0.001
3	O	1.449	-1.246	0.000
4	N	-1.331	1.608	0.000
5	N	1.331	1.608	0.000
6	C	-2.656	1.488	0.000
7	C	2.656	1.488	-0.001
8	C	-0.700	2.839	0.000
9	C	0.700	2.839	0.000
10	C	-3.363	0.267	-0.001
11	C	3.364	0.267	-0.001
12	C	-4.788	0.345	0.000
13	C	4.789	0.345	-0.001
14	C	-5.594	-0.771	0.000
15	C	5.594	-0.771	0.000
16	C	-4.975	-2.057	0.000
17	C	4.975	-2.057	0.000
18	C	-3.590	-2.183	0.000
19	C	3.590	-2.183	0.001
20	C	-2.730	-1.055	-0.001
21	C	2.730	-1.055	0.000
22	O	-5.676	-3.223	0.001
23	O	5.676	-3.223	0.001
24	C	-7.106	-3.165	0.001
25	C	7.106	-3.165	0.001
26	H	-7.490	-2.659	0.903
27	H	7.490	-2.659	0.902
28	H	-7.490	-2.659	-0.901
29	H	7.490	-2.660	-0.902
30	H	-7.439	-4.209	0.001
31	H	7.439	-4.209	0.001
32	C	-1.448	4.049	0.001
33	C	1.449	4.049	0.001

34	N	-2.137	4.996	0.001
35	N	2.137	4.996	0.001
36	H	-3.261	2.410	0.000
37	H	3.261	2.410	-0.001
38	H	-5.247	1.338	0.000
39	H	5.247	1.338	-0.001
40	H	-6.678	-0.663	0.000
41	H	6.678	-0.664	-0.001
42	H	-3.138	-3.175	0.000
43	H	3.138	-3.175	0.001

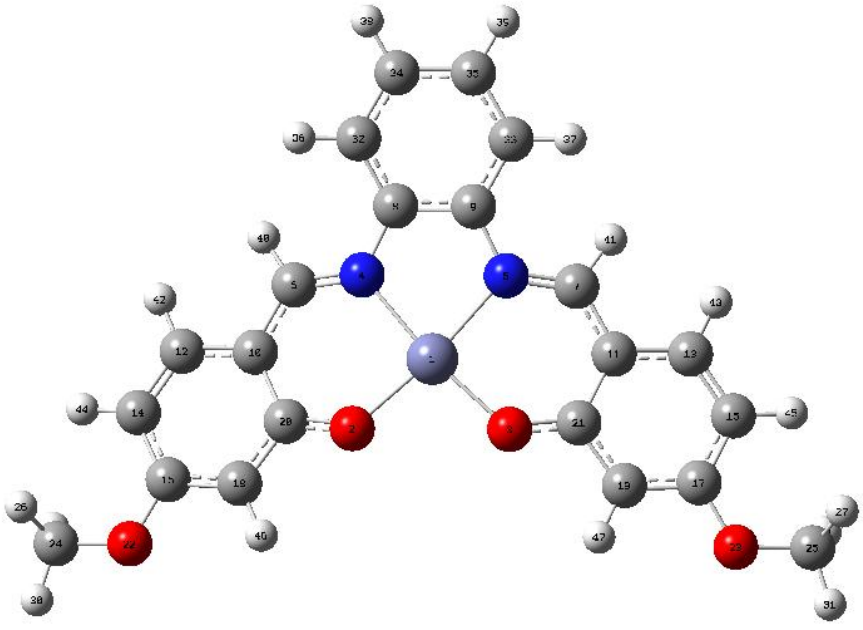
Structural parameters

R(1-2)	1.937
R(1-3)	1.937
R(1-4)	2.057
R(1-5)	2.057
R(2-20)	1.296
R(3-21)	1.296
R(4-6)	1.331
R(4-8)	1.383
R(5-7)	1.331
R(5-9)	1.383
R(6-10)	1.411
R(6-36)	1.102
R(7-11)	1.411
R(7-37)	1.102
R(8-9)	1.400
R(8-32)	1.423
R(9-33)	1.423
R(10-12)	1.427
R(10-20)	1.466
R(11-13)	1.427
R(11-21)	1.466
R(12-14)	1.376
R(12-38)	1.094
R(13-15)	1.376
R(13-39)	1.094
R(14-16)	1.427
R(14-40)	1.089
R(15-17)	1.427
R(15-41)	1.089
R(16-18)	1.391
R(16-22)	1.360
R(17-19)	1.391
R(17-23)	1.360
R(18-20)	1.417
R(18-42)	1.090
R(19-21)	1.418
R(19-43)	1.090
R(22-24)	1.431
R(23-25)	1.431
R(24-28)	1.103
R(24-30)	1.096
R(24-26)	1.103
R(25-31)	1.096
R(25-29)	1.103
R(25-27)	1.103

R(32-34)	1.171
R(33-35)	1.171
A(2-1-3)	96.79
A(2-1-4)	91.29
A(2-1-5)	171.94
A(1-2-20)	129.91
A(3-1-4)	171.92
A(3-1-5)	91.27
A(1-3-21)	129.93
A(4-1-5)	80.66
A(1-4-6)	125.14
A(1-4-8)	112.51
A(1-5-7)	125.15
A(1-5-9)	112.51
A(2-20-10)	124.06
A(2-20-18)	118.85
A(3-21-11)	124.06
A(3-21-19)	118.85
A(6-4-8)	122.35
A(4-6-10)	125.24
A(4-6-36)	118.08
A(4-8-9)	117.17
A(4-8-32)	121.08
A(7-5-9)	122.34
A(5-7-11)	125.24
A(5-7-37)	118.08
A(5-9-8)	117.16
A(5-9-33)	121.09
A(10-6-36)	116.68
A(6-10-12)	116.92
A(6-10-20)	124.35
A(11-7-37)	116.68
A(7-11-13)	116.92
A(7-11-21)	124.34
A(9-8-32)	121.75
A(8-9-33)	121.75
A(8-32-34)	175.73
A(9-33-35)	175.73
A(12-10-20)	118.73
A(10-12-14)	122.69
A(10-12-38)	117.94
A(10-20-18)	117.09
A(13-11-21)	118.73
A(11-13-15)	122.68
A(11-13-39)	117.94
A(11-21-19)	117.09
A(14-12-38)	119.38
A(12-14-16)	118.49
A(12-14-40)	120.16
A(15-13-39)	119.38
A(13-15-17)	118.49
A(13-15-41)	120.16
A(16-14-40)	121.35
A(14-16-18)	120.85
A(14-16-22)	123.32
A(17-15-41)	121.35
A(15-17-19)	120.85
A(15-17-23)	123.32

A(18-16-22)	115.83
A(16-18-20)	122.16
A(16-18-42)	119.67
A(16-22-24)	118.67
A(19-17-23)	115.83
A(17-19-21)	122.16
A(17-19-43)	119.67
A(17-23-25)	118.66
A(20-18-42)	118.17
A(21-19-43)	118.17
A(22-24-28)	111.52
A(22-24-30)	105.35
A(22-24-26)	111.52
A(23-25-31)	105.35
A(23-25-29)	111.52
A(23-25-27)	111.53
A(28-24-30)	109.31
A(28-24-26)	109.72
A(30-24-26)	109.30
A(31-25-29)	109.30
A(31-25-27)	109.31
A(29-25-27)	109.72

Complex 4



Cartesian coordinates

		X	Y	Z
1	Zn	0.061	-0.353	0.000
2	O	-1.217	-0.593	1.445
3	O	-1.217	-0.593	-1.445
4	N	1.589	-0.036	1.323
5	N	1.589	-0.036	-1.323

6	C	1.400	0.262	2.595
7	C	1.400	0.262	-2.595
8	C	2.852	-0.010	0.716
9	C	2.852	-0.010	-0.716
10	C	0.167	0.182	3.295
11	C	0.167	0.182	-3.295
12	C	0.175	0.551	4.669
13	C	0.175	0.551	-4.669
14	C	-0.951	0.501	5.464
15	C	-0.951	0.501	-5.464
16	C	-2.173	0.067	4.876
17	C	-2.173	0.067	-4.876
18	C	-2.231	-0.293	3.534
19	C	-2.231	-0.293	-3.534
20	C	-1.091	-0.249	2.689
21	C	-1.091	-0.249	-2.689
22	O	-3.348	-0.023	5.565
23	O	-3.348	-0.023	-5.565
24	C	-3.353	0.339	6.947
25	C	-3.353	0.339	-6.947
26	H	-2.681	-0.305	7.540
27	H	-2.681	-0.305	-7.540
28	H	-3.072	1.397	7.092
29	H	-3.072	1.397	-7.092
30	H	-4.386	0.191	7.284
31	H	-4.386	0.191	-7.284
32	C	4.081	-0.037	1.401
33	C	4.081	-0.037	-1.401
34	C	5.288	-0.036	0.701
35	C	5.288	-0.036	-0.701
36	H	4.092	-0.086	2.492
37	H	4.092	-0.086	-2.492
38	H	6.231	-0.061	1.250
39	H	6.231	-0.061	-1.250
40	H	2.259	0.620	3.187
41	H	2.259	0.620	-3.187
42	H	1.124	0.878	5.108
43	H	1.124	0.878	-5.108
44	H	-0.895	0.788	6.513
45	H	-0.895	0.788	-6.513
46	H	-3.178	-0.616	3.101
47	H	-3.178	-0.616	-3.101

Structural parameters

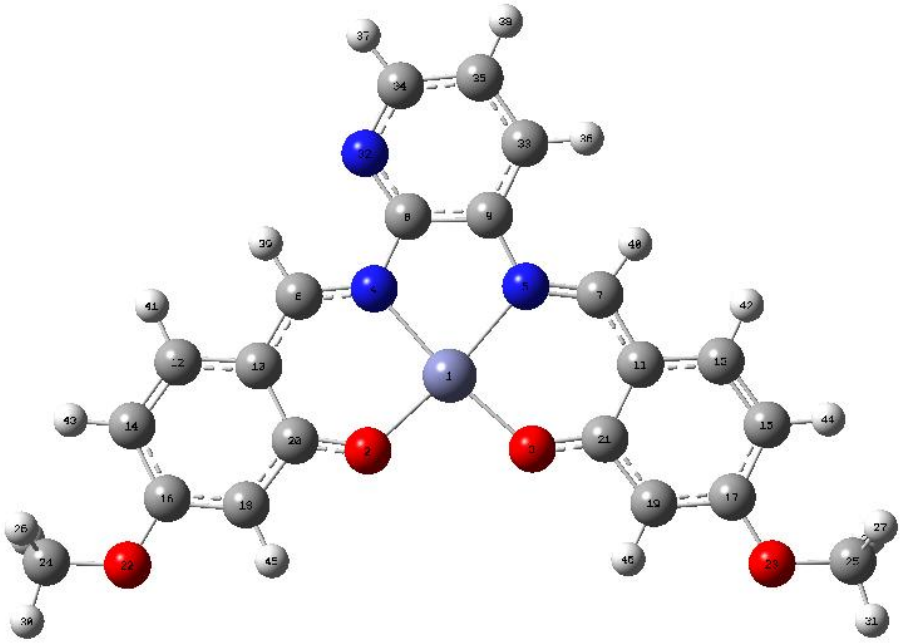
R(1-2)	1.944
R(1-3)	1.944
R(1-4)	2.046
R(1-5)	2.046
R(2-20)	1.297
R(3-21)	1.297
R(4-6)	1.319
R(4-8)	1.401
R(5-9)	1.401
R(5-7)	1.319
R(6-10)	1.420
R(6-40)	1.103
R(7-11)	1.420

R(7-41)	1.103
R(8-9)	1.432
R(8-32)	1.407
R(9-33)	1.407
R(10-20)	1.462
R(10-12)	1.423
R(11-13)	1.423
R(11-21)	1.462
R(12-14)	1.380
R(12-42)	1.095
R(13-15)	1.380
R(13-43)	1.095
R(14-16)	1.424
R(14-44)	1.089
R(15-17)	1.424
R(15-45)	1.089
R(16-18)	1.391
R(16-22)	1.364
R(17-19)	1.391
R(17-23)	1.364
R(18-20)	1.419
R(18-46)	1.091
R(19-21)	1.419
R(19-47)	1.091
R(22-24)	1.429
R(23-25)	1.429
R(24-28)	1.104
R(24-30)	1.097
R(24-26)	1.104
R(25-31)	1.097
R(25-29)	1.104
R(25-27)	1.104
R(32-34)	1.395
R(32-36)	1.092
R(33-35)	1.395
R(33-37)	1.092
R(34-35)	1.402
R(34-38)	1.092
R(35-39)	1.092
A(2-1-3)	96.05
A(2-1-4)	91.68
A(2-1-5)	172.23
A(1-2-20)	128.08
A(3-1-4)	172.23
A(3-1-5)	91.68
A(1-3-21)	128.08
A(4-1-5)	80.58
A(1-4-6)	123.43
A(1-4-8)	113.30
A(1-5-9)	113.30
A(1-5-7)	123.43
A(2-20-10)	124.01
A(2-20-18)	119.00
A(3-21-11)	124.01
A(3-21-19)	119.00
A(6-4-8)	122.87
A(4-6-10)	125.96
A(4-6-40)	118.60

A(4-8-9)	115.67
A(4-8-32)	125.16
A(9-5-7)	122.87
A(5-9-8)	115.67
A(5-9-33)	125.16
A(5-7-11)	125.96
A(5-7-41)	118.60
A(10-6-40)	115.43
A(6-10-20)	124.01
A(6-10-12)	117.20
A(11-7-41)	115.43
A(7-11-13)	117.20
A(7-11-21)	124.01
A(9-8-32)	119.12
A(8-9-33)	119.12
A(8-32-34)	120.76
A(8-32-36)	119.75
A(9-33-35)	120.76
A(9-33-37)	119.75
A(20-10-12)	118.79
A(10-20-18)	116.98
A(10-12-14)	122.87
A(10-12-42)	117.96
A(13-11-21)	118.79
A(11-13-15)	122.87
A(11-13-43)	117.96
A(11-21-19)	116.98
A(14-12-42)	119.16
A(12-14-16)	118.27
A(12-14-44)	120.25
A(15-13-43)	119.16
A(13-15-17)	118.27
A(13-15-45)	120.25
A(16-14-44)	121.48
A(14-16-18)	120.85
A(14-16-22)	123.37
A(17-15-45)	121.48
A(15-17-19)	120.85
A(15-17-23)	123.37
A(18-16-22)	115.78
A(16-18-20)	122.23
A(16-18-46)	119.66
A(16-22-24)	118.38
A(19-17-23)	115.78
A(17-19-21)	122.23
A(17-19-47)	119.66
A(17-23-25)	118.38
A(20-18-46)	118.11
A(21-19-47)	118.11
A(22-24-28)	111.63
A(22-24-30)	105.48
A(22-24-26)	111.65
A(23-25-31)	105.48
A(23-25-29)	111.63
A(23-25-27)	111.65
A(28-24-30)	109.25
A(28-24-26)	109.49
A(30-24-26)	109.24

A(31-25-29)	109.25
A(31-25-27)	109.24
A(29-25-27)	109.49
A(34-32-36)	119.47
A(32-34-35)	120.11
A(32-34-38)	119.71
A(35-33-37)	119.47
A(33-35-34)	120.11
A(33-35-39)	119.71
A(35-34-38)	120.17
A(34-35-39)	120.17

Complex 5



Cartesian coordinates

		X	Y	Z
1	Zn	-0.010	0.009	-0.130
2	O	1.423	-1.315	-0.184
3	O	-1.459	-1.278	-0.244
4	N	1.316	1.536	0.008
5	N	-1.342	1.582	-0.049
6	C	2.632	1.404	0.087
7	C	-2.649	1.443	0.082
8	C	0.727	2.805	0.014
9	C	-0.707	2.830	-0.029
10	C	3.337	0.178	0.062
11	C	-3.362	0.217	0.054
12	C	4.755	0.244	0.175
13	C	-4.776	0.286	0.206
14	C	5.560	-0.875	0.162
15	C	-5.585	-0.830	0.195
16	C	4.939	-2.152	0.029

17	C	-4.974	-2.106	0.027
18	C	3.558	-2.266	-0.084
19	C	-3.595	-2.223	-0.118
20	C	2.701	-1.135	-0.073
21	C	-2.735	-1.094	-0.109
22	O	5.636	-3.324	0.005
23	O	-5.674	-3.276	0.000
24	C	7.060	-3.272	0.119
25	C	-7.094	-3.221	0.151
26	H	7.515	-2.710	-0.715
27	H	-7.568	-2.645	-0.663
28	H	7.374	-2.826	1.078
29	H	-7.384	-2.790	1.125
30	H	7.394	-4.315	0.078
31	H	-7.434	-4.263	0.101
32	N	1.481	3.912	0.044
33	C	-1.321	4.091	-0.067
34	C	0.861	5.100	0.028
35	C	-0.531	5.241	-0.034
36	H	-2.408	4.180	-0.133
37	H	1.511	5.981	0.056
38	H	-0.984	6.234	-0.064
39	H	3.218	2.332	0.178
40	H	-3.268	2.342	0.238
41	H	5.213	1.233	0.275
42	H	-5.231	1.274	0.333
43	H	6.640	-0.775	0.251
44	H	-6.663	-0.728	0.312
45	H	3.105	-3.253	-0.185
46	H	-3.147	-3.209	-0.241

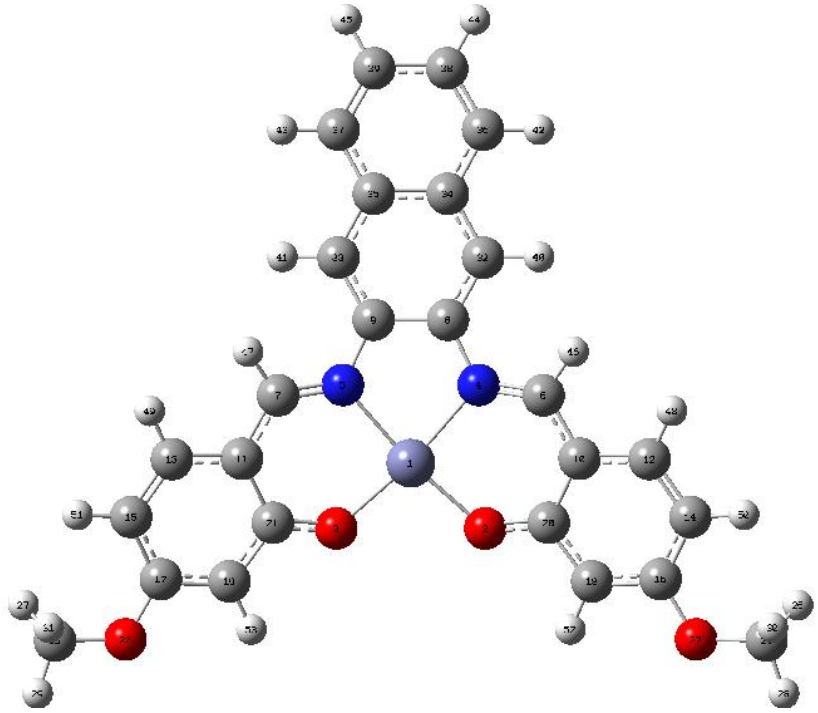
Structural parameters

R(1-2)	1.951
R(1-3)	1.942
R(1-4)	2.027
R(1-5)	2.063
R(2-20)	1.295
R(3-21)	1.296
R(4-6)	1.325
R(4-8)	1.399
R(5-9)	1.400
R(5-7)	1.321
R(6-10)	1.415
R(6-39)	1.101
R(7-11)	1.418
R(7-40)	1.103
R(8-9)	1.434
R(8-32)	1.340
R(9-33)	1.404
R(10-20)	1.464
R(10-12)	1.425
R(11-13)	1.424
R(11-21)	1.463
R(12-14)	1.378
R(12-41)	1.094
R(13-15)	1.379
R(13-42)	1.095

R(14-16)	1.425
R(14-43)	1.089
R(15-17)	1.425
R(15-44)	1.089
R(16-18)	1.391
R(16-22)	1.364
R(17-19)	1.391
R(17-23)	1.364
R(18-20)	1.420
R(18-45)	1.091
R(19-21)	1.419
R(19-46)	1.091
R(22-24)	1.429
R(23-25)	1.429
R(24-28)	1.104
R(24-30)	1.097
R(24-26)	1.104
R(25-31)	1.097
R(25-29)	1.104
R(25-27)	1.104
R(32-34)	1.340
R(33-35)	1.396
R(33-36)	1.092
R(34-35)	1.400
R(34-37)	1.095
R(35-38)	1.092
A(2-1-3)	95.56
A(2-1-4)	91.88
A(2-1-5)	172.97
A(1-2-20)	128.86
A(3-1-4)	172.56
A(3-1-5)	91.46
A(1-3-21)	129.38
A(4-1-5)	81.10
A(1-4-6)	125.38
A(1-4-8)	114.06
A(1-5-9)	112.76
A(1-5-7)	124.23
A(2-20-10)	124.13
A(2-20-18)	118.92
A(3-21-11)	124.14
A(3-21-19)	118.89
A(6-4-8)	120.55
A(4-6-10)	125.42
A(4-6-39)	116.74
A(4-8-9)	115.90
A(4-8-32)	120.82
A(9-5-7)	122.79
A(5-9-8)	116.01
A(5-9-33)	126.99
A(5-7-11)	125.92
A(5-7-40)	118.94
A(10-6-39)	117.83
A(6-10-20)	124.22
A(6-10-12)	116.99
A(11-7-40)	115.14
A(7-11-13)	117.11
A(7-11-21)	124.14

A(9-8-32)	123.28
A(8-9-33)	117.00
A(8-32-34)	118.18
A(9-33-35)	119.45
A(9-33-36)	120.69
A(20-10-12)	118.79
A(10-20-18)	116.95
A(10-12-14)	122.83
A(10-12-41)	117.80
A(13-11-21)	118.75
A(11-13-15)	122.89
A(11-13-42)	117.96
A(11-21-19)	116.97
A(14-12-41)	119.37
A(12-14-16)	118.31
A(12-14-43)	120.25
A(15-13-42)	119.15
A(13-15-17)	118.29
A(13-15-44)	120.25
A(16-14-43)	121.44
A(14-16-18)	120.92
A(14-16-22)	123.30
A(17-15-44)	121.47
A(15-17-19)	120.84
A(15-17-23)	123.34
A(18-16-22)	115.78
A(16-18-20)	122.20
A(16-18-45)	119.66
A(16-22-24)	118.43
A(19-17-23)	115.82
A(17-19-21)	122.25
A(17-19-46)	119.67
A(17-23-25)	118.42
A(20-18-45)	118.14
A(21-19-46)	118.08
A(22-24-28)	111.62
A(22-24-30)	105.45
A(22-24-26)	111.64
A(23-25-31)	105.45
A(23-25-29)	111.61
A(23-25-27)	111.63
A(28-24-30)	109.26
A(28-24-26)	109.53
A(30-24-26)	109.24
A(31-25-29)	109.25
A(31-25-27)	109.24
A(29-25-27)	109.55
A(32-34-35)	123.32
A(32-34-37)	116.03
A(35-33-36)	119.86
A(33-35-34)	118.75
A(33-35-38)	120.85
A(35-34-37)	120.65
A(34-35-38)	120.40

Complex 6



Cartesian coordinates

		X	Y	Z
1	Zn	0.000	-0.679	-0.381
2	O	1.448	-1.948	-0.649
3	O	-1.448	-1.948	-0.649
4	N	1.321	0.841	-0.025
5	N	-1.321	0.841	-0.025
6	C	2.584	0.640	0.301
7	C	-2.584	0.640	0.301
8	C	0.725	2.109	0.007
9	C	-0.725	2.109	0.007
10	C	3.283	-0.592	0.207
11	C	-3.283	-0.592	0.207
12	C	4.647	-0.599	0.612
13	C	-4.647	-0.599	0.612
14	C	5.440	-1.726	0.549
15	C	-5.440	-1.726	0.549
16	C	4.861	-2.933	0.065
17	C	-4.860	-2.933	0.065
18	C	3.527	-2.976	-0.330
19	C	-3.527	-2.976	-0.330
20	C	2.684	-1.836	-0.273
21	C	-2.684	-1.837	-0.273
22	O	5.549	-4.105	-0.043
23	O	-5.549	-4.106	-0.043
24	C	6.922	-4.126	0.353
25	C	-6.922	-4.127	0.353
26	H	7.532	-3.437	-0.257
27	H	-7.531	-3.438	-0.257
28	H	7.260	-5.156	0.182
29	H	-7.259	-5.156	0.181

30	H	7.041	-3.877	1.421
31	H	-7.041	-3.878	1.421
32	C	1.406	3.319	-0.018
33	C	-1.407	3.319	-0.018
34	C	0.720	4.560	-0.012
35	C	-0.721	4.560	-0.012
36	C	1.406	5.806	-0.028
37	C	-1.407	5.806	-0.028
38	C	0.709	7.000	-0.037
39	C	-0.710	7.000	-0.037
40	H	2.498	3.332	-0.072
41	H	-2.498	3.332	-0.072
42	H	2.499	5.805	-0.031
43	H	-2.500	5.804	-0.031
44	H	1.249	7.949	-0.046
45	H	-1.250	7.949	-0.046
46	H	3.167	1.490	0.696
47	H	-3.167	1.489	0.696
48	H	5.079	0.339	0.977
49	H	-5.079	0.338	0.977
50	H	6.482	-1.681	0.864
51	H	-6.482	-1.682	0.864
52	H	3.101	-3.913	-0.691
53	H	-3.101	-3.913	-0.691

Structural parameters

R(1-2)	1.945
R(1-3)	1.945
R(1-4)	2.045
R(1-5)	2.045
R(2-20)	1.297
R(3-21)	1.297
R(4-6)	1.320
R(4-8)	1.402
R(5-9)	1.401
R(5-7)	1.320
R(6-10)	1.419
R(6-46)	1.103
R(7-11)	1.419
R(7-47)	1.103
R(8-9)	1.450
R(8-32)	1.389
R(9-33)	1.389
R(10-20)	1.462
R(10-12)	1.423
R(11-13)	1.423
R(11-21)	1.462
R(12-14)	1.379
R(12-48)	1.095
R(13-15)	1.380
R(13-49)	1.095
R(14-16)	1.424
R(14-50)	1.089
R(15-17)	1.424
R(15-51)	1.089
R(16-18)	1.391
R(16-22)	1.364

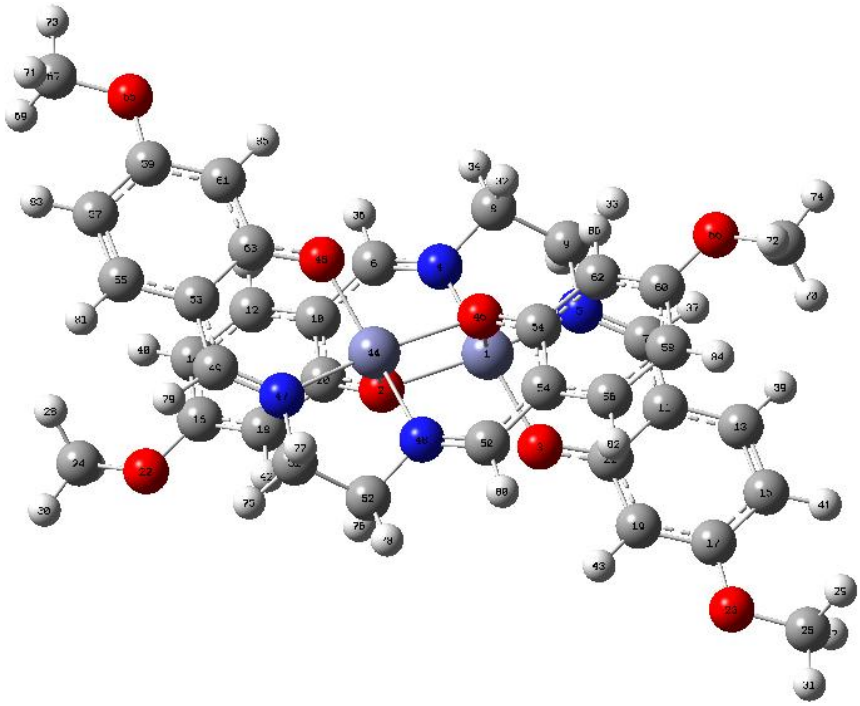
R(17-19)	1.391
R(17-23)	1.364
R(18-20)	1.419
R(18-52)	1.091
R(19-21)	1.419
R(19-53)	1.091
R(22-24)	1.429
R(23-25)	1.429
R(24-30)	1.104
R(24-28)	1.097
R(24-26)	1.104
R(25-29)	1.097
R(25-31)	1.104
R(25-27)	1.104
R(32-34)	1.418
R(32-40)	1.093
R(33-35)	1.418
R(33-41)	1.093
R(34-35)	1.441
R(34-36)	1.423
R(35-37)	1.423
R(36-38)	1.382
R(36-42)	1.094
R(37-43)	1.094
R(37-39)	1.382
R(38-39)	1.418
R(38-44)	1.092
R(39-45)	1.092
A(2-1-3)	96.28
A(2-1-4)	91.61
A(2-1-5)	172.06
A(1-2-20)	127.85
A(3-1-4)	172.05
A(3-1-5)	91.61
A(1-3-21)	127.85
A(4-1-5)	80.48
A(1-4-6)	123.22
A(1-4-8)	113.69
A(1-5-9)	113.69
A(1-5-7)	123.22
A(2-20-10)	123.99
A(2-20-18)	119.03
A(3-21-11)	123.98
A(3-21-19)	119.03
A(6-4-8)	122.62
A(4-6-10)	125.95
A(4-6-46)	118.46
A(4-8-9)	115.16
A(4-8-32)	125.41
A(9-5-7)	122.62
A(5-9-8)	115.16
A(5-9-33)	125.41
A(5-7-11)	125.95
A(5-7-47)	118.45
A(10-6-46)	115.59
A(6-10-20)	123.97
A(6-10-12)	117.23
A(11-7-47)	115.59

A(7-11-13)	117.22
A(7-11-21)	123.98
A(9-8-32)	119.37
A(8-9-33)	119.37
A(8-32-34)	121.68
A(8-32-40)	120.06
A(9-33-35)	121.68
A(9-33-41)	120.07
A(20-10-12)	118.80
A(10-20-18)	116.98
A(10-12-14)	122.85
A(10-12-48)	117.96
A(13-11-21)	118.80
A(11-13-15)	122.84
A(11-13-49)	117.97
A(11-21-19)	116.99
A(14-12-48)	119.19
A(12-14-16)	118.29
A(12-14-50)	120.24
A(15-13-49)	119.18
A(13-15-17)	118.28
A(13-15-51)	120.24
A(16-14-50)	121.47
A(14-16-18)	120.86
A(14-16-22)	123.37
A(17-15-51)	121.48
A(15-17-19)	120.87
A(15-17-23)	123.37
A(18-16-22)	115.77
A(16-18-20)	122.21
A(16-18-52)	119.66
A(16-22-24)	118.41
A(19-17-23)	115.76
A(17-19-21)	122.20
A(17-19-53)	119.67
A(17-23-25)	118.41
A(20-18-52)	118.12
A(21-19-53)	118.13
A(22-24-30)	111.63
A(22-24-28)	105.46
A(22-24-26)	111.64
A(23-25-29)	105.46
A(23-25-31)	111.63
A(23-25-27)	111.64
A(30-24-28)	109.24
A(30-24-26)	109.52
A(28-24-26)	109.24
A(29-25-31)	109.25
A(29-25-27)	109.24
A(31-25-27)	109.51
A(34-32-40)	118.24
A(32-34-35)	118.93
A(32-34-36)	122.24
A(35-33-41)	118.23
A(33-35-34)	118.94
A(33-35-37)	122.24
A(35-34-36)	118.82
A(34-35-37)	118.82

A(34-36-38)	120.90
A(34-36-42)	118.72
A(35-37-43)	118.70
A(35-37-39)	120.90
A(38-36-42)	120.38
A(36-38-39)	120.29
A(36-38-44)	120.05
A(43-37-39)	120.40
A(37-39-38)	120.28
A(37-39-45)	120.05
A(39-38-44)	119.67
A(38-39-45)	119.67

IV. Optimised molecular structure for ZnL dimers

Complex 1D



Cartesian coordinates

		X	Y	Z
1	Zn	0.865	0.389	1.232
2	O	-0.762	1.131	0.208
3	O	2.269	1.460	0.353
4	N	-0.494	-0.291	2.621
5	N	2.163	-0.138	2.736
6	C	-1.702	0.130	2.830
7	C	3.458	0.017	2.692
8	C	0.135	-1.270	3.491
9	C	1.528	-0.743	3.901
10	C	-2.396	1.089	2.011
11	C	4.183	0.704	1.668
12	C	-3.653	1.546	2.461
13	C	5.596	0.728	1.782
14	C	-4.424	2.455	1.749
15	C	6.415	1.390	0.885
16	C	-3.926	2.926	0.514
17	C	5.801	2.082	-0.192
18	C	-2.688	2.488	0.033
19	C	4.417	2.090	-0.340
20	C	-1.901	1.556	0.736
21	C	3.550	1.409	0.557
22	O	-4.585	3.817	-0.286
23	O	6.503	2.778	-1.142
24	C	-5.863	4.283	0.148
25	C	7.924	2.815	-1.031
26	H	-5.794	4.824	1.108

27	H	8.249	3.293	-0.090
28	H	-6.585	3.453	0.246
29	H	8.368	1.806	-1.100
30	H	-6.206	4.973	-0.632
31	H	8.270	3.419	-1.880
32	H	0.256	-2.201	2.909
33	H	2.137	-1.560	4.333
34	H	-0.476	-1.496	4.385
35	H	1.395	0.029	4.682
36	H	-2.261	-0.254	3.705
37	H	4.070	-0.396	3.517
38	H	-4.031	1.164	3.415
39	H	6.050	0.198	2.626
40	H	-5.391	2.773	2.136
41	H	7.496	1.380	1.017
42	H	-2.331	2.859	-0.929
43	H	3.970	2.634	-1.172
44	Zn	-0.865	-0.389	-1.231
45	O	-2.269	-1.460	-0.353
46	O	0.762	-1.131	-0.208
47	N	-2.163	0.138	-2.736
48	N	0.494	0.291	-2.621
49	C	-3.458	-0.017	-2.692
50	C	1.702	-0.130	-2.830
51	C	-1.528	0.743	-3.901
52	C	-0.135	1.270	-3.491
53	C	-4.183	-0.705	-1.668
54	C	2.396	-1.089	-2.011
55	C	-5.596	-0.728	-1.782
56	C	3.653	-1.546	-2.461
57	C	-6.415	-1.390	-0.885
58	C	4.424	-2.455	-1.749
59	C	-5.801	-2.082	0.192
60	C	3.926	-2.926	-0.514
61	C	-4.417	-2.090	0.340
62	C	2.688	-2.488	-0.033
63	C	-3.550	-1.409	-0.557
64	C	1.901	-1.556	-0.736
65	O	-6.503	-2.778	1.142
66	O	4.585	-3.817	0.286
67	C	-7.924	-2.816	1.031
68	C	5.863	-4.283	-0.148
69	H	-8.368	-1.807	1.100
70	H	6.585	-3.453	-0.246
71	H	-8.249	-3.293	0.090
72	H	5.794	-4.823	-1.108
73	H	-8.270	-3.419	1.880
74	H	6.206	-4.973	0.632
75	H	-2.137	1.560	-4.333
76	H	-0.256	2.201	-2.909
77	H	-1.395	-0.029	-4.682
78	H	0.476	1.496	-4.385
79	H	-4.070	0.396	-3.517
80	H	2.261	0.254	-3.705
81	H	-6.050	-0.198	-2.626
82	H	4.031	-1.164	-3.415
83	H	-7.496	-1.380	-1.017
84	H	5.391	-2.773	-2.136

85	H	-3.970	-2.635	1.172
86	H	2.331	-2.859	0.929

Structural parameters

R(1-3)	1.972
R(1-4)	2.059
R(1-5)	2.056
R(2-20)	1.326
R(3-21)	1.298
R(4-6)	1.296
R(4-8)	1.453
R(5-9)	1.459
R(5-7)	1.304
R(6-10)	1.439
R(6-36)	1.107
R(7-11)	1.431
R(7-37)	1.108
R(8-9)	1.545
R(8-32)	1.104
R(8-34)	1.106
R(9-35)	1.107
R(9-33)	1.106
R(10-20)	1.445
R(10-12)	1.412
R(11-13)	1.417
R(11-21)	1.461
R(12-14)	1.388
R(12-38)	1.094
R(13-15)	1.384
R(13-39)	1.095
R(14-16)	1.413
R(14-40)	1.089
R(15-17)	1.420
R(15-41)	1.089
R(16-18)	1.398
R(16-22)	1.367
R(17-19)	1.391
R(17-23)	1.370
R(18-20)	1.408
R(18-42)	1.091
R(19-21)	1.422
R(19-43)	1.091
R(22-24)	1.428
R(23-25)	1.426
R(24-30)	1.097
R(24-28)	1.104
R(24-26)	1.104
R(25-29)	1.104
R(25-31)	1.097
R(25-27)	1.104
R(44-45)	1.972
R(44-48)	2.059
R(44-47)	2.056
R(45-63)	1.298
R(46-64)	1.326
R(47-51)	1.459
R(47-49)	1.304

R(48-50)	1.296
R(48-52)	1.453
R(49-53)	1.431
R(49-79)	1.108
R(50-54)	1.439
R(50-80)	1.107
R(51-52)	1.545
R(51-77)	1.107
R(51-75)	1.106
R(52-76)	1.104
R(52-78)	1.106
R(53-55)	1.417
R(53-63)	1.461
R(54-56)	1.412
R(54-64)	1.445
R(55-57)	1.384
R(55-81)	1.095
R(56-58)	1.388
R(56-82)	1.094
R(57-59)	1.420
R(57-83)	1.089
R(58-60)	1.413
R(58-84)	1.089
R(59-61)	1.391
R(59-65)	1.370
R(60-62)	1.398
R(60-66)	1.367
R(61-63)	1.422
R(61-85)	1.091
R(62-64)	1.408
R(62-86)	1.091
R(65-67)	1.426
R(66-68)	1.427
R(67-73)	1.097
R(67-69)	1.104
R(67-71)	1.104
R(68-70)	1.104
R(68-74)	1.097
R(68-72)	1.104
A(3-1-4)	161.73
A(3-1-5)	90.88
A(1-3-21)	127.68
A(4-1-5)	80.70
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A(1-5-9)	114.55
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A(2-20-10)	122.83
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A(3-21-11)	124.51
A(3-21-19)	118.99
A(6-4-8)	121.74
A(4-6-10)	125.06
A(4-6-36)	119.02
A(4-8-9)	108.61
A(4-8-32)	107.48
A(4-8-34)	112.52
A(9-5-7)	120.56

A(5-9-8)	108.81
A(5-9-35)	109.10
A(5-9-33)	112.21
A(5-7-11)	125.76
A(5-7-37)	118.66
A(10-6-36)	115.92
A(6-10-20)	123.51
A(6-10-12)	117.63
A(11-7-37)	115.57
A(7-11-13)	117.12
A(7-11-21)	123.79
A(9-8-32)	109.17
A(9-8-34)	110.67
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A(8-9-33)	110.38
A(32-8-34)	108.30
A(35-9-33)	107.76
A(20-10-12)	118.79
A(10-20-18)	117.60
A(10-12-14)	122.86
A(10-12-38)	118.17
A(13-11-21)	119.05
A(11-13-15)	123.09
A(11-13-39)	117.89
A(11-21-19)	116.49
A(14-12-38)	118.97
A(12-14-16)	118.14
A(12-14-40)	120.13
A(15-13-39)	119.02
A(13-15-17)	117.96
A(13-15-41)	120.32
A(16-14-40)	121.72
A(14-16-18)	120.54
A(14-16-22)	123.99
A(17-15-41)	121.72
A(15-17-19)	120.88
A(15-17-23)	123.46
A(18-16-22)	115.47
A(16-18-20)	122.02
A(16-18-42)	119.10
A(16-22-24)	117.81
A(19-17-23)	115.66
A(17-19-21)	122.51
A(17-19-43)	119.44
A(17-23-25)	118.06
A(20-18-42)	118.86
A(21-19-43)	118.04
A(22-24-30)	105.61
A(22-24-28)	111.52
A(22-24-26)	111.62
A(23-25-29)	111.80
A(23-25-31)	105.60
A(23-25-27)	111.77
A(30-24-28)	109.34
A(30-24-26)	109.24
A(28-24-26)	109.41
A(29-25-31)	109.16
A(29-25-27)	109.26

A(31-25-27)	109.15
A(45-44-48)	161.72
A(45-44-47)	90.88
A(44-45-63)	127.68
A(48-44-47)	80.70
A(44-48-50)	128.06
A(44-48-52)	109.94
A(44-47-51)	114.55
A(44-47-49)	124.88
A(45-63-53)	124.50
A(45-63-61)	119.00
A(46-64-54)	122.83
A(46-64-62)	119.56
A(51-47-49)	120.56
A(47-51-52)	108.82
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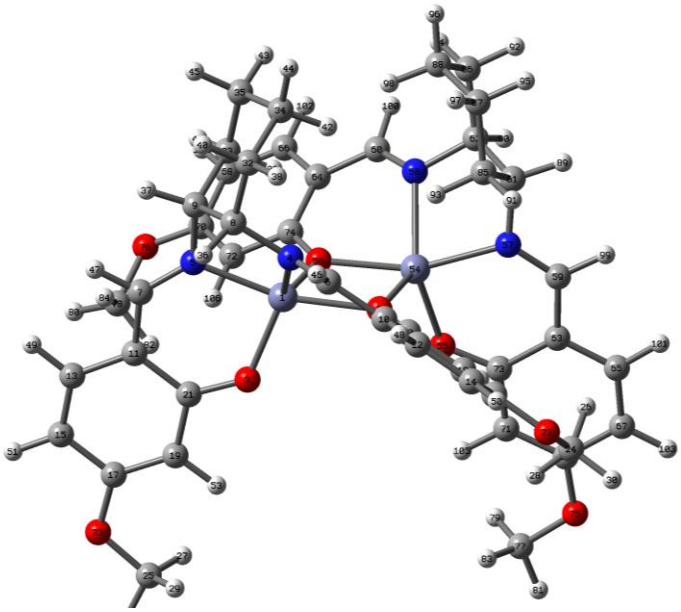
A(47-51-75)	112.22
A(47-49-53)	125.76
A(47-49-79)	118.67
A(50-48-52)	121.73
A(48-50-54)	125.05
A(48-50-80)	119.02
A(48-52-51)	108.61
A(48-52-76)	107.48
A(48-52-78)	112.52
A(53-49-79)	115.57
A(49-53-55)	117.12
A(49-53-63)	123.80
A(54-50-80)	115.92
A(50-54-56)	117.63
A(50-54-64)	123.51
A(52-51-77)	108.49
A(52-51-75)	110.37
A(51-52-76)	109.17
A(51-52-78)	110.67
A(77-51-75)	107.75
A(76-52-78)	108.31
A(55-53-63)	119.05
A(53-55-57)	123.09
A(53-55-81)	117.89
A(53-63-61)	116.50
A(56-54-64)	118.80
A(54-56-58)	122.86
A(54-56-82)	118.17
A(54-64-62)	117.60
A(57-55-81)	119.02
A(55-57-59)	117.96
A(55-57-83)	120.32
A(58-56-82)	118.97
A(56-58-60)	118.14
A(56-58-84)	120.14
A(59-57-83)	121.72
A(57-59-61)	120.88
A(57-59-65)	123.45
A(60-58-84)	121.71
A(58-60-62)	120.54
A(58-60-66)	123.99
A(61-59-65)	115.66

A(59-61-63)	122.52
A(59-61-85)	119.45
A(59-65-67)	118.07
A(62-60-66)	115.47
A(60-62-64)	122.02
A(60-62-86)	119.10
A(60-66-68)	117.81
A(63-61-85)	118.04
A(64-62-86)	118.86
A(65-67-73)	105.60
A(65-67-69)	111.81
A(65-67-71)	111.77
A(66-68-70)	111.52
A(66-68-74)	105.61
A(66-68-72)	111.62
A(73-67-69)	109.16
A(73-67-71)	109.15
A(69-67-71)	109.25
A(70-68-74)	109.34
A(70-68-72)	109.41
A(74-68-72)	109.25

Complex 2D



Cartesian coordinates

		X	Y	Z
1	Zn	1.348	-0.313	0.886
2	O	-0.698	-0.274	1.068
3	O	1.994	1.546	1.121
4	N	1.187	-1.918	2.261
5	N	3.269	-1.008	0.923
6	C	0.337	-1.895	3.250
7	C	4.348	-0.286	1.039

8	C	2.421	-2.718	2.403
9	C	3.285	-2.446	1.132
10	C	-0.883	-1.139	3.304
11	C	4.399	1.145	1.039
12	C	-1.650	-1.178	4.499
13	C	5.682	1.760	1.053
14	C	-2.826	-0.473	4.643
15	C	5.854	3.126	1.096
16	C	-3.285	0.325	3.563
17	C	4.698	3.954	1.155
18	C	-2.567	0.383	2.366
19	C	3.423	3.401	1.166
20	C	-1.362	-0.337	2.210
21	C	3.211	1.987	1.106
22	O	-4.439	1.004	3.799
23	O	4.961	5.293	1.205
24	C	-4.933	1.864	2.762
25	C	3.846	6.181	1.295
26	H	-5.175	1.299	1.847
27	H	3.188	6.093	0.413
28	H	-4.202	2.651	2.513
29	H	3.255	5.994	2.208
30	H	-5.843	2.320	3.168
31	H	4.273	7.191	1.334
32	C	2.171	-4.226	2.598
33	C	2.705	-3.160	-0.105
34	C	1.588	-4.897	1.348
35	C	2.495	-4.661	0.133
36	H	2.991	-2.335	3.271
37	H	4.313	-2.811	1.326
38	H	1.516	-4.383	3.471
39	H	1.737	-2.688	-0.350
40	H	3.138	-4.698	2.850
41	H	3.365	-2.976	-0.967
42	H	0.586	-4.480	1.143
43	H	2.062	-5.124	-0.769
44	H	1.454	-5.976	1.531
45	H	3.470	-5.155	0.301
46	H	0.551	-2.489	4.160
47	H	5.318	-0.806	1.163
48	H	-1.285	-1.790	5.330
49	H	6.564	1.111	1.024
50	H	-3.412	-0.498	5.563
51	H	6.839	3.593	1.106
52	H	-2.895	0.988	1.522
53	H	2.521	4.011	1.219
54	Zn	-1.348	-0.313	-0.886
55	O	-1.994	1.546	-1.121
56	O	0.698	-0.274	-1.068
57	N	-3.269	-1.008	-0.923
58	N	-1.187	-1.918	-2.261
59	C	-4.348	-0.286	-1.039
60	C	-0.337	-1.895	-3.250
61	C	-3.285	-2.446	-1.132
62	C	-2.421	-2.718	-2.403
63	C	-4.399	1.145	-1.039
64	C	0.883	-1.139	-3.304
65	C	-5.682	1.760	-1.053

66	C	1.650	-1.178	-4.499
67	C	-5.854	3.126	-1.096
68	C	2.826	-0.473	-4.643
69	C	-4.698	3.954	-1.155
70	C	3.285	0.325	-3.563
71	C	-3.423	3.401	-1.166
72	C	2.567	0.383	-2.366
73	C	-3.211	1.987	-1.106
74	C	1.362	-0.337	-2.210
75	O	-4.961	5.293	-1.205
76	O	4.439	1.004	-3.799
77	C	-3.846	6.181	-1.295
78	C	4.933	1.864	-2.762
79	H	-3.255	5.994	-2.208
80	H	5.843	2.320	-3.168
81	H	-4.273	7.191	-1.334
82	H	4.202	2.651	-2.513
83	H	-3.188	6.093	-0.413
84	H	5.175	1.299	-1.847
85	C	-2.705	-3.160	0.105
86	C	-2.171	-4.226	-2.598
87	C	-2.495	-4.661	-0.133
88	C	-1.588	-4.897	-1.348
89	H	-4.313	-2.811	-1.326
90	H	-2.991	-2.335	-3.271
91	H	-3.365	-2.976	0.967
92	H	-3.138	-4.698	-2.850
93	H	-1.737	-2.688	0.350
94	H	-1.516	-4.383	-3.471
95	H	-3.470	-5.155	-0.301
96	H	-1.454	-5.976	-1.531
97	H	-2.062	-5.124	0.769
98	H	-0.586	-4.480	-1.143
99	H	-5.318	-0.806	-1.163
100	H	-0.551	-2.489	-4.160
101	H	-6.564	1.111	-1.024
102	H	1.285	-1.790	-5.330
103	H	-6.839	3.593	-1.106
104	H	3.412	-0.498	-5.563
105	H	-2.521	4.011	-1.219
106	H	2.895	0.988	-1.522

Structural parameters

R(1-5)	2.042
R(1-3)	1.982
R(1-2)	2.055
R(1-4)	2.120
R(2-20)	1.322
R(3-21)	1.295
R(4-6)	1.305
R(4-8)	1.477
R(5-9)	1.454
R(5-7)	1.304
R(6-10)	1.436
R(6-46)	1.107
R(7-11)	1.431
R(7-47)	1.108

R(8-9)	1.561
R(8-32)	1.541
R(8-36)	1.107
R(9-33)	1.541
R(9-37)	1.109
R(10-20)	1.439
R(10-12)	1.421
R(11-13)	1.424
R(11-21)	1.458
R(12-14)	1.379
R(12-48)	1.095
R(13-15)	1.377
R(13-49)	1.095
R(14-16)	1.419
R(14-50)	1.091
R(15-17)	1.422
R(15-51)	1.090
R(16-18)	1.397
R(16-22)	1.359
R(17-19)	1.390
R(17-23)	1.366
R(18-20)	1.413
R(18-52)	1.089
R(19-21)	1.430
R(19-53)	1.090
R(22-24)	1.434
R(23-25)	1.428
R(24-30)	1.096
R(24-26)	1.102
R(24-28)	1.103
R(25-31)	1.097
R(25-29)	1.104
R(25-27)	1.104
R(32-34)	1.534
R(32-40)	1.106
R(32-38)	1.103
R(33-35)	1.533
R(33-41)	1.102
R(33-39)	1.104
R(34-35)	1.534
R(34-44)	1.102
R(34-42)	1.104
R(35-45)	1.106
R(35-43)	1.102
R(54-57)	2.042
R(54-55)	1.982
R(54-58)	2.120
R(54-56)	2.055
R(55-73)	1.295
R(56-74)	1.322
R(57-61)	1.454
R(57-59)	1.304
R(58-60)	1.305
R(58-62)	1.477
R(59-63)	1.431
R(59-99)	1.108
R(60-64)	1.436
R(60-100)	1.107

R(61-62)	1.561
R(61-85)	1.541
R(61-89)	1.109
R(62-86)	1.541
R(62-90)	1.107
R(63-65)	1.424
R(63-73)	1.458
R(64-66)	1.421
R(64-74)	1.439
R(65-67)	1.377
R(65-101)	1.095
R(66-68)	1.379
R(66-102)	1.095
R(67-69)	1.422
R(67-103)	1.090
R(68-70)	1.419
R(68-104)	1.091
R(69-71)	1.390
R(69-75)	1.366
R(70-72)	1.397
R(70-76)	1.359
R(71-73)	1.430
R(71-105)	1.090
R(72-74)	1.413
R(72-106)	1.089
R(75-77)	1.428
R(76-78)	1.434
R(77-81)	1.097
R(77-79)	1.104
R(77-83)	1.104
R(78-80)	1.096
R(78-84)	1.102
R(78-82)	1.103
R(85-87)	1.533
R(85-91)	1.102
R(85-93)	1.104
R(86-88)	1.534
R(86-92)	1.106
R(86-94)	1.103
R(87-88)	1.534
R(87-95)	1.106
R(87-97)	1.102
R(88-96)	1.102
R(88-98)	1.104
A(5-1-3)	90.62
A(5-1-2)	160.25
A(5-1-4)	78.59
A(1-5-9)	110.47
A(1-5-7)	126.27
A(3-1-2)	107.21
A(3-1-4)	131.13
A(1-3-21)	128.63
A(2-1-4)	83.17
A(1-2-20)	125.14
A(1-4-6)	121.89
A(1-4-8)	114.12
A(2-20-10)	121.11
A(2-20-18)	119.95

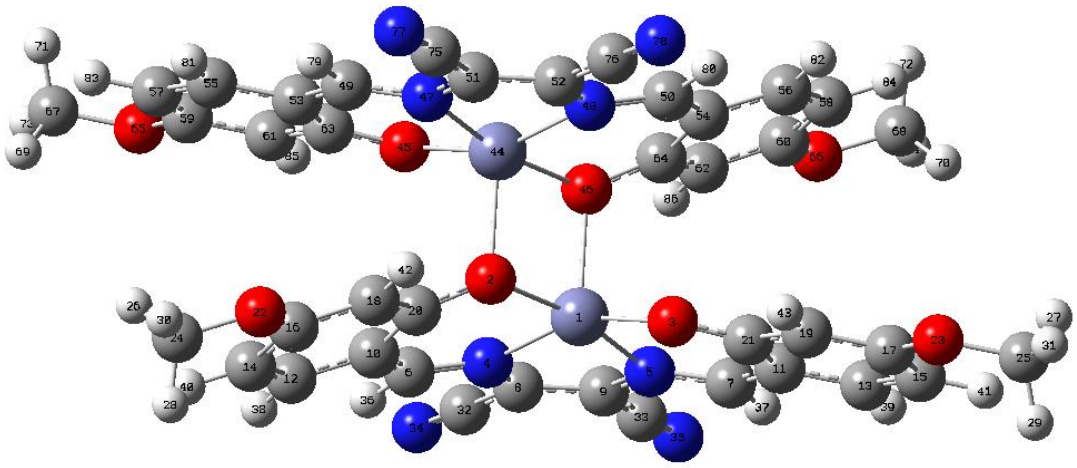
A(3-21-11)	124.71
A(3-21-19)	118.41
A(6-4-8)	118.77
A(4-6-10)	126.24
A(4-6-46)	119.18
A(4-8-9)	106.87
A(4-8-32)	113.99
A(4-8-36)	108.55
A(9-5-7)	121.72
A(5-9-8)	106.44
A(5-9-33)	109.82
A(5-9-37)	111.19
A(5-7-11)	125.63
A(5-7-47)	118.35
A(10-6-46)	114.57
A(6-10-20)	123.22
A(6-10-12)	118.40
A(11-7-47)	116.01
A(7-11-13)	117.64
A(7-11-21)	123.29
A(9-8-32)	111.29
A(9-8-36)	107.02
A(8-9-33)	111.37
A(8-9-37)	108.25
A(32-8-36)	108.85
A(8-32-34)	112.75
A(8-32-40)	107.77
A(8-32-38)	109.62
A(33-9-37)	109.73
A(9-33-35)	112.37
A(9-33-41)	108.97
A(9-33-39)	108.03
A(20-10-12)	118.38
A(10-20-18)	118.94
A(10-12-14)	122.29
A(10-12-48)	118.26
A(13-11-21)	118.96
A(11-13-15)	122.76
A(11-13-49)	117.97
A(11-21-19)	116.88
A(14-12-48)	119.45
A(12-14-16)	118.96
A(12-14-50)	122.27
A(15-13-49)	119.27
A(13-15-17)	118.51
A(13-15-51)	122.51
A(16-14-50)	118.77
A(14-16-18)	120.59
A(14-16-22)	115.06
A(17-15-51)	118.96
A(15-17-19)	120.93
A(15-17-23)	114.57
A(18-16-22)	124.35
A(16-18-20)	120.83
A(16-18-52)	122.14
A(16-22-24)	117.78
A(19-17-23)	124.50
A(17-19-21)	121.93

A(17-19-53)	122.46
A(17-23-25)	117.50
A(20-18-52)	117.02
A(21-19-53)	115.60
A(22-24-30)	105.49
A(22-24-26)	111.64
A(22-24-28)	111.28
A(23-25-31)	105.67
A(23-25-29)	111.37
A(23-25-27)	111.44
A(30-24-26)	109.76
A(30-24-28)	109.68
A(26-24-28)	108.94
A(31-25-29)	109.59
A(31-25-27)	109.55
A(29-25-27)	109.15
A(34-32-40)	109.34
A(34-32-38)	110.96
A(32-34-35)	110.68
A(32-34-44)	109.83
A(32-34-42)	109.33
A(40-32-38)	106.12
A(35-33-41)	111.55
A(35-33-39)	109.45
A(33-35-34)	110.76
A(33-35-45)	109.87
A(33-35-43)	109.75
A(41-33-39)	106.23
A(35-34-44)	110.71
A(35-34-42)	109.33
A(34-35-45)	109.38
A(34-35-43)	110.58
A(44-34-42)	106.88
A(45-35-43)	106.40
A(57-54-55)	90.62
A(57-54-58)	78.59
A(57-54-56)	160.25
A(54-57-61)	110.47
A(54-57-59)	126.27
A(55-54-58)	131.13
A(55-54-56)	107.21
A(54-55-73)	128.63
A(58-54-56)	83.17
A(54-58-60)	121.89
A(54-58-62)	114.12
A(54-56-74)	125.14
A(55-73-63)	124.71
A(55-73-71)	118.41
A(56-74-64)	121.10
A(56-74-72)	119.96
A(61-57-59)	121.72
A(57-61-62)	106.44
A(57-61-85)	109.82
A(57-61-89)	111.19
A(57-59-63)	125.63
A(57-59-99)	118.35
A(60-58-62)	118.77
A(58-60-64)	126.24

A(58-60-100)	119.18
A(58-62-61)	106.87
A(58-62-86)	113.99
A(58-62-90)	108.55
A(63-59-99)	116.02
A(59-63-65)	117.64
A(59-63-73)	123.29
A(64-60-100)	114.57
A(60-64-66)	118.40
A(60-64-74)	123.22
A(62-61-85)	111.37
A(62-61-89)	108.25
A(61-62-86)	111.29
A(61-62-90)	107.02
A(85-61-89)	109.73
A(61-85-87)	112.37
A(61-85-91)	108.97
A(61-85-93)	108.03
A(86-62-90)	108.85
A(62-86-88)	112.76
A(62-86-92)	107.77
A(62-86-94)	109.62
A(65-63-73)	118.96
A(63-65-67)	122.76
A(63-65-101)	117.97
A(63-73-71)	116.88
A(66-64-74)	118.38
A(64-66-68)	122.29
A(64-66-102)	118.26
A(64-74-72)	118.94
A(67-65-101)	119.27
A(65-67-69)	118.51
A(65-67-103)	122.51
A(68-66-102)	119.45
A(66-68-70)	118.96
A(66-68-104)	122.27
A(69-67-103)	118.96
A(67-69-71)	120.93
A(67-69-75)	114.57
A(70-68-104)	118.77
A(68-70-72)	120.59
A(68-70-76)	115.06
A(71-69-75)	124.50
A(69-71-73)	121.93
A(69-71-105)	122.46
A(69-75-77)	117.50
A(72-70-76)	124.35
A(70-72-74)	120.84
A(70-72-106)	122.14
A(70-76-78)	117.78
A(73-71-105)	115.60
A(74-72-106)	117.02
A(75-77-81)	105.67
A(75-77-79)	111.37
A(75-77-83)	111.44
A(76-78-80)	105.49
A(76-78-84)	111.64
A(76-78-82)	111.28

A(81-77-79)	109.59
A(81-77-83)	109.55
A(79-77-83)	109.16
A(80-78-84)	109.76
A(80-78-82)	109.68
A(84-78-82)	108.94
A(87-85-91)	111.55
A(87-85-93)	109.45
A(85-87-88)	110.77
A(85-87-95)	109.87
A(85-87-97)	109.75
A(91-85-93)	106.23
A(88-86-92)	109.34
A(88-86-94)	110.97
A(86-88-87)	110.67
A(86-88-96)	109.83
A(86-88-98)	109.33
A(92-86-94)	106.12
A(88-87-95)	109.39
A(88-87-97)	110.58
A(87-88-96)	110.72
A(87-88-98)	109.33
A(95-87-97)	106.40
A(96-88-98)	106.88

Complex 3D



Cartesian coordinates

		X	Y	Z
1	Zn	-0.937	-0.894	-0.880
2	O	0.744	0.220	-1.108
3	O	-2.275	0.438	-1.427
4	N	0.248	-2.589	-1.051
5	N	-2.394	-2.362	-0.822
6	C	1.506	-2.634	-1.452
7	C	-3.702	-2.146	-0.894
8	C	-0.465	-3.739	-0.745
9	C	-1.852	-3.614	-0.616

10	C	2.279	-1.512	-1.859
11	C	-4.303	-0.900	-1.176
12	C	3.550	-1.783	-2.435
13	C	-5.729	-0.875	-1.229
14	C	4.380	-0.787	-2.914
15	C	-6.445	0.259	-1.542
16	C	3.942	0.559	-2.821
17	C	-5.726	1.456	-1.835
18	C	2.704	0.866	-2.246
19	C	-4.336	1.481	-1.798
20	C	1.863	-0.130	-1.724
21	C	-3.565	0.337	-1.463
22	O	4.662	1.623	-3.260
23	O	-6.331	2.630	-2.163
24	C	5.941	1.382	-3.856
25	C	-7.760	2.669	-2.229
26	H	6.633	0.907	-3.142
27	H	-8.218	2.432	-1.254
28	H	5.851	0.757	-4.761
29	H	-8.148	1.980	-2.998
30	H	6.324	2.372	-4.133
31	H	-8.010	3.700	-2.507
32	C	0.190	-4.995	-0.613
33	C	-2.680	-4.735	-0.320
34	N	0.800	-5.991	-0.531
35	N	-3.434	-5.599	-0.086
36	H	1.996	-3.618	-1.535
37	H	-4.383	-3.001	-0.747
38	H	3.870	-2.826	-2.507
39	H	-6.265	-1.804	-1.015
40	H	5.346	-1.042	-3.348
41	H	-7.533	0.229	-1.574
42	H	2.392	1.909	-2.175
43	H	-3.808	2.408	-2.025
44	Zn	0.937	0.894	0.880
45	O	2.275	-0.438	1.427
46	O	-0.744	-0.220	1.108
47	N	2.394	2.362	0.822
48	N	-0.248	2.589	1.051
49	C	3.702	2.147	0.894
50	C	-1.506	2.634	1.453
51	C	1.852	3.614	0.616
52	C	0.465	3.739	0.745
53	C	4.303	0.900	1.176
54	C	-2.279	1.512	1.859
55	C	5.729	0.875	1.228
56	C	-3.550	1.782	2.435
57	C	6.445	-0.259	1.542
58	C	-4.380	0.787	2.914
59	C	5.726	-1.456	1.835
60	C	-3.942	-0.559	2.821
61	C	4.336	-1.481	1.798
62	C	-2.704	-0.866	2.246
63	C	3.565	-0.337	1.463
64	C	-1.863	0.130	1.724
65	O	6.332	-2.630	2.163
66	O	-4.662	-1.624	3.260
67	C	7.760	-2.669	2.229

68	C	-5.940	-1.383	3.857
69	H	8.218	-2.432	1.254
70	H	-6.633	-0.907	3.142
71	H	8.148	-1.980	2.998
72	H	-5.851	-0.758	4.761
73	H	8.011	-3.699	2.507
74	H	-6.323	-2.372	4.133
75	C	2.680	4.735	0.320
76	C	-0.190	4.995	0.613
77	N	3.434	5.599	0.086
78	N	-0.800	5.991	0.530
79	H	4.383	3.001	0.747
80	H	-1.996	3.618	1.535
81	H	6.264	1.805	1.015
82	H	-3.870	2.826	2.508
83	H	7.533	-0.229	1.574
84	H	-5.345	1.042	3.348
85	H	3.808	-2.408	2.025
86	H	-2.392	-1.909	2.175

Structural parameters

R(1-3)	1.966
R(2-20)	1.325
R(3-21)	1.294
R(4-6)	1.321
R(4-8)	1.387
R(5-7)	1.328
R(5-9)	1.379
R(6-10)	1.422
R(6-36)	1.102
R(7-11)	1.413
R(7-37)	1.103
R(8-9)	1.399
R(8-32)	1.422
R(9-33)	1.425
R(10-12)	1.421
R(10-20)	1.450
R(11-13)	1.427
R(11-21)	1.468
R(12-14)	1.382
R(12-38)	1.094
R(13-15)	1.377
R(13-39)	1.094
R(14-16)	1.418
R(14-40)	1.089
R(15-17)	1.427
R(15-41)	1.089
R(16-18)	1.399
R(16-22)	1.358
R(17-19)	1.391
R(17-23)	1.361
R(18-20)	1.404
R(18-42)	1.090
R(19-21)	1.419
R(19-43)	1.091
R(22-24)	1.432

R(23-25)	1.430
R(24-30)	1.096
R(24-26)	1.103
R(24-28)	1.103
R(25-27)	1.103
R(25-31)	1.096
R(25-29)	1.103
R(32-34)	1.171
R(33-35)	1.170
R(44-45)	1.966
R(45-63)	1.294
R(46-64)	1.325
R(47-49)	1.328
R(47-51)	1.379
R(48-50)	1.321
R(48-52)	1.387
R(49-53)	1.413
R(49-79)	1.103
R(50-54)	1.422
R(50-80)	1.102
R(51-52)	1.399
R(51-75)	1.425
R(52-76)	1.422
R(53-55)	1.427
R(53-63)	1.469
R(54-64)	1.450
R(54-56)	1.421
R(55-57)	1.377
R(55-81)	1.094
R(56-58)	1.382
R(56-82)	1.094
R(57-59)	1.427
R(57-83)	1.089
R(58-60)	1.418
R(58-84)	1.089
R(59-61)	1.391
R(59-65)	1.361
R(60-62)	1.399
R(60-66)	1.358
R(61-63)	1.419
R(61-85)	1.091
R(62-64)	1.404
R(62-86)	1.090
R(65-67)	1.430
R(66-68)	1.432
R(67-73)	1.096
R(67-69)	1.103
R(67-71)	1.103
R(68-70)	1.103
R(68-74)	1.096
R(68-72)	1.103
R(75-77)	1.170
R(76-78)	1.171
A(1-3-21)	129.28
A(2-20-10)	122.53
A(2-20-18)	119.44
A(3-21-11)	124.19
A(3-21-19)	118.98

A(6-4-8)	121.88
A(4-6-10)	125.31
A(4-6-36)	118.43
A(4-8-9)	117.09
A(4-8-32)	121.07
A(7-5-9)	122.84
A(5-7-11)	124.99
A(5-7-37)	118.39
A(5-9-8)	117.19
A(5-9-33)	121.14
A(10-6-36)	116.19
A(6-10-12)	116.87
A(6-10-20)	124.72
A(11-7-37)	116.61
A(7-11-13)	116.61
A(7-11-21)	124.62
A(9-8-32)	121.81
A(8-9-33)	121.65
A(8-32-34)	175.85
A(9-33-35)	175.40
A(12-10-20)	118.41
A(10-12-14)	122.73
A(10-12-38)	118.05
A(10-20-18)	118.02
A(13-11-21)	118.73
A(11-13-15)	122.84
A(11-13-39)	117.85
A(11-21-19)	116.84
A(14-12-38)	119.21
A(12-14-16)	118.38
A(12-14-40)	120.16
A(15-13-39)	119.31
A(13-15-17)	118.39
A(13-15-41)	120.25
A(16-14-40)	121.46
A(14-16-18)	120.56
A(14-16-22)	124.01
A(17-15-41)	121.36
A(15-17-19)	120.87
A(15-17-23)	123.28
A(18-16-22)	115.43
A(16-18-20)	121.79
A(16-18-42)	119.30
A(16-22-24)	118.42
A(19-17-23)	115.85
A(17-19-21)	122.33
A(17-19-43)	119.54
A(17-23-25)	118.61
A(20-18-42)	118.88
A(21-19-43)	118.13
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A(22-24-26)	111.34
A(22-24-28)	111.38
A(23-25-27)	111.58
A(23-25-31)	105.39
A(23-25-29)	111.54
A(30-24-26)	109.46
A(30-24-28)	109.43

A(26-24-28)	109.73
A(27-25-31)	109.29
A(27-25-29)	109.63
A(31-25-29)	109.30
A(44-45-63)	129.28
A(45-63-53)	124.19
A(45-63-61)	118.98
A(46-64-54)	122.52
A(46-64-62)	119.44
A(49-47-51)	122.84
A(47-49-53)	124.99
A(47-49-79)	118.39
A(47-51-52)	117.19
A(47-51-75)	121.14
A(50-48-52)	121.88
A(48-50-54)	125.30
A(48-50-80)	118.42
A(48-52-51)	117.09
A(48-52-76)	121.07
A(53-49-79)	116.60
A(49-53-55)	116.61
A(49-53-63)	124.61
A(54-50-80)	116.20
A(50-54-64)	124.72
A(50-54-56)	116.86
A(52-51-75)	121.64
A(51-52-76)	121.81
A(51-75-77)	175.40
A(52-76-78)	175.86
A(55-53-63)	118.73
A(53-55-57)	122.84
A(53-55-81)	117.85
A(53-63-61)	116.84
A(64-54-56)	118.42
A(54-64-62)	118.02
A(54-56-58)	122.72
A(54-56-82)	118.06
A(57-55-81)	119.32
A(55-57-59)	118.39
A(55-57-83)	120.25
A(58-56-82)	119.21
A(56-58-60)	118.39
A(56-58-84)	120.16
A(59-57-83)	121.36
A(57-59-61)	120.87
A(57-59-65)	123.28
A(60-58-84)	121.45
A(58-60-62)	120.55
A(58-60-66)	124.02
A(61-59-65)	115.85
A(59-61-63)	122.33
A(59-61-85)	119.53
A(59-65-67)	118.62
A(62-60-66)	115.43
A(60-62-64)	121.80
A(60-62-86)	119.30
A(60-66-68)	118.42
A(63-61-85)	118.14

A(64-62-86)	118.89
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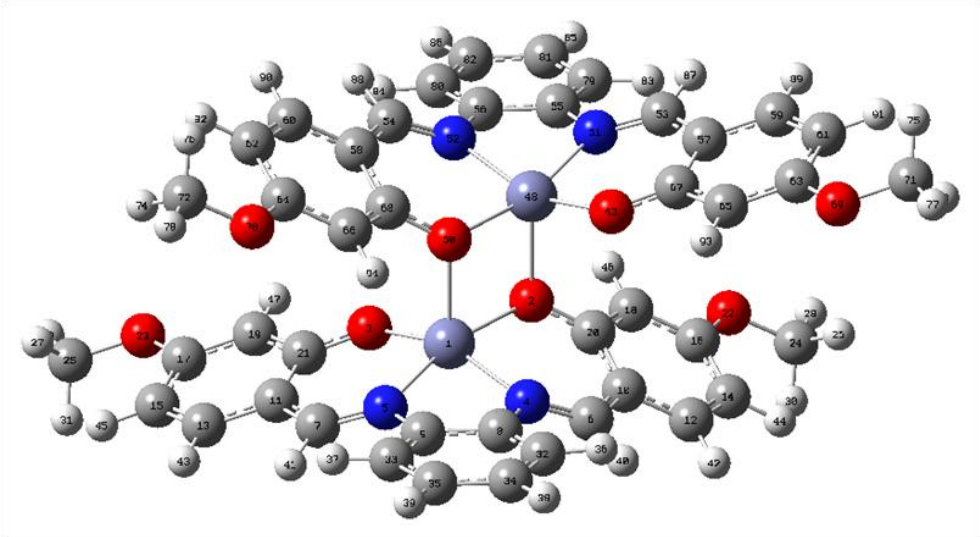
A(65-67-71)	111.54
A(66-68-70)	111.33
A(66-68-74)	105.40
A(66-68-72)	111.38
A(73-67-69)	109.29
A(73-67-71)	109.30
A(69-67-71)	109.63
A(70-68-74)	109.47
A(70-68-72)	109.73
A(74-68-72)	109.43

Complex 4D



Cartesian coordinates

		X	Y	Z
1	Zn	1.040	0.708	-0.928
2	O	-0.679	-0.389	-1.101
3	O	2.342	-0.748	-1.170
4	N	-0.079	2.357	-1.477
5	N	2.519	2.133	-1.086
6	C	-1.192	2.326	-2.166
7	C	3.787	1.877	-1.323
8	C	0.599	3.553	-1.201
9	C	2.007	3.431	-0.980
10	C	-1.966	1.158	-2.457
11	C	4.373	0.583	-1.423
12	C	-3.087	1.318	-3.309
13	C	5.775	0.528	-1.650
14	C	-3.917	0.268	-3.663
15	C	6.473	-0.657	-1.777
16	C	-3.628	-1.019	-3.147
17	C	5.745	-1.876	-1.690

18	C	-2.530	-1.218	-2.306
19	C	4.370	-1.873	-1.486
20	C	-1.687	-0.158	-1.923
21	C	3.622	-0.672	-1.345
22	O	-4.367	-2.132	-3.423
23	O	6.327	-3.109	-1.800
24	C	-5.495	-1.991	-4.288
25	C	7.735	-3.172	-2.024
26	H	-6.249	-1.306	-3.863
27	H	8.301	-2.714	-1.195
28	H	-5.927	-2.996	-4.374
29	H	7.977	-4.240	-2.080
30	H	-5.197	-1.635	-5.289
31	H	8.019	-2.685	-2.974
32	C	-0.013	4.812	-1.081
33	C	2.748	4.577	-0.642
34	C	0.745	5.942	-0.770
35	C	2.125	5.824	-0.550
36	H	-1.097	4.895	-1.192
37	H	3.814	4.485	-0.422
38	H	0.255	6.912	-0.667
39	H	2.713	6.703	-0.278
40	H	-1.569	3.265	-2.607
41	H	4.477	2.723	-1.488
42	H	-3.300	2.319	-3.698
43	H	6.319	1.476	-1.717
44	H	-4.770	0.441	-4.317
45	H	7.549	-0.645	-1.944
46	H	-2.322	-2.218	-1.921
47	H	3.830	-2.819	-1.435
48	Zn	-1.040	-0.708	0.928
49	O	-2.342	0.748	1.170
50	O	0.679	0.389	1.101
51	N	-2.519	-2.133	1.086
52	N	0.079	-2.357	1.477
53	C	-3.787	-1.877	1.323
54	C	1.192	-2.326	2.166
55	C	-2.007	-3.431	0.980
56	C	-0.599	-3.553	1.201
57	C	-4.373	-0.583	1.423
58	C	1.966	-1.158	2.457
59	C	-5.775	-0.528	1.650
60	C	3.087	-1.318	3.309
61	C	-6.473	0.657	1.777
62	C	3.917	-0.268	3.663
63	C	-5.745	1.876	1.690
64	C	3.628	1.019	3.147
65	C	-4.370	1.873	1.486
66	C	2.530	1.218	2.306
67	C	-3.622	0.672	1.345
68	C	1.687	0.158	1.923
69	O	-6.327	3.109	1.800
70	O	4.367	2.132	3.423
71	C	-7.735	3.172	2.024
72	C	5.495	1.991	4.288
73	H	-8.301	2.714	1.195
74	H	6.249	1.306	3.863
75	H	-8.019	2.685	2.974

76	H	5.197	1.635	5.289
77	H	-7.977	4.240	2.080
78	H	5.927	2.996	4.374
79	C	-2.748	-4.577	0.642
80	C	0.013	-4.812	1.081
81	C	-2.125	-5.824	0.550
82	C	-0.745	-5.942	0.770
83	H	-3.814	-4.485	0.422
84	H	1.097	-4.895	1.192
85	H	-2.713	-6.703	0.278
86	H	-0.255	-6.912	0.667
87	H	-4.477	-2.723	1.488
88	H	1.569	-3.265	2.607
89	H	-6.319	-1.476	1.717
90	H	3.300	-2.319	3.698
91	H	-7.549	0.645	1.944
92	H	4.770	-0.441	4.317
93	H	-3.830	2.819	1.435
94	H	2.322	2.218	1.921

Structural parameters

R(1-3)	1.967
R(1-5)	2.060
R(2-20)	1.321
R(3-21)	1.295
R(4-6)	1.310
R(4-8)	1.402
R(5-9)	1.400
R(5-7)	1.315
R(6-10)	1.431
R(6-40)	1.104
R(7-11)	1.424
R(7-41)	1.104
R(8-9)	1.431
R(8-32)	1.405
R(9-33)	1.406
R(10-12)	1.417
R(10-20)	1.447
R(11-13)	1.421
R(11-21)	1.464
R(12-14)	1.385
R(12-42)	1.094
R(13-15)	1.381
R(13-43)	1.095
R(14-16)	1.416
R(14-44)	1.089
R(15-17)	1.422
R(15-45)	1.089
R(16-18)	1.398
R(16-22)	1.365
R(17-19)	1.391
R(17-23)	1.368
R(18-20)	1.408
R(18-46)	1.091
R(19-21)	1.422
R(19-47)	1.091
R(22-24)	1.428

R(23-25)	1.427
R(24-30)	1.104
R(24-28)	1.097
R(24-26)	1.104
R(25-29)	1.097
R(25-31)	1.104
R(25-27)	1.104
R(32-34)	1.396
R(32-36)	1.092
R(33-35)	1.396
R(33-37)	1.092
R(34-35)	1.402
R(34-38)	1.092
R(35-39)	1.092
R(48-49)	1.967
R(48-51)	2.060
R(49-67)	1.295
R(50-68)	1.321
R(51-55)	1.400
R(51-53)	1.315
R(52-54)	1.310
R(52-56)	1.402
R(53-57)	1.424
R(53-87)	1.104
R(54-58)	1.431
R(54-88)	1.104
R(55-56)	1.431
R(55-79)	1.406
R(56-80)	1.405
R(57-59)	1.421
R(57-67)	1.464
R(58-68)	1.447
R(58-60)	1.417
R(59-61)	1.381
R(59-89)	1.095
R(60-62)	1.385
R(60-90)	1.094
R(61-63)	1.422
R(61-91)	1.089
R(62-64)	1.416
R(62-92)	1.089
R(63-65)	1.391
R(63-69)	1.368
R(64-66)	1.398
R(64-70)	1.365
R(65-67)	1.422
R(65-93)	1.091
R(66-68)	1.407
R(66-94)	1.091
R(69-71)	1.427
R(70-72)	1.428
R(71-75)	1.104
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R(72-78)	1.097
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R(72-74)	1.104
R(79-81)	1.396

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A(3-21-11)	124.39
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A(6-4-8)	122.34
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A(4-8-9)	115.69
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A(6-10-12)	117.25
A(6-10-20)	124.23
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A(7-11-13)	116.85
A(7-11-21)	124.36
A(9-8-32)	119.47
A(8-9-33)	119.09
A(8-32-34)	120.51
A(8-32-36)	119.46
A(9-33-35)	120.56
A(9-33-37)	119.59
A(12-10-20)	118.52
A(10-12-14)	122.82
A(10-12-42)	118.10
A(10-20-18)	117.97
A(13-11-21)	118.77
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A(11-21-19)	116.69
A(14-12-42)	119.07
A(12-14-16)	118.27
A(12-14-44)	120.17
A(15-13-43)	119.05
A(13-15-17)	118.11
A(13-15-45)	120.27
A(16-14-44)	121.55
A(14-16-18)	120.63
A(14-16-22)	123.83
A(17-15-45)	121.62
A(15-17-19)	120.85
A(15-17-23)	123.37
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A(16-22-24)	118.03
A(19-17-23)	115.78
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A(17-23-25)	118.16
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A(21-19-47)	117.95
A(22-24-30)	111.57
A(22-24-28)	105.55
A(22-24-26)	111.56
A(23-25-29)	105.56
A(23-25-31)	111.70
A(23-25-27)	111.71
A(30-24-28)	109.28
A(30-24-26)	109.46
A(28-24-26)	109.32
A(29-25-31)	109.19
A(29-25-27)	109.21
A(31-25-27)	109.36
A(34-32-36)	119.99
A(32-34-35)	120.09
A(32-34-38)	119.74
A(35-33-37)	119.83
A(33-35-34)	120.26
A(33-35-39)	119.64
A(35-34-38)	120.15
A(34-35-39)	120.07
A(49-48-51)	91.57
A(48-49-67)	128.85
A(48-51-55)	111.91
A(48-51-53)	124.85
A(49-67-57)	124.39
A(49-67-65)	118.92
A(50-68-58)	122.42
A(50-68-66)	119.60
A(55-51-53)	123.17
A(51-55-56)	115.31
A(51-55-79)	125.56
A(51-53-57)	125.88
A(51-53-87)	118.67
A(54-52-56)	122.34
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A(52-54-88)	118.63
A(52-56-55)	115.69
A(52-56-80)	124.79
A(57-53-87)	115.43
A(53-57-59)	116.85
A(53-57-67)	124.36
A(58-54-88)	115.41
A(54-58-68)	124.23
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A(56-55-79)	119.09
A(55-56-80)	119.47
A(55-79-81)	120.56
A(55-79-83)	119.60
A(56-80-82)	120.50
A(56-80-84)	119.46

A(59-57-67)	118.77
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A(57-59-89)	117.84
A(57-67-65)	116.69
A(68-58-60)	118.52
A(58-68-66)	117.97
A(58-60-62)	122.82
A(58-60-90)	118.10
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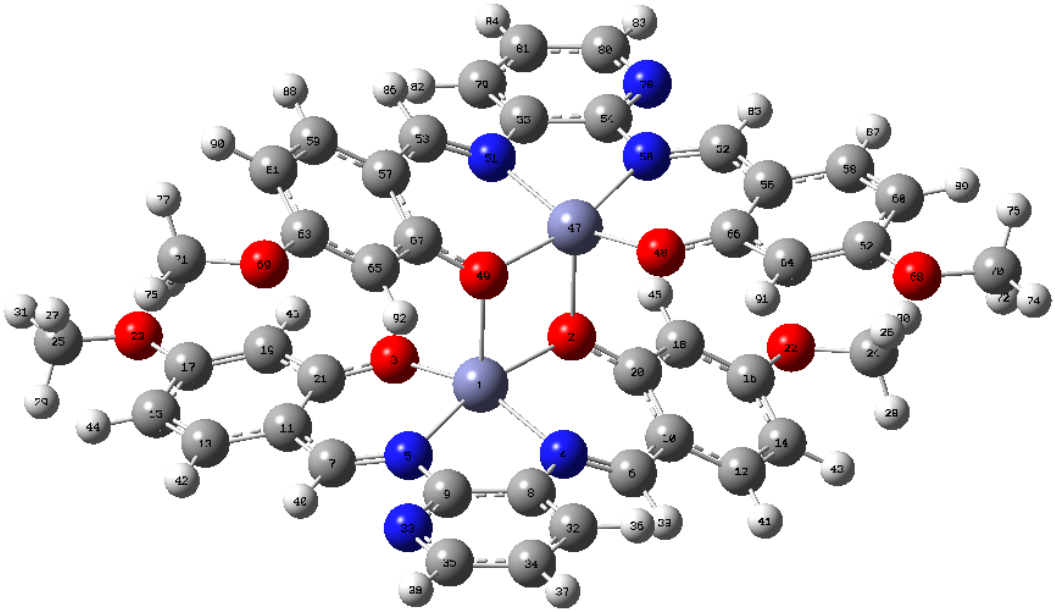
A(59-61-63)	118.11
A(59-61-91)	120.27
A(62-60-90)	119.07
A(60-62-64)	118.27
A(60-62-92)	120.17
A(63-61-91)	121.62
A(61-63-65)	120.85
A(61-63-69)	123.37
A(64-62-92)	121.55
A(62-64-66)	120.62
A(62-64-70)	123.83
A(65-63-69)	115.78
A(63-65-67)	122.46
A(63-65-93)	119.59
A(63-69-71)	118.16
A(66-64-70)	115.54
A(64-66-68)	121.78
A(64-66-94)	119.47
A(64-70-72)	118.03
A(67-65-93)	117.95
A(68-66-94)	118.74
A(69-71-75)	111.70
A(69-71-77)	105.56
A(69-71-73)	111.71
A(70-72-78)	105.55
A(70-72-76)	111.57
A(70-72-74)	111.56
A(75-71-77)	109.19
A(75-71-73)	109.36
A(77-71-73)	109.21
A(78-72-76)	109.28
A(78-72-74)	109.32
A(76-72-74)	109.46
A(81-79-83)	119.82
A(79-81-82)	120.25
A(79-81-85)	119.64
A(82-80-84)	119.99
A(80-82-81)	120.10
A(80-82-86)	119.74
A(82-81-85)	120.08
A(81-82-86)	120.14

Complex 5D



Cartesian coordinates

		X	Y	Z
1	Zn	-0.990	-0.884	0.826
2	O	0.738	-1.109	-0.229
3	O	-2.283	-1.387	-0.576
4	N	0.168	-1.122	2.540
5	N	-2.457	-0.902	2.249
6	C	1.314	-1.751	2.603
7	C	-3.748	-1.045	2.021
8	C	-0.551	-0.773	3.690
9	C	-1.971	-0.658	3.537
10	C	2.108	-2.158	1.481
11	C	-4.334	-1.305	0.752
12	C	3.273	-2.924	1.759
13	C	-5.755	-1.429	0.718
14	C	4.104	-3.383	0.752
15	C	-6.440	-1.712	-0.445
16	C	3.781	-3.079	-0.587
17	C	-5.703	-1.895	-1.642
18	C	2.652	-2.332	-0.898
19	C	-4.326	-1.790	-1.659
20	C	1.789	-1.836	0.111
21	C	-3.571	-1.482	-0.481
22	O	4.623	-3.547	-1.643
23	O	-6.397	-2.197	-2.855
24	C	5.986	-3.528	-1.211
25	C	-7.786	-1.896	-2.698
26	H	6.194	-2.597	-0.727
27	H	-7.896	-0.893	-2.343
28	H	6.154	-4.332	-0.524
29	H	-8.220	-2.573	-1.992
30	H	6.631	-3.642	-2.058
31	H	-8.282	-1.998	-3.640
32	C	-0.010	-0.497	4.953
33	N	-2.792	-0.331	4.543
34	C	-0.871	-0.162	6.001

35	C	-2.248	-0.100	5.747
36	H	1.071	-0.517	5.105
37	H	-0.483	0.069	6.994
38	H	-2.948	0.168	6.546
39	H	1.705	-2.048	3.592
40	H	-4.425	-0.972	2.888
41	H	3.503	-3.150	2.805
42	H	-6.300	-1.290	1.658
43	H	4.995	-3.966	0.989
44	H	-7.528	-1.800	-0.446
45	H	2.400	-2.095	-1.933
46	H	-3.753	-1.934	-2.577
47	Zn	0.990	0.884	-0.826
48	O	2.283	1.387	0.576
49	O	-0.738	1.109	0.229
50	N	2.457	0.902	-2.249
51	N	-0.168	1.122	-2.540
52	C	3.748	1.045	-2.021
53	C	-1.314	1.751	-2.603
54	C	1.971	0.658	-3.537
55	C	0.551	0.773	-3.690
56	C	4.334	1.305	-0.752
57	C	-2.108	2.158	-1.481
58	C	5.755	1.429	-0.718
59	C	-3.273	2.924	-1.759
60	C	6.440	1.712	0.445
61	C	-4.104	3.383	-0.752
62	C	5.703	1.895	1.642
63	C	-3.781	3.079	0.587
64	C	4.326	1.790	1.659
65	C	-2.652	2.332	0.898
66	C	3.571	1.482	0.481
67	C	-1.789	1.836	-0.111
68	O	6.397	2.197	2.855
69	O	-4.623	3.547	1.643
70	C	7.786	1.896	2.698
71	C	-5.986	3.528	1.211
72	H	7.896	0.893	2.343
73	H	-6.194	2.597	0.727
74	H	8.282	1.998	3.640
75	H	-6.631	3.642	2.058
76	H	8.220	2.573	1.992
77	H	-6.154	4.332	0.524
78	N	2.792	0.331	-4.543
79	C	0.010	0.497	-4.953
80	C	2.248	0.100	-5.747
81	C	0.871	0.162	-6.001
82	H	-1.071	0.517	-5.105
83	H	2.948	-0.168	-6.546
84	H	0.483	-0.069	-6.994
85	H	4.425	0.972	-2.888
86	H	-1.705	2.048	-3.592
87	H	6.300	1.290	-1.658
88	H	-3.503	3.150	-2.805
89	H	7.528	1.800	0.446
90	H	-4.995	3.966	-0.989
91	H	3.753	1.934	2.577
92	H	-2.400	2.095	1.933

Structural parameters

R(1-3)	1.973
R(1-5)	2.044
R(2-20)	1.322
R(3-21)	1.294
R(4-6)	1.309
R(4-8)	1.400
R(5-9)	1.398
R(5-7)	1.319
R(6-10)	1.434
R(6-39)	1.104
R(7-11)	1.422
R(7-40)	1.101
R(8-9)	1.432
R(8-32)	1.401
R(9-33)	1.340
R(10-20)	1.442
R(10-12)	1.421
R(11-13)	1.427
R(11-21)	1.460
R(12-14)	1.384
R(12-41)	1.095
R(13-15)	1.379
R(13-42)	1.095
R(14-16)	1.410
R(14-43)	1.091
R(15-17)	1.418
R(15-44)	1.091
R(16-18)	1.389
R(16-22)	1.430
R(17-19)	1.381
R(17-23)	1.430
R(18-20)	1.418
R(18-45)	1.092
R(19-21)	1.433
R(19-46)	1.092
R(22-24)	1.430
R(23-25)	1.430
R(24-28)	1.070
R(24-30)	1.070
R(24-26)	1.070
R(25-31)	1.070
R(25-29)	1.070
R(25-27)	1.070
R(32-34)	1.397
R(32-36)	1.092
R(33-35)	1.341
R(34-35)	1.401
R(34-37)	1.091
R(35-38)	1.095
R(47-48)	1.973
R(47-50)	2.044
R(48-66)	1.294
R(49-67)	1.322
R(50-54)	1.398
R(50-52)	1.319
R(51-53)	1.309

R(51-55)	1.400
R(52-56)	1.422
R(52-85)	1.101
R(53-57)	1.434
R(53-86)	1.104
R(54-55)	1.432
R(54-78)	1.340
R(55-79)	1.401
R(56-58)	1.427
R(56-66)	1.460
R(57-67)	1.442
R(57-59)	1.421
R(58-60)	1.379
R(58-87)	1.095
R(59-61)	1.384
R(59-88)	1.095
R(60-62)	1.418
R(60-89)	1.091
R(61-63)	1.410
R(61-90)	1.091
R(62-64)	1.381
R(62-68)	1.430
R(63-65)	1.389
R(63-69)	1.430
R(64-66)	1.433
R(64-91)	1.092
R(65-67)	1.418
R(65-92)	1.092
R(68-70)	1.430
R(69-71)	1.430
R(70-76)	1.070
R(70-74)	1.070
R(70-72)	1.070
R(71-75)	1.070
R(71-77)	1.070
R(71-73)	1.070
R(78-80)	1.341
R(79-81)	1.397
R(79-82)	1.092
R(80-81)	1.401
R(80-83)	1.095
R(81-84)	1.091
A(3-1-5)	91.28
A(1-3-21)	128.17
A(1-5-9)	112.97
A(1-5-7)	125.69
A(2-20-10)	122.90
A(2-20-18)	119.55
A(3-21-11)	124.97
A(3-21-19)	118.62
A(6-4-8)	122.02
A(4-6-10)	125.75
A(4-6-39)	118.83
A(4-8-9)	116.16
A(4-8-32)	126.22
A(9-5-7)	121.23
A(5-9-8)	115.42
A(5-9-33)	121.43

A(5-7-11)	125.24
A(5-7-40)	117.26
A(10-6-39)	115.36
A(6-10-20)	123.83
A(6-10-12)	116.97
A(11-7-40)	117.50
A(7-11-13)	116.55
A(7-11-21)	124.10
A(9-8-32)	117.60
A(8-9-33)	123.14
A(8-32-34)	119.03
A(8-32-36)	120.26
A(9-33-35)	117.88
A(20-10-12)	119.19
A(10-20-18)	117.55
A(10-12-14)	121.87
A(10-12-41)	118.09
A(13-11-21)	119.33
A(11-13-15)	122.16
A(11-13-42)	117.64
A(11-21-19)	116.41
A(14-12-41)	120.04
A(12-14-16)	118.81
A(12-14-43)	120.65
A(15-13-42)	120.20
A(13-15-17)	118.71
A(13-15-44)	120.82
A(16-14-43)	120.53
A(14-16-18)	120.97
A(14-16-22)	119.73
A(17-15-44)	120.47
A(15-17-19)	121.26
A(15-17-23)	119.40
A(18-16-22)	119.29
A(16-18-20)	121.58
A(16-18-45)	121.17
A(16-22-24)	109.50
A(19-17-23)	119.34
A(17-19-21)	122.12
A(17-19-46)	121.55
A(17-23-25)	109.50
A(20-18-45)	117.24
A(21-19-46)	116.33
A(22-24-28)	109.47
A(22-24-30)	109.48
A(22-24-26)	109.47
A(23-25-31)	109.47
A(23-25-29)	109.47
A(23-25-27)	109.47
A(28-24-30)	109.47
A(28-24-26)	109.47
A(30-24-26)	109.47
A(31-25-29)	109.47
A(31-25-27)	109.47
A(29-25-27)	109.48
A(34-32-36)	120.69
A(32-34-35)	118.72
A(32-34-37)	120.94

A(33-35-34)	123.61
A(33-35-38)	115.91
A(35-34-37)	120.33
A(34-35-38)	120.47
A(48-47-50)	91.28
A(47-48-66)	128.17
A(47-50-54)	112.97
A(47-50-52)	125.69
A(48-66-56)	124.97
A(48-66-64)	118.62
A(49-67-57)	122.90
A(49-67-65)	119.55
A(54-50-52)	121.23
A(50-54-55)	115.42
A(50-54-78)	121.43
A(50-52-56)	125.24
A(50-52-85)	117.26
A(53-51-55)	122.02
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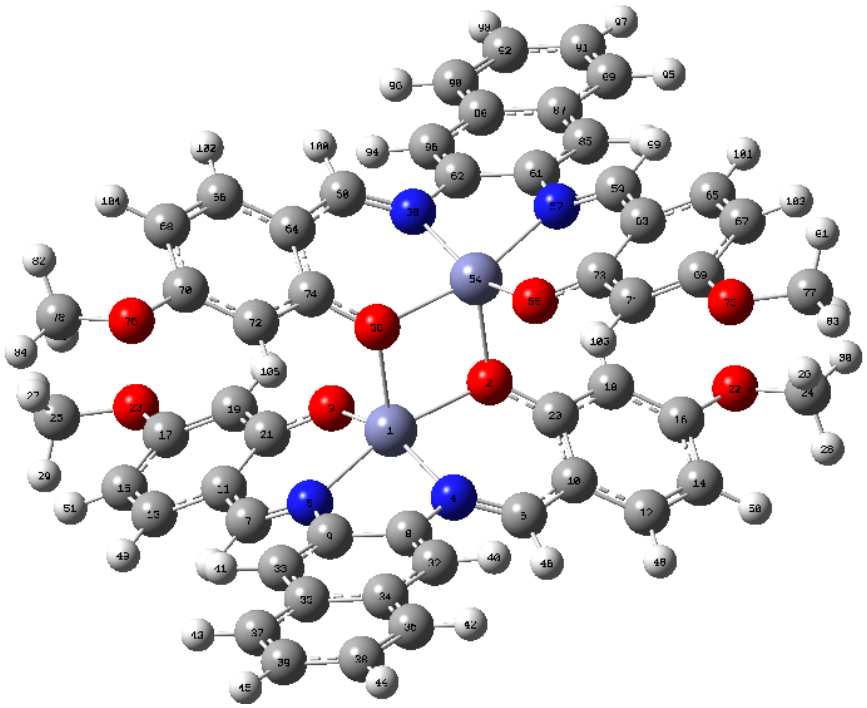
A(51-53-86)	118.83
A(51-55-54)	116.16
A(51-55-79)	126.22
A(56-52-85)	117.50
A(52-56-58)	116.55
A(52-56-66)	124.10
A(57-53-86)	115.36
A(53-57-67)	123.83
A(53-57-59)	116.97
A(55-54-78)	123.14
A(54-55-79)	117.60
A(54-78-80)	117.88
A(55-79-81)	119.03
A(55-79-82)	120.26
A(58-56-66)	119.33
A(56-58-60)	122.16
A(56-58-87)	117.64
A(56-66-64)	116.41
A(67-57-59)	119.19
A(57-67-65)	117.55
A(57-59-61)	121.87
A(57-59-88)	118.09
A(60-58-87)	120.20
A(58-60-62)	118.71
A(58-60-89)	120.82
A(61-59-88)	120.04
A(59-61-63)	118.81
A(59-61-90)	120.65
A(62-60-89)	120.47
A(60-62-64)	121.26
A(60-62-68)	119.40
A(63-61-90)	120.53
A(61-63-65)	120.97
A(61-63-69)	119.73
A(64-62-68)	119.34
A(62-64-66)	122.12
A(62-64-91)	121.55
A(62-68-70)	109.50
A(65-63-69)	119.29

A(63-65-67)	121.58
A(63-65-92)	121.17
A(63-69-71)	109.50
A(66-64-91)	116.33
A(67-65-92)	117.24
A(68-70-76)	109.47
A(68-70-74)	109.47
A(68-70-72)	109.47
A(69-71-75)	109.48
A(69-71-77)	109.47
A(69-71-73)	109.47
A(76-70-74)	109.47
A(76-70-72)	109.48
A(74-70-72)	109.47
A(75-71-77)	109.47
A(75-71-73)	109.47
A(77-71-73)	109.47
A(78-80-81)	123.61
A(78-80-83)	115.91
A(81-79-82)	120.69
A(79-81-80)	118.72
A(79-81-84)	120.94
A(81-80-83)	120.47
A(80-81-84)	120.33

Complex 6D



Cartesian coordinates

		X	Y	Z
1	Zn	-0.059	-0.885	1.290
2	O	0.179	-1.113	-0.732
3	O	-1.995	-1.216	1.404
4	N	1.945	-1.380	1.456
5	N	0.138	-1.006	3.335
6	C	2.615	-2.115	0.606
7	C	-0.841	-1.286	4.168
8	C	2.458	-1.051	2.720
9	C	1.465	-0.838	3.753
10	C	2.191	-2.467	-0.719
11	C	-2.214	-1.451	3.823
12	C	3.020	-3.364	-1.445
13	C	-3.117	-1.708	4.897
14	C	2.707	-3.770	-2.731
15	C	-4.468	-1.899	4.692
16	C	1.532	-3.274	-3.333
17	C	-4.968	-1.851	3.367
18	C	0.698	-2.395	-2.655
19	C	-4.129	-1.622	2.293
20	C	0.995	-1.956	-1.340
21	C	-2.722	-1.411	2.457
22	O	1.187	-3.686	-4.658
23	O	-6.365	-2.048	3.135
24	C	2.373	-3.786	-5.451
25	C	-7.093	-1.762	4.333
26	H	2.983	-2.921	-5.290
27	H	-6.790	-0.810	4.715
28	H	2.917	-4.663	-5.171
29	H	-6.892	-2.520	5.061
30	H	2.106	-3.846	-6.485

31	H	-8.140	-1.744	4.117
32	C	3.802	-0.873	3.009
33	C	1.876	-0.457	5.023
34	C	4.235	-0.506	4.309
35	C	3.250	-0.296	5.339
36	C	5.610	-0.322	4.626
37	C	3.687	0.086	6.638
38	C	6.001	0.044	5.900
39	C	5.032	0.249	6.914
40	H	4.546	-0.977	2.215
41	H	1.134	-0.252	5.799
42	H	6.355	-0.478	3.841
43	H	2.939	0.247	7.419
44	H	7.061	0.178	6.129
45	H	5.352	0.540	7.917
46	H	3.580	-2.545	0.928
47	H	-0.598	-1.438	5.234
48	H	3.927	-3.736	-0.959
49	H	-2.707	-1.744	5.912
50	H	3.358	-4.459	-3.271
51	H	-5.140	-2.086	5.531
52	H	-0.216	-2.013	-3.114
53	H	-4.506	-1.593	1.269
54	Zn	0.059	0.885	-1.290
55	O	1.995	1.216	-1.404
56	O	-0.179	1.113	0.732
57	N	-0.138	1.006	-3.335
58	N	-1.945	1.380	-1.456
59	C	0.841	1.286	-4.168
60	C	-2.615	2.115	-0.606
61	C	-1.465	0.838	-3.753
62	C	-2.458	1.051	-2.720
63	C	2.214	1.451	-3.823
64	C	-2.191	2.467	0.719
65	C	3.117	1.708	-4.897
66	C	-3.020	3.364	1.445
67	C	4.468	1.899	-4.692
68	C	-2.707	3.770	2.731
69	C	4.968	1.851	-3.367
70	C	-1.532	3.274	3.333
71	C	4.129	1.622	-2.293
72	C	-0.698	2.395	2.655
73	C	2.722	1.411	-2.457
74	C	-0.995	1.956	1.340
75	O	6.365	2.048	-3.135
76	O	-1.187	3.686	4.658
77	C	7.093	1.762	-4.333
78	C	-2.373	3.786	5.451
79	H	6.790	0.810	-4.715
80	H	-2.983	2.921	5.290
81	H	6.892	2.520	-5.061
82	H	-2.917	4.663	5.171
83	H	8.140	1.744	-4.117
84	H	-2.106	3.846	6.485
85	C	-1.876	0.457	-5.023
86	C	-3.802	0.873	-3.009
87	C	-3.250	0.296	-5.339
88	C	-4.235	0.506	-4.309

89	C	-3.687	-0.086	-6.638
90	C	-5.610	0.322	-4.626
91	C	-5.032	-0.249	-6.914
92	C	-6.001	-0.044	-5.900
93	H	-1.134	0.252	-5.799
94	H	-4.546	0.977	-2.215
95	H	-2.939	-0.247	-7.419
96	H	-6.355	0.478	-3.841
97	H	-5.352	-0.540	-7.917
98	H	-7.061	-0.178	-6.129
99	H	0.598	1.438	-5.234
100	H	-3.580	2.545	-0.928
101	H	2.707	1.744	-5.912
102	H	-3.927	3.736	0.959
103	H	5.140	2.086	-5.531
104	H	-3.358	4.459	3.271
105	H	4.506	1.593	-1.269
106	H	0.216	2.013	3.114

Structural parameters

R(1-3)	1.968
R(1-5)	2.058
R(2-20)	1.321
R(3-21)	1.294
R(4-6)	1.308
R(4-8)	1.403
R(5-9)	1.401
R(5-7)	1.315
R(6-10)	1.435
R(6-46)	1.104
R(7-11)	1.426
R(7-47)	1.104
R(8-9)	1.448
R(8-32)	1.386
R(9-33)	1.388
R(10-20)	1.442
R(10-12)	1.421
R(11-13)	1.426
R(11-21)	1.458
R(12-14)	1.385
R(12-48)	1.095
R(13-15)	1.380
R(13-49)	1.095
R(14-16)	1.410
R(14-50)	1.091
R(15-17)	1.417
R(15-51)	1.091
R(16-18)	1.389
R(16-22)	1.430
R(17-19)	1.382
R(17-23)	1.430
R(18-20)	1.418
R(18-52)	1.092
R(19-21)	1.432
R(19-53)	1.092
R(22-24)	1.430
R(23-25)	1.430

R(24-28)	1.070
R(24-30)	1.070
R(24-26)	1.070
R(25-31)	1.070
R(25-29)	1.070
R(25-27)	1.070
R(32-34)	1.419
R(32-40)	1.093
R(33-35)	1.419
R(33-41)	1.093
R(34-35)	1.441
R(34-36)	1.422
R(35-37)	1.423
R(36-38)	1.382
R(36-42)	1.093
R(37-39)	1.382
R(37-43)	1.094
R(38-39)	1.418
R(38-44)	1.092
R(39-45)	1.092
R(54-55)	1.968
R(54-57)	2.058
R(55-73)	1.294
R(56-74)	1.321
R(57-61)	1.401
R(57-59)	1.315
R(58-60)	1.308
R(58-62)	1.403
R(59-63)	1.426
R(59-99)	1.104
R(60-64)	1.435
R(60-100)	1.104
R(61-62)	1.448
R(61-85)	1.388
R(62-86)	1.386
R(63-65)	1.426
R(63-73)	1.458
R(64-74)	1.442
R(64-66)	1.421
R(65-67)	1.380
R(65-101)	1.095
R(66-68)	1.385
R(66-102)	1.095
R(67-69)	1.417
R(67-103)	1.091
R(68-70)	1.410
R(68-104)	1.091
R(69-71)	1.382
R(69-75)	1.430
R(70-72)	1.389
R(70-76)	1.430
R(71-73)	1.432
R(71-105)	1.092
R(72-74)	1.418
R(72-106)	1.092
R(75-77)	1.430
R(76-78)	1.430
R(77-81)	1.070

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R(77-79)	1.070
R(78-84)	1.070
R(78-82)	1.070
R(78-80)	1.070
R(85-87)	1.419
R(85-93)	1.093
R(86-88)	1.419
R(86-94)	1.093
R(87-88)	1.441
R(87-89)	1.423
R(88-90)	1.422
R(89-91)	1.382
R(89-95)	1.094
R(90-92)	1.382
R(90-96)	1.093
R(91-92)	1.418
R(91-97)	1.092
R(92-98)	1.092
A(3-1-5)	91.52
A(1-3-21)	128.68
A(1-5-9)	112.31
A(1-5-7)	124.81
A(2-20-10)	122.73
A(2-20-18)	119.66
A(3-21-11)	124.83
A(3-21-19)	118.74
A(6-4-8)	121.98
A(4-6-10)	125.89
A(4-6-46)	118.54
A(4-8-9)	115.24
A(4-8-32)	124.87
A(9-5-7)	122.77
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A(5-9-33)	125.87
A(5-7-11)	126.02
A(5-7-47)	118.51
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A(7-11-13)	116.65
A(7-11-21)	123.98
A(9-8-32)	119.84
A(8-9-33)	119.33
A(8-32-34)	121.34
A(8-32-40)	119.81
A(9-33-35)	121.45
A(9-33-41)	120.02
A(20-10-12)	119.20
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A(11-21-19)	116.43
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A(15-17-19)	121.21
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A(30-24-26)	109.47
A(31-25-29)	109.47
A(31-25-27)	109.47
A(29-25-27)	109.47
A(34-32-40)	118.81
A(32-34-35)	118.93
A(32-34-36)	122.18
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A(34-35-37)	118.75
A(34-36-38)	120.88
A(34-36-42)	118.70
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A(36-38-44)	120.05
A(39-37-43)	120.38
A(37-39-38)	120.33
A(37-39-45)	120.01
A(39-38-44)	119.69
A(38-39-45)	119.66
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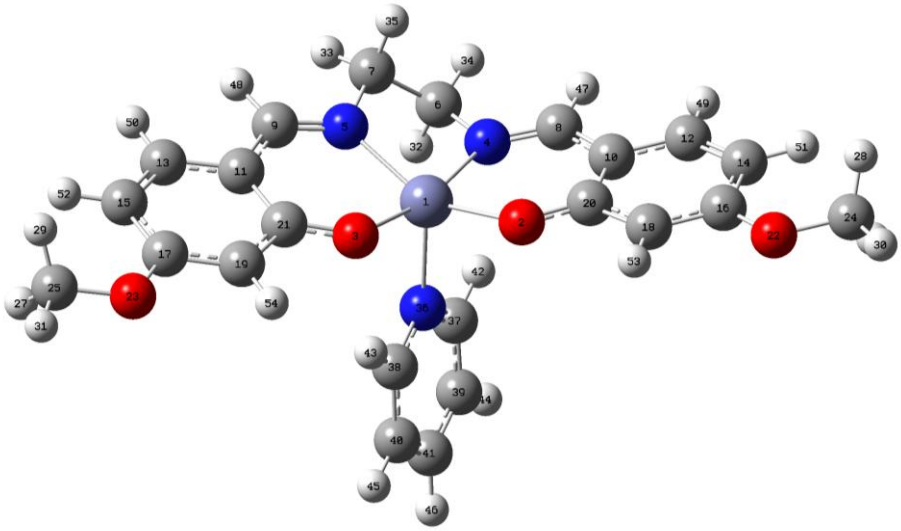
A(57-61-85)	125.87
A(57-59-63)	126.02
A(57-59-99)	118.51
A(60-58-62)	121.98
A(58-60-64)	125.89
A(58-60-100)	118.54
A(58-62-61)	115.24
A(58-62-86)	124.87
A(63-59-99)	115.44
A(59-63-65)	116.65
A(59-63-73)	123.98
A(64-60-100)	115.53
A(60-64-74)	123.77
A(60-64-66)	117.03
A(62-61-85)	119.33
A(61-62-86)	119.84
A(61-85-87)	121.45
A(61-85-93)	120.02
A(62-86-88)	121.34
A(62-86-94)	119.81
A(65-63-73)	119.35
A(63-65-67)	122.18
A(63-65-101)	117.82
A(63-73-71)	116.43
A(74-64-66)	119.20
A(64-74-72)	117.61
A(64-66-68)	121.86
A(64-66-102)	118.10
A(67-65-101)	120.00
A(65-67-69)	118.68
A(65-67-103)	120.80
A(68-66-102)	120.04
A(66-68-70)	118.81
A(66-68-104)	120.65
A(69-67-103)	120.52
A(67-69-71)	121.21
A(67-69-75)	119.44
A(70-68-104)	120.54
A(68-70-72)	120.98
A(68-70-76)	119.69
A(71-69-75)	119.35
A(69-71-73)	122.14
A(69-71-105)	121.56
A(69-75-77)	109.50
A(72-70-76)	119.33
A(70-72-74)	121.53
A(70-72-106)	121.26
A(70-76-78)	109.50
A(73-71-105)	116.30
A(74-72-106)	117.21
A(75-77-81)	109.46
A(75-77-83)	109.48
A(75-77-79)	109.47

A(76-78-84)	109.47
A(76-78-82)	109.47
A(76-78-80)	109.47
A(81-77-83)	109.47
A(81-77-79)	109.47
A(83-77-79)	109.47
A(84-78-82)	109.47
A(84-78-80)	109.47
A(82-78-80)	109.47
A(87-85-93)	118.51
A(85-87-88)	119.10
A(85-87-89)	122.14
A(88-86-94)	118.81
A(86-88-87)	118.93
A(86-88-90)	122.18
A(88-87-89)	118.75
A(87-88-90)	118.88
A(87-89-91)	120.90
A(87-89-95)	118.72
A(88-90-92)	120.88
A(88-90-96)	118.70
A(91-89-95)	120.38
A(89-91-92)	120.33
A(89-91-97)	120.01
A(92-90-96)	120.41
A(90-92-91)	120.25
A(90-92-98)	120.05
A(92-91-97)	119.66
A(91-92-98)	119.69

V. Optimised molecular structure for ZnL·py adducts

Adduct 1·py



Cartesian coordinates

		X	Y	Z
1	Zn	0.002	-0.411	-0.331
2	O	1.492	0.879	-0.115
3	O	-1.514	0.847	-0.100
4	N	1.385	-1.840	-0.992
5	N	-1.219	-1.577	-1.541
6	C	0.729	-3.047	-1.462
7	C	-0.517	-2.630	-2.268
8	C	2.659	-1.645	-1.200
9	C	-2.508	-1.445	-1.697
10	C	3.388	-0.463	-0.862
11	C	-3.324	-0.405	-1.152
12	C	4.787	-0.474	-1.090
13	C	-4.717	-0.469	-1.408
14	C	5.603	0.610	-0.817
15	C	-5.608	0.490	-0.960
16	C	4.998	1.786	-0.297
17	C	-5.093	1.587	-0.220
18	C	3.626	1.846	-0.073
19	C	-3.731	1.690	0.050
20	C	2.759	0.749	-0.337
21	C	-2.773	0.717	-0.381
22	O	5.701	2.920	0.012
23	O	-5.873	2.601	0.269
24	C	7.110	2.918	-0.206
25	C	-7.275	2.553	0.009
26	H	7.617	2.146	0.401
27	H	-7.744	1.658	0.456
28	H	7.359	2.766	-1.271
29	H	-7.491	2.576	-1.074
30	H	7.459	3.910	0.107

31	H	-7.693	3.452	0.479
32	H	0.397	-3.643	-0.590
33	H	-1.167	-3.504	-2.467
34	H	1.395	-3.683	-2.077
35	H	-0.181	-2.229	-3.243
36	N	-0.053	-0.978	1.734
37	C	0.682	-1.982	2.249
38	C	-0.734	-0.181	2.584
39	C	0.750	-2.247	3.617
40	C	-0.716	-0.373	3.966
41	C	0.034	-1.427	4.494
42	H	1.245	-2.576	1.524
43	H	-1.290	0.628	2.102
44	H	1.358	-3.075	3.983
45	H	-1.283	0.300	4.613
46	H	0.066	-1.603	5.572
47	H	3.245	-2.452	-1.685
48	H	-3.042	-2.190	-2.320
49	H	5.235	-1.387	-1.496
50	H	-5.095	-1.317	-1.988
51	H	6.674	0.552	-1.005
52	H	-6.671	0.398	-1.182
53	H	3.185	2.764	0.317
54	H	-3.361	2.552	0.608

Structural parameters

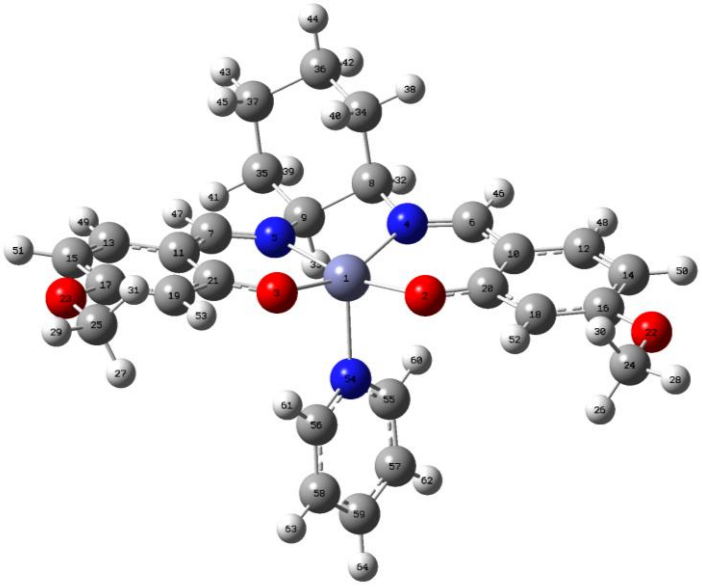
R(1-3)	1.983
R(1-2)	1.983
R(1-5)	2.077
R(1-4)	2.095
R(2-20)	1.293
R(3-21)	1.297
R(4-8)	1.306
R(4-6)	1.452
R(5-7)	1.459
R(5-9)	1.305
R(6-7)	1.542
R(6-32)	1.107
R(6-34)	1.107
R(7-33)	1.107
R(7-35)	1.106
R(8-10)	1.429
R(8-47)	1.109
R(9-11)	1.430
R(9-48)	1.108
R(10-20)	1.463
R(10-12)	1.418
R(11-13)	1.417
R(11-21)	1.469
R(12-14)	1.383
R(12-49)	1.095
R(13-15)	1.384
R(13-50)	1.095
R(14-16)	1.422
R(14-51)	1.089
R(15-17)	1.420
R(15-52)	1.089

R(16-18)	1.391
R(16-22)	1.369
R(17-19)	1.392
R(17-23)	1.369
R(18-20)	1.423
R(18-53)	1.091
R(19-54)	1.091
R(19-21)	1.432
R(22-24)	1.426
R(23-25)	1.427
R(24-30)	1.097
R(24-26)	1.104
R(24-28)	1.104
R(25-31)	1.097
R(25-29)	1.104
R(25-27)	1.104
R(36-37)	1.347
R(36-38)	1.349
R(37-39)	1.395
R(37-42)	1.093
R(38-40)	1.396
R(38-43)	1.093
R(39-41)	1.398
R(39-44)	1.091
R(40-41)	1.397
R(40-45)	1.091
R(41-46)	1.092
A(3-1-2)	98.57
A(3-1-5)	88.55
A(3-1-4)	166.83
A(1-3-21)	130.82
A(2-1-5)	150.55
A(2-1-4)	88.97
A(1-2-20)	130.72
A(5-1-4)	79.72
A(1-5-7)	114.36
A(1-5-9)	126.39
A(1-4-8)	126.34
A(1-4-6)	111.79
A(2-20-10)	124.47
A(2-20-18)	119.19
A(3-21-11)	123.66
A(3-21-19)	121.12
A(8-4-6)	120.86
A(4-8-10)	125.70
A(4-8-47)	118.48
A(4-6-7)	108.00
A(4-6-32)	109.14
A(4-6-34)	112.68
A(7-5-9)	119.25
A(5-7-6)	108.89
A(5-7-33)	112.14
A(5-7-35)	108.90
A(5-9-11)	126.31
A(5-9-48)	118.36
A(7-6-32)	108.35
A(7-6-34)	110.59
A(6-7-33)	110.77

A(6-7-35)	108.24
A(32-6-34)	108.00
A(33-7-35)	107.81
A(10-8-47)	115.82
A(8-10-20)	123.43
A(8-10-12)	117.36
A(11-9-48)	115.33
A(9-11-13)	117.38
A(9-11-21)	122.78
A(20-10-12)	119.19
A(10-20-18)	116.34
A(10-12-14)	122.99
A(10-12-49)	117.97
A(13-11-21)	119.83
A(11-13-15)	122.96
A(11-13-50)	118.00
A(11-21-19)	115.22
A(14-12-49)	119.04
A(12-14-16)	118.02
A(12-14-51)	120.30
A(15-13-50)	119.05
A(13-15-17)	118.03
A(13-15-52)	120.29
A(16-14-51)	121.68
A(14-16-18)	120.92
A(14-16-22)	123.35
A(17-15-52)	121.68
A(15-17-19)	120.87
A(15-17-23)	123.43
A(18-16-22)	115.73
A(16-18-20)	122.53
A(16-18-53)	119.52
A(16-22-24)	118.09
A(19-17-23)	115.70
A(17-19-54)	119.31
A(17-19-21)	123.10
A(17-23-25)	118.06
A(20-18-53)	117.95
A(54-19-21)	117.60
A(22-24-30)	105.57
A(22-24-26)	111.76
A(22-24-28)	111.76
A(23-25-31)	105.58
A(23-25-29)	111.70
A(23-25-27)	111.73
A(30-24-26)	109.19
A(30-24-28)	109.15
A(26-24-28)	109.30
A(31-25-29)	109.21
A(31-25-27)	109.20
A(29-25-27)	109.32
A(37-36-38)	118.32
A(36-37-39)	122.89
A(36-37-42)	115.64
A(36-38-40)	122.45
A(36-38-43)	114.56
A(39-37-42)	121.47
A(37-39-41)	118.64

A(37-39-44)	119.99
A(40-38-43)	122.98
A(38-40-41)	118.99
A(38-40-45)	119.70
A(41-39-44)	121.37
A(39-41-40)	118.69
A(39-41-46)	120.60
A(41-40-45)	121.31
A(40-41-46)	120.70

Adduct 2·py



Cartesian coordinates

		X	Y	Z
1	Zn	-0.033	0.137	-0.001
2	O	-1.608	-0.914	-0.680
3	O	1.358	-1.202	-0.508
4	N	-1.140	1.860	-0.162
5	N	1.467	1.540	0.359
6	C	-2.432	1.926	-0.364
7	C	2.750	1.325	0.287
8	C	-0.362	3.090	-0.072
9	C	0.896	2.815	0.810
10	C	-3.308	0.826	-0.603
11	C	3.379	0.108	-0.135
12	C	-4.698	1.105	-0.734
13	C	4.801	0.091	-0.174
14	C	-5.629	0.131	-1.014
15	C	5.524	-1.010	-0.577
16	C	-5.180	-1.207	-1.192
17	C	4.817	-2.176	-0.974
18	C	-3.834	-1.532	-1.081
19	C	3.427	-2.211	-0.948
20	C	-2.841	-0.546	-0.774
21	C	2.652	-1.087	-0.527

22	O	-6.172	-2.103	-1.476
23	O	5.610	-3.218	-1.365
24	C	-5.791	-3.462	-1.693
25	C	4.963	-4.420	-1.784
26	H	-5.317	-3.896	-0.795
27	H	4.356	-4.855	-0.972
28	H	-6.721	-4.000	-1.913
29	H	5.769	-5.114	-2.051
30	H	-5.099	-3.554	-2.548
31	H	4.319	-4.246	-2.664
32	H	-0.954	3.889	0.420
33	H	0.525	2.639	1.840
34	C	0.048	3.576	-1.476
35	C	1.815	4.049	0.833
36	C	0.942	4.821	-1.413
37	C	2.196	4.556	-0.567
38	H	-0.865	3.773	-2.062
39	H	1.268	4.847	1.367
40	H	0.580	2.754	-1.986
41	H	2.713	3.850	1.443
42	H	0.374	5.661	-0.972
43	H	2.801	5.473	-0.476
44	H	1.225	5.134	-2.431
45	H	2.829	3.813	-1.082
46	H	-2.911	2.926	-0.362
47	H	3.455	2.131	0.560
48	H	-5.028	2.142	-0.609
49	H	5.333	0.999	0.128
50	H	-6.693	0.348	-1.115
51	H	6.614	-1.017	-0.608
52	H	-3.464	-2.548	-1.216
53	H	2.860	-3.091	-1.253
54	N	-0.382	-0.601	1.981
55	C	-1.235	-0.037	2.857
56	C	0.197	-1.773	2.310
57	C	-1.530	-0.606	4.097
58	C	-0.042	-2.410	3.528
59	C	-0.918	-1.815	4.441
60	H	-1.699	0.899	2.534
61	H	0.854	-2.190	1.542
62	H	-2.229	-0.111	4.773
63	H	0.451	-3.358	3.752
64	H	-1.126	-2.288	5.403

Structural parameters

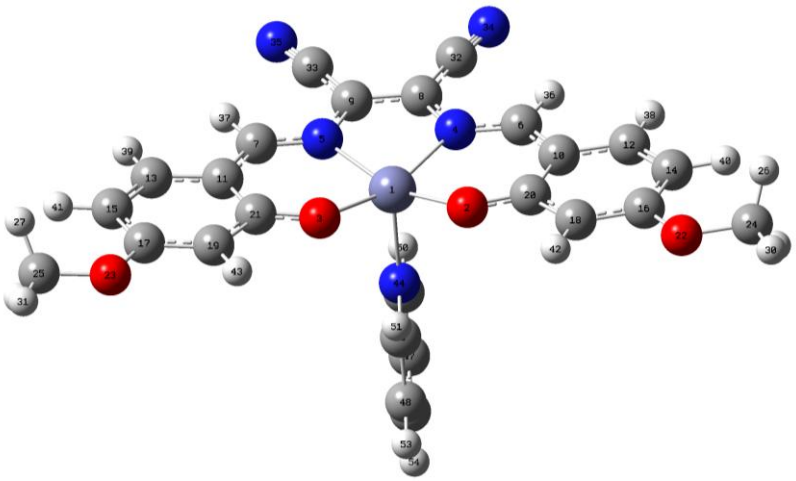
R(1-3)	1.997
R(1-4)	2.054
R(1-2)	2.012
R(2-20)	1.290
R(3-21)	1.299
R(4-8)	1.459
R(4-6)	1.310
R(5-7)	1.303
R(5-9)	1.468
R(6-10)	1.426
R(6-46)	1.109
R(7-11)	1.433

R(7-47)	1.105
R(8-9)	1.560
R(8-34)	1.542
R(8-32)	1.110
R(9-35)	1.539
R(9-33)	1.109
R(10-12)	1.424
R(10-20)	1.459
R(11-21)	1.452
R(11-13)	1.423
R(12-14)	1.376
R(12-48)	1.095
R(13-15)	1.378
R(13-49)	1.095
R(14-16)	1.423
R(14-50)	1.090
R(15-17)	1.420
R(15-51)	1.090
R(16-18)	1.389
R(16-22)	1.367
R(17-19)	1.391
R(17-23)	1.367
R(18-20)	1.432
R(18-52)	1.090
R(19-21)	1.429
R(19-53)	1.090
R(22-24)	1.427
R(23-25)	1.427
R(24-28)	1.097
R(24-26)	1.104
R(24-30)	1.104
R(25-29)	1.097
R(25-31)	1.104
R(25-27)	1.104
R(34-36)	1.534
R(34-38)	1.103
R(34-40)	1.104
R(35-37)	1.537
R(35-39)	1.105
R(35-41)	1.103
R(36-37)	1.535
R(36-42)	1.106
R(36-44)	1.102
R(37-43)	1.102
R(37-45)	1.103
R(54-56)	1.348
R(54-55)	1.346
R(55-57)	1.396
R(55-60)	1.094
R(56-58)	1.396
R(56-61)	1.093
R(57-59)	1.398
R(57-62)	1.091
R(58-59)	1.398
R(58-63)	1.091
R(59-64)	1.092
A(3-1-4)	156.67
A(3-1-2)	96.28

A(1-3-21)	129.64
A(4-1-2)	89.41
A(1-4-8)	114.51
A(1-4-6)	125.91
A(1-2-20)	128.59
A(2-20-10)	124.43
A(2-20-18)	118.79
A(3-21-11)	124.56
A(3-21-19)	118.30
A(8-4-6)	119.55
A(4-8-9)	108.46
A(4-8-34)	110.55
A(4-8-32)	110.49
A(4-6-10)	126.32
A(4-6-46)	118.17
A(7-5-9)	122.90
A(5-7-11)	126.03
A(5-7-47)	119.60
A(5-9-8)	107.02
A(5-9-35)	117.95
A(5-9-33)	106.09
A(10-6-46)	115.51
A(6-10-12)	117.58
A(6-10-20)	123.29
A(11-7-47)	114.37
A(7-11-21)	123.98
A(7-11-13)	117.16
A(9-8-34)	110.87
A(9-8-32)	107.87
A(8-9-35)	110.43
A(8-9-33)	106.47
A(34-8-32)	108.57
A(8-34-36)	111.92
A(8-34-38)	108.71
A(8-34-40)	108.30
A(35-9-33)	108.24
A(9-35-37)	113.48
A(9-35-39)	106.92
A(9-35-41)	110.49
A(12-10-20)	119.08
A(10-12-14)	122.69
A(10-12-48)	117.99
A(10-20-18)	116.78
A(21-11-13)	118.86
A(11-21-19)	117.14
A(11-13-15)	122.84
A(11-13-49)	117.93
A(14-12-48)	119.32
A(12-14-16)	118.54
A(12-14-50)	122.56
A(15-13-49)	119.23
A(13-15-17)	118.47
A(13-15-51)	122.53
A(16-14-50)	118.90
A(14-16-18)	121.04
A(14-16-22)	114.42
A(17-15-51)	118.99
A(15-17-19)	120.86

A(15-17-23)	114.65
A(18-16-22)	124.54
A(16-18-20)	121.87
A(16-18-52)	122.47
A(16-22-24)	117.48
A(19-17-23)	124.49
A(17-19-21)	121.83
A(17-19-53)	122.36
A(17-23-25)	117.53
A(20-18-52)	115.65
A(21-19-53)	115.81
A(22-24-28)	105.71
A(22-24-26)	111.46
A(22-24-30)	111.40
A(23-25-29)	105.70
A(23-25-31)	111.49
A(23-25-27)	111.45
A(28-24-26)	109.54
A(28-24-30)	109.57
A(26-24-30)	109.10
A(29-25-31)	109.52
A(29-25-27)	109.50
A(31-25-27)	109.12
A(36-34-38)	111.07
A(36-34-40)	110.03
A(34-36-37)	111.01
A(34-36-42)	109.48
A(34-36-44)	110.01
A(38-34-40)	106.64
A(37-35-39)	108.90
A(37-35-41)	111.19
A(35-37-36)	110.90
A(35-37-43)	109.59
A(35-37-45)	110.19
A(39-35-41)	105.43
A(37-36-42)	109.33
A(37-36-44)	110.41
A(36-37-43)	110.48
A(36-37-45)	109.11
A(42-36-44)	106.49
A(43-37-45)	106.47
A(56-54-55)	118.54
A(54-56-58)	122.42
A(54-56-61)	114.76
A(54-55-57)	122.74
A(54-55-60)	115.77
A(57-55-60)	121.49
A(55-57-59)	118.61
A(55-57-62)	120.03
A(58-56-61)	122.81
A(56-58-59)	118.89
A(56-58-63)	119.85
A(59-57-62)	121.36
A(57-59-58)	118.79
A(57-59-64)	120.56
A(59-58-63)	121.27
A(58-59-64)	120.65

Adduct 3·py



Cartesian coordinates

		X	Y	Z
1	Zn	0.003	0.100	-0.231
2	O	-1.475	-1.170	-0.602
3	O	1.487	-1.170	-0.585
4	N	-1.334	1.695	-0.438
5	N	1.338	1.696	-0.432
6	C	-2.655	1.582	-0.521
7	C	2.660	1.586	-0.509
8	C	-0.700	2.922	-0.424
9	C	0.702	2.922	-0.420
10	C	-3.370	0.365	-0.606
11	C	3.377	0.370	-0.593
12	C	-4.791	0.461	-0.677
13	C	4.798	0.470	-0.662
14	C	-5.610	-0.641	-0.789
15	C	5.621	-0.629	-0.773
16	C	-5.006	-1.933	-0.840
17	C	5.021	-1.923	-0.824
18	C	-3.625	-2.077	-0.775
19	C	3.640	-2.071	-0.759
20	C	-2.749	-0.965	-0.652
21	C	2.761	-0.961	-0.637
22	O	-5.720	-3.088	-0.956
23	O	5.738	-3.076	-0.939
24	C	-7.145	-3.004	-1.050
25	C	7.162	-2.988	-1.035
26	H	-7.459	-2.432	-1.940
27	H	7.473	-2.415	-1.926
28	H	-7.587	-2.553	-0.146
29	H	7.604	-2.535	-0.132
30	H	-7.492	-4.040	-1.144
31	H	7.512	-4.022	-1.130
32	C	-1.443	4.137	-0.427
33	C	1.444	4.138	-0.420
34	N	-2.130	5.085	-0.423
35	N	2.129	5.087	-0.414

36	H	-3.259	2.505	-0.540
37	H	3.261	2.510	-0.525
38	H	-5.239	1.458	-0.643
39	H	5.243	1.469	-0.628
40	H	-6.691	-0.517	-0.840
41	H	6.701	-0.502	-0.824
42	H	-3.186	-3.074	-0.824
43	H	3.204	-3.069	-0.808
44	N	-0.007	-0.213	1.868
45	C	-0.074	0.742	2.814
46	C	0.045	-1.505	2.256
47	C	-0.092	0.452	4.179
48	C	0.031	-1.882	3.599
49	C	-0.039	-0.887	4.578
50	H	-0.114	1.773	2.454
51	H	0.100	-2.235	1.446
52	H	-0.147	1.261	4.908
53	H	0.074	-2.938	3.867
54	H	-0.052	-1.150	5.638

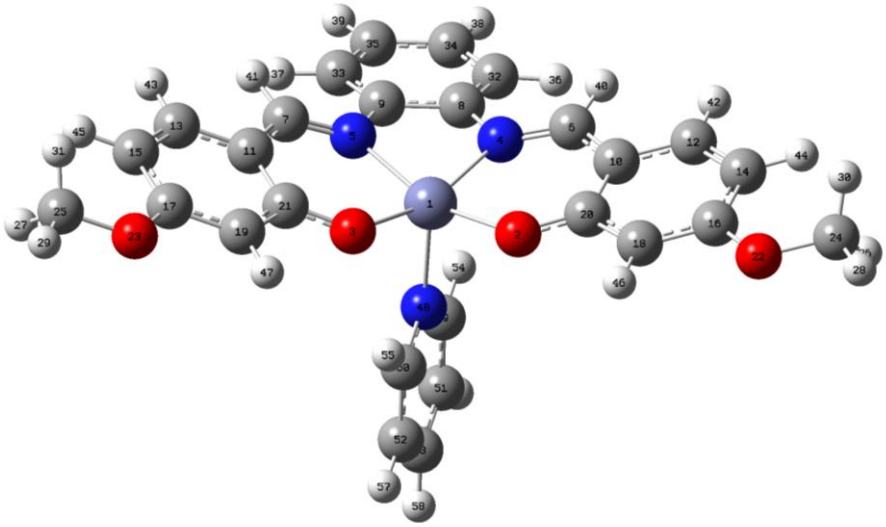
Structural parameters

R(1-2)	1.983
R(1-3)	1.985
R(2-20)	1.292
R(3-21)	1.292
R(4-6)	1.329
R(4-8)	1.381
R(5-7)	1.328
R(5-9)	1.381
R(6-10)	1.414
R(6-36)	1.103
R(7-11)	1.414
R(7-37)	1.103
R(8-9)	1.402
R(8-32)	1.424
R(9-33)	1.424
R(10-12)	1.426
R(10-20)	1.468
R(11-13)	1.426
R(11-21)	1.468
R(12-14)	1.377
R(12-38)	1.094
R(13-15)	1.377
R(13-39)	1.094
R(14-16)	1.427
R(14-40)	1.089
R(15-17)	1.426
R(15-41)	1.089
R(16-18)	1.390
R(16-22)	1.363
R(17-19)	1.390
R(17-23)	1.363
R(18-20)	1.421
R(18-42)	1.091
R(19-21)	1.421
R(19-43)	1.091
R(22-24)	1.430

R(23-25)	1.430
R(24-26)	1.103
R(24-30)	1.097
R(24-28)	1.103
R(25-31)	1.097
R(25-27)	1.103
R(25-29)	1.103
R(32-34)	1.171
R(33-35)	1.171
R(44-46)	1.349
R(44-45)	1.347
R(45-47)	1.395
R(45-50)	1.093
R(46-48)	1.395
R(46-51)	1.092
R(47-49)	1.398
R(47-52)	1.091
R(48-49)	1.398
R(48-53)	1.091
R(49-54)	1.092
A(2-1-3)	96.52
A(1-2-20)	129.80
A(1-3-21)	129.83
A(2-20-10)	124.05
A(2-20-18)	119.16
A(3-21-11)	124.05
A(3-21-19)	119.17
A(6-4-8)	122.20
A(4-6-10)	125.40
A(4-6-36)	118.31
A(4-8-9)	117.37
A(4-8-32)	121.19
A(7-5-9)	122.15
A(5-7-11)	125.43
A(5-7-37)	118.30
A(5-9-8)	117.39
A(5-9-33)	121.20
A(10-6-36)	116.29
A(6-10-12)	116.65
A(6-10-20)	124.60
A(11-7-37)	116.27
A(7-11-13)	116.64
A(7-11-21)	124.62
A(9-8-32)	121.43
A(8-9-33)	121.41
A(8-32-34)	175.52
A(9-33-35)	175.56
A(12-10-20)	118.73
A(10-12-14)	122.87
A(10-12-38)	117.88
A(10-20-18)	116.78
A(13-11-21)	118.73
A(11-13-15)	122.88
A(11-13-39)	117.87
A(11-21-19)	116.78
A(14-12-38)	119.25
A(12-14-16)	118.40
A(12-14-40)	120.18

A(15-13-39)	119.25
A(13-15-17)	118.39
A(13-15-41)	120.18
A(16-14-40)	121.42
A(14-16-18)	120.83
A(14-16-22)	123.29
A(17-15-41)	121.43
A(15-17-19)	120.83
A(15-17-23)	123.30
A(18-16-22)	115.88
A(16-18-20)	122.39
A(16-18-42)	119.54
A(16-22-24)	118.53
A(19-17-23)	115.88
A(17-19-21)	122.39
A(17-19-43)	119.51
A(17-23-25)	118.51
A(20-18-42)	118.08
A(21-19-43)	118.09
A(22-24-26)	111.56
A(22-24-30)	105.41
A(22-24-28)	111.65
A(23-25-31)	105.41
A(23-25-27)	111.56
A(23-25-29)	111.65
A(26-24-30)	109.26
A(26-24-28)	109.60
A(30-24-28)	109.24
A(31-25-27)	109.26
A(31-25-29)	109.24
A(27-25-29)	109.60
A(46-44-45)	118.59
A(44-46-48)	122.36
A(44-46-51)	115.34
A(44-45-47)	122.71
A(44-45-50)	116.07
A(47-45-50)	121.23
A(45-47-49)	118.59
A(45-47-52)	119.99
A(48-46-51)	122.30
A(46-48-49)	118.87
A(46-48-53)	119.83
A(49-47-52)	121.42
A(47-49-48)	118.88
A(47-49-54)	120.53
A(49-48-53)	121.30
A(48-49-54)	120.59

Adduct 4·py



Cartesian coordinates

		X	Y	Z
1	Zn	0.010	0.055	0.020
2	O	-1.445	-1.296	0.033
3	O	1.517	-1.253	0.099
4	N	-1.324	1.488	-0.693
5	N	1.325	1.517	-0.662
6	C	-2.563	1.245	-1.070
7	C	2.575	1.309	-1.015
8	C	-0.729	2.748	-0.841
9	C	0.704	2.764	-0.819
10	C	-3.262	0.017	-0.916
11	C	3.305	0.097	-0.855
12	C	-4.617	-0.014	-1.348
13	C	4.660	0.099	-1.282
14	C	-5.414	-1.136	-1.246
15	C	5.485	-1.004	-1.178
16	C	-4.845	-2.316	-0.690
17	C	4.942	-2.197	-0.625
18	C	-3.520	-2.340	-0.270
19	C	3.617	-2.251	-0.207
20	C	-2.671	-1.201	-0.358
21	C	2.744	-1.133	-0.297
22	O	-5.538	-3.485	-0.537
23	O	5.661	-3.350	-0.473
24	C	-6.899	-3.524	-0.964
25	C	7.023	-3.359	-0.900
26	H	-7.524	-2.804	-0.408
27	H	7.631	-2.627	-0.340
28	H	-7.245	-4.543	-0.749
29	H	7.390	-4.371	-0.688
30	H	-6.993	-3.330	-2.047
31	H	7.112	-3.159	-1.982
32	C	-1.425	3.967	-0.946
33	C	1.375	3.998	-0.901
34	C	-0.737	5.177	-1.051

35	C	0.665	5.192	-1.027
36	H	-2.517	3.967	-0.921
37	H	2.465	4.023	-0.836
38	H	-1.296	6.112	-1.126
39	H	1.204	6.141	-1.083
40	H	-3.130	2.048	-1.574
41	H	3.131	2.128	-1.504
42	H	-5.039	0.903	-1.774
43	H	5.062	1.026	-1.705
44	H	-6.448	-1.107	-1.585
45	H	6.519	-0.950	-1.514
46	H	-3.101	-3.260	0.140
47	H	3.220	-3.183	0.198
48	N	-0.041	0.368	2.122
49	C	-0.517	1.471	2.730
50	C	0.362	-0.668	2.886
51	C	-0.603	1.589	4.118
52	C	0.307	-0.633	4.280
53	C	-0.183	0.515	4.909
54	H	-0.841	2.280	2.070
55	H	0.745	-1.529	2.333
56	H	-0.992	2.505	4.564
57	H	0.643	-1.496	4.858
58	H	-0.238	0.573	5.998

Structural parameters

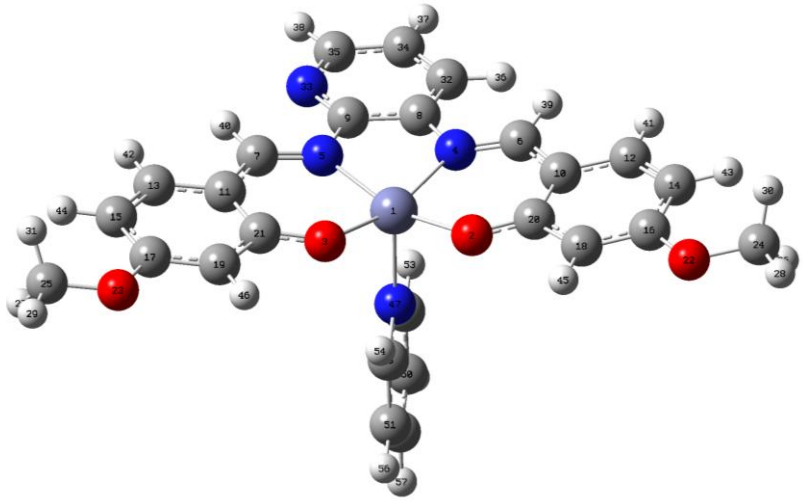
R(1-2)	1.985
R(1-3)	1.997
R(2-20)	1.291
R(3-21)	1.295
R(4-6)	1.318
R(4-8)	1.401
R(5-9)	1.401
R(5-7)	1.316
R(6-10)	1.422
R(6-40)	1.104
R(7-11)	1.423
R(7-41)	1.104
R(8-9)	1.433
R(8-32)	1.408
R(9-33)	1.407
R(10-12)	1.422
R(10-20)	1.465
R(11-13)	1.421
R(11-21)	1.462
R(12-14)	1.381
R(12-42)	1.095
R(13-15)	1.381
R(13-43)	1.095
R(14-16)	1.424
R(14-44)	1.089
R(15-17)	1.422
R(15-45)	1.089
R(16-18)	1.390
R(16-22)	1.367
R(17-19)	1.391
R(17-23)	1.367

R(18-20)	1.423
R(18-46)	1.091
R(19-21)	1.421
R(19-47)	1.091
R(22-24)	1.427
R(23-25)	1.427
R(24-30)	1.104
R(24-28)	1.097
R(24-26)	1.104
R(25-29)	1.097
R(25-31)	1.104
R(25-27)	1.104
R(32-34)	1.396
R(32-36)	1.092
R(33-35)	1.396
R(33-37)	1.092
R(34-35)	1.402
R(34-38)	1.092
R(35-39)	1.092
R(48-49)	1.347
R(48-50)	1.349
R(49-51)	1.395
R(49-54)	1.093
R(50-52)	1.396
R(50-55)	1.093
R(51-53)	1.398
R(51-56)	1.091
R(52-53)	1.398
R(52-57)	1.091
R(53-58)	1.092
A(2-1-3)	96.15
A(1-2-20)	130.11
A(1-3-21)	129.99
A(2-20-10)	124.06
A(2-20-18)	119.30
A(3-21-11)	123.90
A(3-21-19)	119.35
A(6-4-8)	122.35
A(4-6-10)	126.20
A(4-6-40)	118.62
A(4-8-9)	115.67
A(4-8-32)	125.18
A(9-5-7)	122.11
A(5-9-8)	115.75
A(5-9-33)	125.14
A(5-7-11)	126.28
A(5-7-41)	118.62
A(10-6-40)	115.17
A(6-10-12)	116.99
A(6-10-20)	124.15
A(11-7-41)	115.08
A(7-11-13)	116.96
A(7-11-21)	124.22
A(9-8-32)	119.08
A(8-9-33)	119.06
A(8-32-34)	120.83
A(8-32-36)	119.55
A(9-33-35)	120.86

A(9-33-37)	119.54
A(12-10-20)	118.85
A(10-12-14)	123.02
A(10-12-42)	117.91
A(10-20-18)	116.63
A(13-11-21)	118.82
A(11-13-15)	123.04
A(11-13-43)	117.91
A(11-21-19)	116.75
A(14-12-42)	119.07
A(12-14-16)	118.17
A(12-14-44)	120.27
A(15-13-43)	119.05
A(13-15-17)	118.14
A(13-15-45)	120.28
A(16-14-44)	121.56
A(14-16-18)	120.87
A(14-16-22)	123.33
A(17-15-45)	121.58
A(15-17-19)	120.83
A(15-17-23)	123.41
A(18-16-22)	115.80
A(16-18-20)	122.44
A(16-18-46)	119.59
A(16-22-24)	118.28
A(19-17-23)	115.76
A(17-19-21)	122.41
A(17-19-47)	119.43
A(17-23-25)	118.24
A(20-18-46)	117.97
A(21-19-47)	118.16
A(22-24-30)	111.71
A(22-24-28)	105.52
A(22-24-26)	111.73
A(23-25-29)	105.52
A(23-25-31)	111.69
A(23-25-27)	111.72
A(30-24-28)	109.18
A(30-24-26)	109.38
A(28-24-26)	109.19
A(29-25-31)	109.20
A(29-25-27)	109.21
A(31-25-27)	109.39
A(34-32-36)	119.60
A(32-34-35)	120.08
A(32-34-38)	119.72
A(35-33-37)	119.58
A(33-35-34)	120.08
A(33-35-39)	119.73
A(35-34-38)	120.18
A(34-35-39)	120.18
A(49-48-50)	118.58
A(48-49-51)	122.69
A(48-49-54)	115.96
A(48-50-52)	122.37
A(48-50-55)	115.00
A(51-49-54)	121.35
A(49-51-53)	118.65

A(49-51-56)	119.96
A(52-50-55)	122.63
A(50-52-53)	118.90
A(50-52-57)	119.80
A(53-51-56)	121.39
A(51-53-52)	118.81
A(51-53-58)	120.57
A(53-52-57)	121.29
A(52-53-58)	120.63

Adduct 5·py



Cartesian coordinates

		X	Y	Z
1	Zn	-0.015	0.064	-0.158
2	O	-1.488	-1.254	-0.373
3	O	1.446	-1.255	-0.422
4	N	-1.358	1.629	-0.456
5	N	1.305	1.599	-0.517
6	C	-2.649	1.486	-0.688
7	C	2.611	1.480	-0.680
8	C	-0.729	2.879	-0.478
9	C	0.706	2.863	-0.524
10	C	-3.367	0.261	-0.707
11	C	3.335	0.261	-0.706
12	C	-4.770	0.341	-0.927
13	C	4.744	0.357	-0.884
14	C	-5.589	-0.769	-0.979
15	C	5.572	-0.745	-0.941
16	C	-4.993	-2.052	-0.815
17	C	4.983	-2.036	-0.819
18	C	-3.625	-2.182	-0.612
19	C	3.611	-2.181	-0.647
20	C	-2.752	-1.060	-0.546
21	C	2.730	-1.068	-0.577

22	O	-5.705	-3.219	-0.850
23	O	5.704	-3.197	-0.864
24	C	-7.112	-3.146	-1.077
25	C	7.116	-3.109	-1.058
26	H	-7.627	-2.585	-0.278
27	H	7.608	-2.563	-0.235
28	H	-7.464	-4.185	-1.072
29	H	7.475	-4.145	-1.069
30	H	-7.344	-2.690	-2.055
31	H	7.365	-2.628	-2.020
32	C	-1.352	4.137	-0.436
33	N	1.450	3.979	-0.559
34	C	-0.571	5.294	-0.471
35	C	0.821	5.162	-0.541
36	H	-2.440	4.214	-0.364
37	H	-1.032	6.283	-0.436
38	H	1.464	6.048	-0.572
39	H	-3.255	2.382	-0.914
40	H	3.185	2.411	-0.813
41	H	-5.213	1.334	-1.056
42	H	5.178	1.357	-0.980
43	H	-6.659	-0.654	-1.145
44	H	6.645	-0.619	-1.077
45	H	-3.189	-3.176	-0.502
46	H	3.184	-3.182	-0.567
47	N	0.018	-0.117	1.971
48	C	-0.220	0.879	2.844
49	C	0.249	-1.356	2.453
50	C	-0.233	0.685	4.226
51	C	0.252	-1.638	3.820
52	C	0.008	-0.600	4.723
53	H	-0.406	1.864	2.408
54	H	0.442	-2.120	1.696
55	H	-0.427	1.526	4.894
56	H	0.444	-2.655	4.164
57	H	0.005	-0.788	5.799

Structural parameters

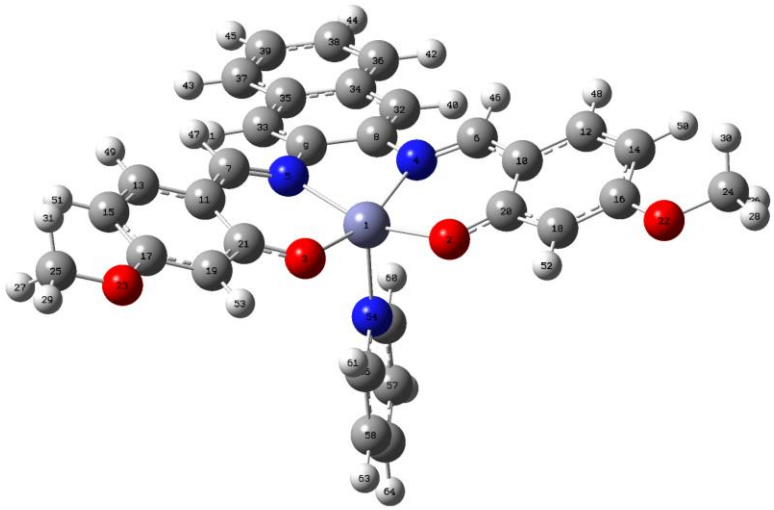
R(1-3)	1.986
R(1-2)	1.989
R(1-4)	2.084
R(1-5)	2.056
R(2-20)	1.290
R(3-21)	1.306
R(4-6)	1.319
R(4-8)	1.399
R(5-9)	1.399
R(5-7)	1.322
R(6-10)	1.420
R(6-39)	1.104
R(7-11)	1.418
R(7-40)	1.102
R(8-9)	1.436
R(8-32)	1.405
R(9-33)	1.341
R(10-12)	1.423
R(10-20)	1.465

R(11-13)	1.423
R(11-21)	1.465
R(12-14)	1.380
R(12-41)	1.095
R(13-15)	1.380
R(13-42)	1.095
R(14-16)	1.424
R(14-43)	1.089
R(15-17)	1.424
R(15-44)	1.089
R(16-18)	1.390
R(16-22)	1.367
R(17-19)	1.390
R(17-23)	1.367
R(18-20)	1.423
R(18-45)	1.091
R(19-21)	1.422
R(19-46)	1.091
R(22-24)	1.428
R(23-25)	1.428
R(24-30)	1.104
R(24-28)	1.097
R(24-26)	1.104
R(25-29)	1.097
R(25-31)	1.104
R(25-27)	1.104
R(32-34)	1.397
R(32-36)	1.092
R(33-35)	1.340
R(34-35)	1.400
R(34-37)	1.092
R(35-38)	1.095
R(47-48)	1.346
R(47-49)	1.349
R(48-50)	1.395
R(48-53)	1.093
R(49-51)	1.395
R(49-54)	1.092
R(50-52)	1.398
R(50-55)	1.091
R(51-52)	1.398
R(51-56)	1.091
R(52-57)	1.092
A(3-1-2)	95.20
A(3-1-4)	162.53
A(3-1-5)	90.03
A(1-3-21)	130.05
A(2-1-4)	90.25
A(2-1-5)	162.08
A(1-2-20)	129.85
A(4-1-5)	80.10
A(1-4-6)	125.06
A(1-4-8)	112.50
A(1-5-9)	113.65
A(1-5-7)	126.08
A(2-20-10)	124.12
A(2-20-18)	119.23
A(3-21-11)	123.10

A(3-21-19)	120.18
A(6-4-8)	122.30
A(4-6-10)	126.18
A(4-6-39)	118.98
A(4-8-9)	116.13
A(4-8-32)	126.85
A(9-5-7)	120.22
A(5-9-8)	115.93
A(5-9-33)	121.00
A(5-7-11)	125.70
A(5-7-40)	117.00
A(10-6-39)	114.82
A(6-10-12)	116.85
A(6-10-20)	124.35
A(11-7-40)	117.31
A(7-11-13)	116.68
A(7-11-21)	124.56
A(9-8-32)	117.01
A(8-9-33)	123.07
A(8-32-34)	119.53
A(8-32-36)	120.49
A(9-33-35)	118.32
A(12-10-20)	118.78
A(10-12-14)	123.06
A(10-12-41)	117.90
A(10-20-18)	116.65
A(13-11-21)	118.76
A(11-13-15)	123.05
A(11-13-42)	117.72
A(11-21-19)	116.71
A(14-12-41)	119.04
A(12-14-16)	118.19
A(12-14-43)	120.27
A(15-13-42)	119.23
A(13-15-17)	118.19
A(13-15-44)	120.27
A(16-14-43)	121.54
A(14-16-18)	120.85
A(14-16-22)	123.28
A(17-15-44)	121.54
A(15-17-19)	120.88
A(15-17-23)	123.31
A(18-16-22)	115.87
A(16-18-20)	122.47
A(16-18-45)	119.57
A(16-22-24)	118.28
A(19-17-23)	115.82
A(17-19-21)	122.41
A(17-19-46)	119.45
A(17-23-25)	118.27
A(20-18-45)	117.96
A(21-19-46)	118.14
A(22-24-30)	111.66
A(22-24-28)	105.50
A(22-24-26)	111.72
A(23-25-29)	105.50
A(23-25-31)	111.65
A(23-25-27)	111.73

A(30-24-28)	109.21
A(30-24-26)	109.43
A(28-24-26)	109.20
A(29-25-31)	109.23
A(29-25-27)	109.21
A(31-25-27)	109.42
A(34-32-36)	119.97
A(32-34-35)	118.69
A(32-34-37)	120.89
A(33-35-34)	123.35
A(33-35-38)	116.03
A(35-34-37)	120.42
A(34-35-38)	120.62
A(48-47-49)	118.59
A(47-48-50)	122.73
A(47-48-53)	115.97
A(47-49-51)	122.36
A(47-49-54)	115.15
A(50-48-53)	121.30
A(48-50-52)	118.60
A(48-50-55)	120.01
A(51-49-54)	122.49
A(49-51-52)	118.88
A(49-51-56)	119.83
A(52-50-55)	121.39
A(50-52-51)	118.83
A(50-52-57)	120.54
A(52-51-56)	121.28
A(51-52-57)	120.62

Adduct 6·py



Cartesian coordinates

		X	Y	Z
1	Zn	0.030	-0.582	0.118
2	O	-1.390	-1.968	0.027
3	O	1.575	-1.848	0.091
4	N	-1.342	0.859	-0.501
5	N	1.298	0.958	-0.472
6	C	-2.562	0.605	-0.933
7	C	2.539	0.803	-0.884
8	C	-0.795	2.148	-0.533
9	C	0.655	2.202	-0.513
10	C	-3.222	-0.652	-0.887
11	C	3.299	-0.398	-0.832
12	C	-4.560	-0.696	-1.369
13	C	4.636	-0.336	-1.309
14	C	-5.321	-1.847	-1.371
15	C	5.487	-1.424	-1.306
16	C	-4.730	-3.045	-0.875
17	C	4.992	-2.662	-0.809
18	C	-3.420	-3.054	-0.411
19	C	3.686	-2.774	-0.345
20	C	-2.607	-1.886	-0.394
21	C	2.785	-1.674	-0.335
22	O	-5.387	-4.242	-0.828
23	O	5.741	-3.804	-0.758
24	C	-6.731	-4.296	-1.307
25	C	7.084	-3.753	-1.239
26	H	-7.399	-3.638	-0.723
27	H	7.700	-3.046	-0.657
28	H	-7.047	-5.338	-1.177
29	H	7.481	-4.767	-1.111
30	H	-6.794	-4.028	-2.376
31	H	7.124	-3.480	-2.308
32	C	-1.521	3.333	-0.518
33	C	1.290	3.437	-0.477
34	C	-0.882	4.599	-0.509
35	C	0.558	4.653	-0.487

36	C	-1.613	5.820	-0.499
37	C	1.196	5.924	-0.455
38	C	-0.961	7.039	-0.474
39	C	0.455	7.092	-0.452
40	H	-2.614	3.301	-0.485
41	H	2.380	3.488	-0.410
42	H	-2.706	5.777	-0.515
43	H	2.289	5.962	-0.437
44	H	-1.538	7.967	-0.471
45	H	0.961	8.060	-0.431
46	H	-3.137	1.426	-1.396
47	H	3.054	1.668	-1.337
48	H	-5.000	0.234	-1.745
49	H	5.001	0.625	-1.687
50	H	-6.344	-1.829	-1.743
51	H	6.506	-1.324	-1.676
52	H	-2.983	-3.987	-0.051
53	H	3.325	-3.739	0.013
54	N	-0.020	-0.421	2.231
55	C	-0.500	0.635	2.916
56	C	0.395	-1.504	2.920
57	C	-0.578	0.656	4.309
58	C	0.347	-1.566	4.313
59	C	-0.147	-0.466	5.022
60	H	-0.832	1.485	2.315
61	H	0.781	-2.322	2.308
62	H	-0.971	1.537	4.819
63	H	0.692	-2.463	4.829
64	H	-0.196	-0.484	6.113

Structural parameters

R(1-2)	1.986
R(1-3)	1.998
R(2-20)	1.291
R(3-21)	1.294
R(4-6)	1.318
R(4-8)	1.401
R(5-9)	1.401
R(5-7)	1.316
R(6-10)	1.421
R(6-46)	1.105
R(7-11)	1.422
R(7-47)	1.104
R(8-9)	1.451
R(8-32)	1.390
R(9-33)	1.389
R(10-20)	1.465
R(10-12)	1.422
R(11-13)	1.421
R(11-21)	1.463
R(12-14)	1.380
R(12-48)	1.095
R(13-15)	1.381
R(13-49)	1.095
R(14-16)	1.424
R(14-50)	1.089
R(15-17)	1.423

R(15-51)	1.089
R(16-18)	1.390
R(16-22)	1.367
R(17-19)	1.391
R(17-23)	1.367
R(18-20)	1.423
R(18-52)	1.091
R(19-21)	1.421
R(19-53)	1.091
R(22-24)	1.428
R(23-25)	1.428
R(24-30)	1.104
R(24-28)	1.097
R(24-26)	1.104
R(25-29)	1.097
R(25-31)	1.104
R(25-27)	1.104
R(32-34)	1.419
R(32-40)	1.093
R(33-35)	1.419
R(33-41)	1.093
R(34-35)	1.441
R(34-36)	1.422
R(35-37)	1.423
R(36-38)	1.383
R(36-42)	1.094
R(37-39)	1.383
R(37-43)	1.094
R(38-44)	1.093
R(38-39)	1.418
R(39-45)	1.092
R(54-55)	1.347
R(54-56)	1.349
R(55-57)	1.395
R(55-60)	1.093
R(56-58)	1.395
R(56-61)	1.093
R(57-59)	1.398
R(57-62)	1.091
R(58-59)	1.398
R(58-63)	1.091
R(59-64)	1.092
A(2-1-3)	96.32
A(1-2-20)	130.13
A(1-3-21)	129.98
A(2-20-10)	124.02
A(2-20-18)	119.35
A(3-21-11)	123.84
A(3-21-19)	119.41
A(6-4-8)	122.10
A(4-6-10)	126.18
A(4-6-46)	118.44
A(4-8-9)	115.10
A(4-8-32)	125.45
A(9-5-7)	121.88
A(5-9-8)	115.20
A(5-9-33)	125.39
A(5-7-11)	126.27

A(5-7-47)	118.41
A(10-6-46)	115.36
A(6-10-20)	124.13
A(6-10-12)	117.00
A(11-7-47)	115.30
A(7-11-13)	116.97
A(7-11-21)	124.17
A(9-8-32)	119.37
A(8-9-33)	119.34
A(8-32-34)	121.70
A(8-32-40)	119.86
A(9-33-35)	121.72
A(9-33-41)	119.88
A(20-10-12)	118.87
A(10-20-18)	116.63
A(10-12-14)	122.99
A(10-12-48)	117.92
A(13-11-21)	118.86
A(11-13-15)	122.99
A(11-13-49)	117.91
A(11-21-19)	116.74
A(14-12-48)	119.09
A(12-14-16)	118.19
A(12-14-50)	120.27
A(15-13-49)	119.09
A(13-15-17)	118.17
A(13-15-51)	120.27
A(16-14-50)	121.54
A(14-16-18)	120.88
A(14-16-22)	123.29
A(17-15-51)	121.57
A(15-17-19)	120.86
A(15-17-23)	123.35
A(18-16-22)	115.82
A(16-18-20)	122.42
A(16-18-52)	119.59
A(16-22-24)	118.30
A(19-17-23)	115.79
A(17-19-21)	122.37
A(17-19-53)	119.43
A(17-23-25)	118.22
A(20-18-52)	117.98
A(21-19-53)	118.19
A(22-24-30)	111.69
A(22-24-28)	105.52
A(22-24-26)	111.72
A(23-25-29)	105.51
A(23-25-31)	111.67
A(23-25-27)	111.70
A(30-24-28)	109.20
A(30-24-26)	109.41
A(28-24-26)	109.20
A(29-25-31)	109.22
A(29-25-27)	109.22
A(31-25-27)	109.41
A(34-32-40)	118.42
A(32-34-35)	118.90
A(32-34-36)	122.28

A(35-33-41)	118.38
A(33-35-34)	118.94
A(33-35-37)	122.27
A(35-34-36)	118.81
A(34-35-37)	118.78
A(34-36-38)	120.95
A(34-36-42)	118.69
A(35-37-39)	120.96
A(35-37-43)	118.67
A(38-36-42)	120.36
A(36-38-44)	120.05
A(36-38-39)	120.25
A(39-37-43)	120.36
A(37-39-38)	120.25
A(37-39-45)	120.05
A(44-38-39)	119.70
A(38-39-45)	119.70
A(55-54-56)	118.59
A(54-55-57)	122.68
A(54-55-60)	116.01
A(54-56-58)	122.36
A(54-56-61)	115.06
A(57-55-60)	121.31
A(55-57-59)	118.66
A(55-57-62)	119.94
A(58-56-61)	122.57
A(56-58-59)	118.90
A(56-58-63)	119.80
A(59-57-62)	121.40
A(57-59-58)	118.81
A(57-59-64)	120.56
A(59-58-63)	121.30
A(58-59-64)	120.63

VI. Parameters of distortion from the planarity of the N_2O_2 coordinated atoms for dimers and adducts.

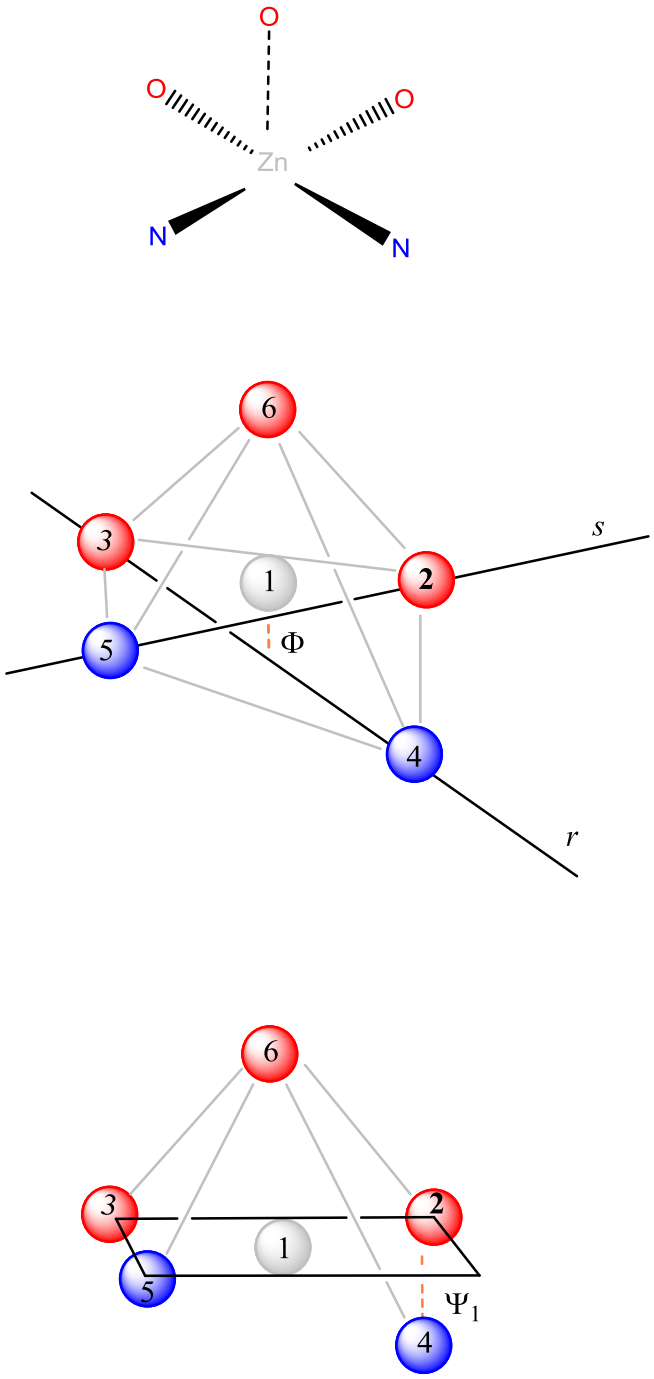
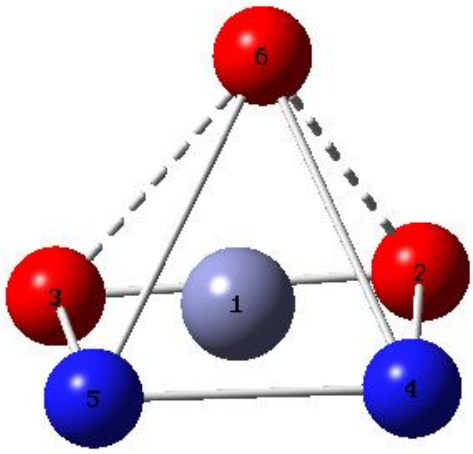


Fig. S3 Graphical representation of distortion parameters Φ and Ψ_1.

Coordination sphere of 1D



Cartesian coordinates

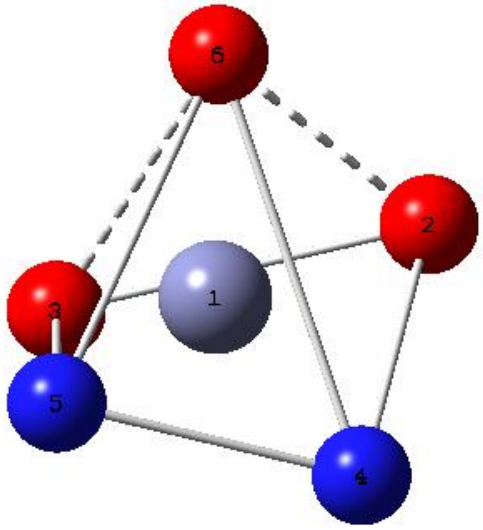
Zn_1	0.8648	0.3886	1.2315
O_2	-0.7622	1.1311	0.2075
O_3	2.2689	1.4598	0.3531
N_4	-0.4940	-0.2909	2.6214
N_5	2.1632	-0.1382	2.7355
O_6	0.7622	-1.1310	-0.2075

d	Å	∠	°
2-3	3.05	2-1-6	83.19
2-4	2.81	3-1-6	97.06
2-5	4.07	4-1-6	101.07
3-4	3.98	5-1-6	110.34
3-5	2.87	2-1-5	162.66
1-6	2.10	3-1-4	161.73
2-6	2.76		
3-6	3.05		
4-6	3.21		
5-6	3.41		

Equations of planes:

α_1 ($O_2O_3N_4$) = -0.226x + 1.654y + z – 2.251 = 0
α_2 ($O_2O_3N_5$) = -0.211x + 1.508y + z – 2.047 = 0
α_3 ($O_2N_4N_5$) = -0.140x + 1.671y + z – 2.204 = 0
α_4 ($O_3N_4N_5$) = -0.130x + 1.503y + z – 2.248 = 0

Coordination sphere of 2D



Cartesian coordinates

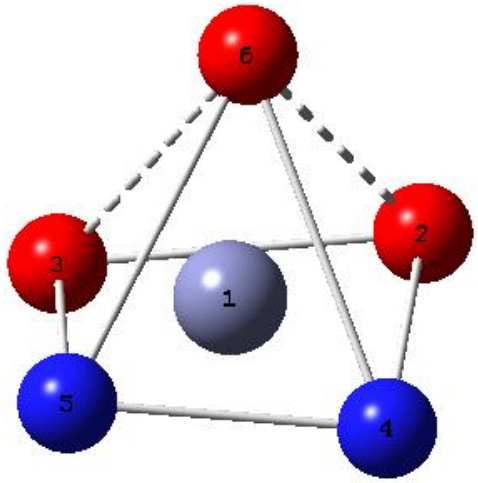
Zn_1	-1.3483	-0.3128	-0.8856
O_2	0.6984	-0.2736	-1.0681
O_3	-1.9937	1.5463	-1.1213
N_4	-1.1872	-1.9180	-2.2613
N_5	-3.2685	-1.0078	-0.9225
O_6	-0.6984	-0.2736	1.0681

d	Å	∠	°
2-3	3.25	2-1-6	76.68
2-4	2.77	3-1-6	101.40
2-5	4.04	4-1-6	127.30
3-4	3.74	5-1-6	108.68
3-5	2.86	2-1-5	160.25
1-6	2.06	3-1-4	131.13
2-6	2.55		
3-6	3.13		
4-6	3.75		
5-6	3.33		

Equations of planes:

α_1 ($O_2O_3N_4$) = -0.289x - 0.396y + z + 1.160 = 0
α_2 ($O_2O_3N_5$) = 0.024x + 0.065y + z + 1.069 = 0
α_3 ($O_2N_4N_5$) = 0.217x - 0.974y + z + 0.650 = 0
α_4 ($O_3N_4N_5$) = 0.555x - 0.200y + z + 2.537 = 0

Coordination sphere of 3D



Cartesian coordinates

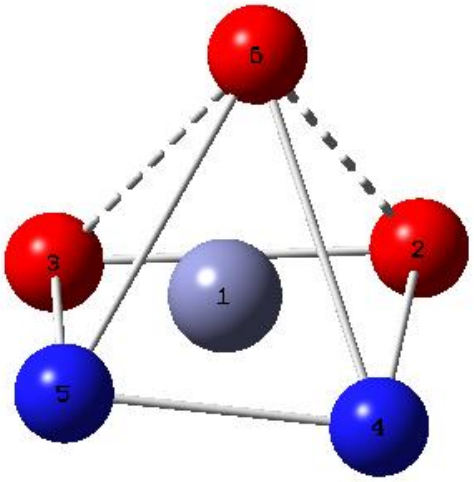
Zn_1	-0.9367	-0.8935	-0.8801
O_2	0.7435	0.2199	-1.1083
O_3	-2.2754	0.4384	-1.4271
N_4	0.2479	-2.5894	-1.0511
N_5	-2.3936	-2.3622	-0.8224
O_6	-0.7435	-0.2199	1.1083

d	Å	∠	°
2-3	3.04	2-1-6	81.65
2-4	2.85	3-1-6	92.22
2-5	4.07	4-1-6	106.64
3-4	3.96	5-1-6	105.36
3-5	2.87	2-1-5	167.36
1-6	2.11	3-1-4	156.80
2-6	2.71		
3-6	3.03		
4-6	3.36		
5-6	3.32		

Equations of planes:

α_1 ($O_2O_3N_4$) = -0.103x + 0.039y + z + 1.178 = 0
α_2 ($O_2O_3N_5$) = -0.090x + 0.221y + z + 1.128 = 0
α_3 ($O_2N_4N_5$) = 0.088x + 0.006y + z + 1.044 = 0
α_4 ($O_3N_4N_5$) = 0.106x + 0.214y + z + 1.577 = 0

Coordination sphere of 4D



Cartesian coordinates

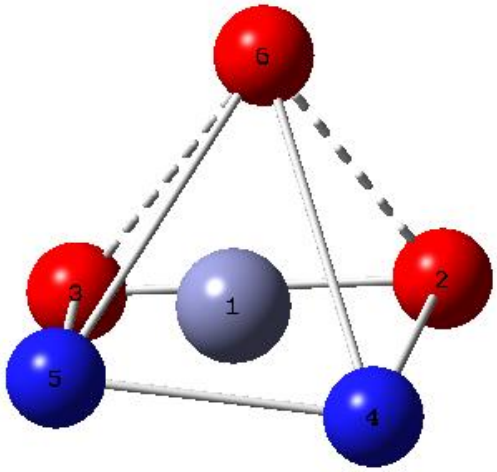
Zn_1	1.0401	0.7077	-0.9284
O_2	-0.6789	-0.3892	-1.1006
O_3	2.3415	-0.7479	-1.1701
N_4	-0.0792	2.3573	-1.4766
N_5	2.5192	2.1327	-1.0862
O_6	0.6789	0.3892	1.1006

d	Å	∠	°
2-3	3.04	2-1-6	81.63
2-4	2.84	3-1-6	96.96
2-5	4.07	4-1-6	106.62
3-4	3.95	5-1-6	107.73
3-5	2.89	2-1-5	165.35
1-6	2.09	3-1-4	156.32
2-6	2.70		
3-6	3.04		
4-6	3.33		
5-6	3.35		

Equations of planes:

α_1 ($O_2O_3N_4$) = 0.038x + 0.129y + z + 1.177 = 0
α_2 ($O_2O_3N_5$) = 0.019x - 0.030y + z + 1.102 = 0
α_3 ($O_2N_4N_5$) = -0.134x + 0.166y + z + 1.074 = 0
α_4 ($O_3N_4N_5$) = -0.150x - 0.019y + z + 1.508 = 0

Coordination sphere of 5D



Cartesian coordinates

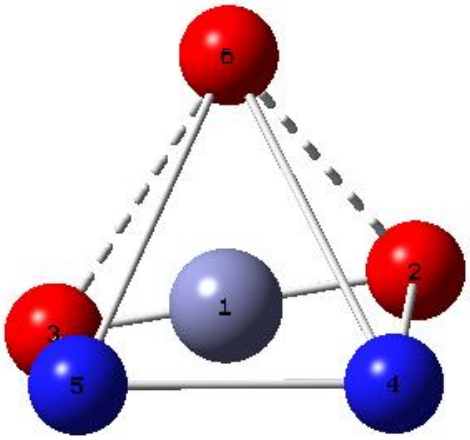
Zn_1	-0.9901	-0.8839	0.8263
O_2	0.7384	-1.1091	-0.2290
O_3	-2.2834	-1.3867	-0.5764
N_4	0.1675	-1.1218	2.5401
N_5	-2.4568	-0.9016	2.2492
O_6	-0.7384	1.1091	0.2290

d	Å	∠	°
2-3	3.05	2-1-6	81.70
2-4	2.83	3-1-6	96.80
2-5	4.05	4-1-6	106.05
3-4	3.97	5-1-6	107.03
3-5	2.87	2-1-5	165.57
1-6	2.10	3-1-4	157.02
2-6	2.70		
3-6	3.04		
4-6	3.34		
5-6	3.33		

Equations of planes:

α_1 ($O_2O_3N_4$) = 6.497x - 71.845y + z - 84.241 = 0
α_2 ($O_2O_3N_5$) = 0.408x - 5.679y + z - 6.369 = 0
α_3 ($O_2N_4N_5$) = 3.795x + 46.604y + z + 49.112 = 0
α_4 ($O_3N_4N_5$) = -0.618x - 6.046y + z - 9.220 = 0

Coordination sphere of 6D



Cartesian coordinates

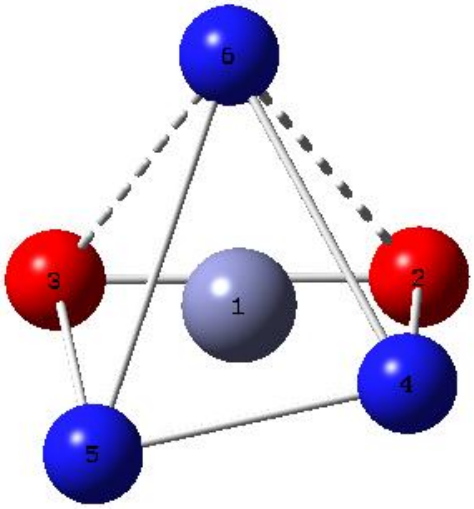
Zn_1	-0.0589	-0.8852	1.2896
O_2	0.1788	-1.1126	-0.7321
O_3	-1.9950	-1.2162	1.4037
N_4	1.9450	-1.3796	1.4559
N_5	0.1378	-1.0059	3.3349
O_6	-0.1788	1.1126	0.7321

d	Å	∠	°
2-3	3.05	2-1-6	81.29
2-4	2.82	3-1-6	96.92
2-5	4.07	4-1-6	107.88
3-4	3.94	5-1-6	109.18
3-5	2.88	2-1-5	164.41
1-6	2.08	3-1-4	155.16
2-6	2.69		
3-6	3.03		
4-6	3.35		
5-6	3.37		

Equations of planes:

α_1 ($O_2O_3N_4$) = 0.451x + 11.178y + z + 13.088 = 0
α_2 ($O_2O_3N_5$) = 2.747x - 37.095y + z - 41.031 = 0
α_3 ($O_2N_4N_5$) = -7.439x - 41.013y + z - 43.569 = 0
α_4 ($O_3N_4N_5$) = -0.278x - 6.372y + z - 9.707 = 0

Coordination sphere of 1·py



Cartesian coordinates

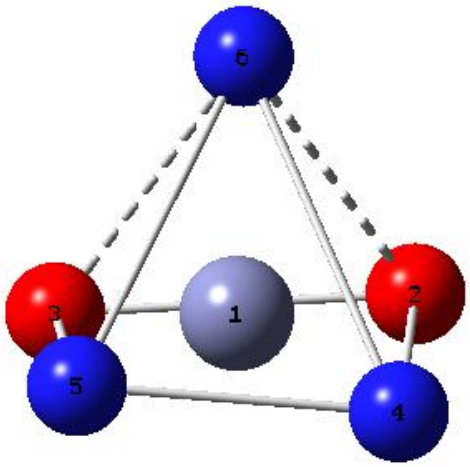
Zn_1	0.0020	-0.4113	-0.3313
O_2	1.4922	0.8787	-0.1145
O_3	-1.5138	0.8465	-0.0999
N_4	1.3846	-1.8398	-0.9919
N_5	-1.2189	-1.5773	-1.5408
N_6	-0.0527	-0.9778	1.7336

d	Å	∠	°
2-3	3.01	2-1-6	94.93
2-4	2.86	3-1-6	92.04
2-5	3.93	4-1-6	98.07
3-4	4.05	5-1-6	113.45
3-5	2.84	2-1-5	150.55
1-6	2.14	3-1-4	166.83
2-6	3.04		
3-6	2.97		
4-6	3.20		
5-6	3.53		

Equations of planes:

α_1 ($O_2O_3N_4$) = 0.007x - 0.324y + z + 0.385 = 0
α_2 ($O_2O_3N_5$) = 0.009x - 0.592y + z + 0.617 = 0
α_3 ($O_2N_4N_5$) = -0.243x - 0.314y + z + 0.748 = 0
α_4 ($O_3N_4N_5$) = -0.274x - 0.625y + z + 0.218 = 0

Coordination sphere of 2·py



Cartesian coordinates

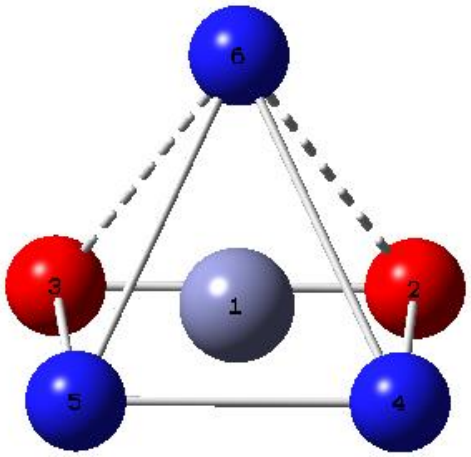
Zn_1	-0.0327	0.1371	-0.0012
O_2	-1.6082	-0.9141	-0.6800
O_3	1.3584	-1.2022	-0.5084
N_4	-1.1398	1.8596	-0.1623
N_5	1.4665	1.5402	0.3591
N_6	-0.3824	-0.6007	1.9811

d	Å	∠	°
2-3	2.99	2-1-6	90.25
2-4	2.86	3-1-6	96.76
2-5	4.07	4-1-6	105.86
3-4	3.97	5-1-6	100.90
3-5	2.87	2-1-5	166.68
1-6	2.14	3-1-4	156.69
2-6	2.95		
3-6	3.10		
4-6	3.35		
5-6	3.26		

Equations of planes:

α_1 ($O_2O_3N_4$) = -0.074x - 0.175y + z + 0.401 = 0
α_2 ($O_2O_3N_5$) = -0.088x - 0.314y + z + 0.253 = 0
α_3 ($O_2N_4N_5$) = -0.218x - 0.151y + z + 0.192 = 0
α_4 ($O_3N_4N_5$) = -0.237x - 0.308y + z + 0.463 = 0

Coordination sphere of 3·py



Cartesian coordinates

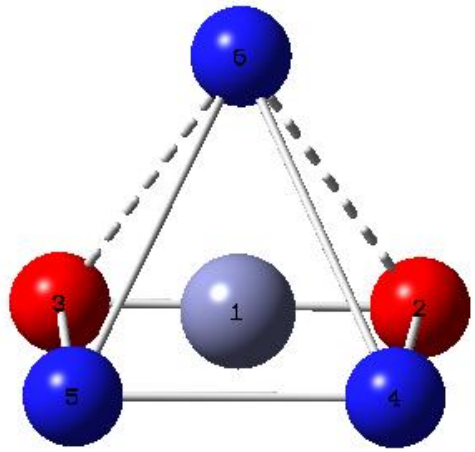
Zn_1	0.0025	0.1002	-0.2314
O_2	-1.4748	-1.1704	-0.6016
O_3	1.4866	-1.1703	-0.5853
N_4	-1.3343	1.6947	-0.4376
N_5	1.3380	1.6958	-0.4316
N_6	-0.0065	-0.2134	1.8676

d	Å	∠	°
2-3	2.96	2-1-6	94.88
2-4	2.87	3-1-6	94.88
2-5	4.02	4-1-6	101.98
3-4	4.02	5-1-6	102.14
3-5	2.87	2-1-5	161.26
1-6	2.12	3-1-4	161.50
2-6	3.03		
3-6	3.03		
4-6	3.27		
5-6	3.28		

Equations of planes:

α_1 ($O_2O_3N_4$) = -0.003x - 0.056y + z + 0.530 = 0
α_2 ($O_2O_3N_5$) = -0.003x - 0.056y + z + 0.530 = 0
α_3 ($O_2N_4N_5$) = -0.004x - 0.056y + z + 0.530 = 0
α_4 ($O_3N_4N_5$) = -0.004x - 0.056y + z + 0.530 = 0

Coordination sphere of 4·py



Cartesian coordinates

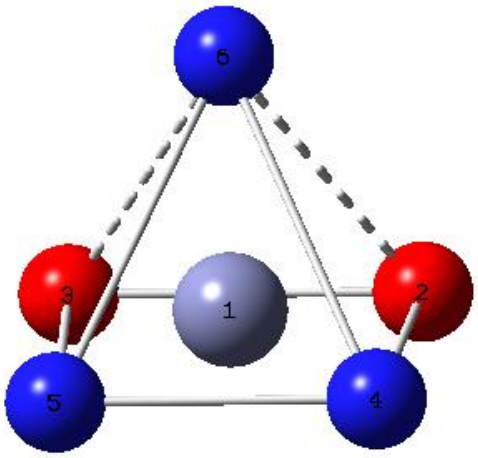
Zn_1	0.0100	0.0549	0.0204
O_2	-1.4446	-1.2960	0.0334
O_3	1.5170	-1.2526	0.0990
N_4	-1.3241	1.4881	-0.6930
N_5	1.3246	1.5172	-0.6616
N_6	-0.0413	0.3678	2.1216

d	Å	∠	°
2-3	2.93	2-1-6	94.36
2-4	2.88	3-1-6	94.34
2-5	4.01	4-1-6	102.81
3-4	4.03	5-1-6	103.64
3-5	2.88	2-1-5	160.58
1-6	2.12	3-1-4	161.26
2-6	3.02		
3-6	3.02		
4-6	3.29		
5-6	3.31		

Equations of planes:

α_1 $(O_2O_3N_4)$ = -0.028x + 0.259y + z + 0.267 = 0
α_2 $(O_2O_3N_5)$ = -0.027x + 0.273y + z + 0.283 = 0
α_3 $(O_2N_4N_5)$ = -0.014x + 0.259y + z + 0.286 = 0
α_4 $(O_3N_4N_5)$ = -0.014x + 0.273y + z + 0.264 = 0

Coordination sphere of 5·py



Cartesian coordinates

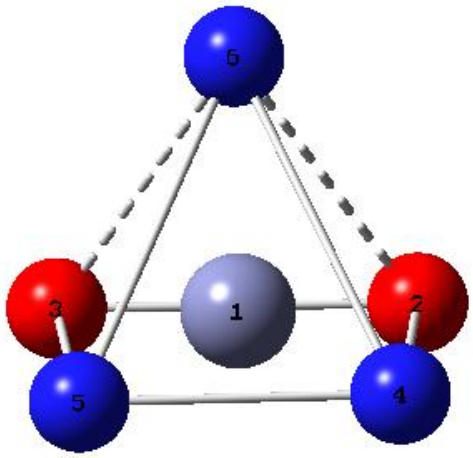
Zn_1	-0.0146	0.0639	-0.1577
O_2	-1.4882	-1.2540	-0.3730
O_3	1.4461	-1.2548	-0.4224
N_4	-1.3584	1.6292	-0.4563
N_5	1.3047	1.5988	-0.5171
N_6	0.0175	-0.1172	1.9714

d	Å	∠	°
2-3	2.93	2-1-6	93.60
2-4	2.89	3-1-6	93.75
2-5	3.99	4-1-6	102.48
3-4	4.02	5-1-6	103.17
3-5	2.86	2-1-5	162.08
1-6	2.14	3-1-4	162.53
2-6	3.01		
3-6	3.01		
4-6	3.29		
5-6	3.29		

Equations of planes:

α_1 ($O_2O_3N_4$) = 0.017x + 0.030y + z + 0.433 = 0
α_2 ($O_2O_3N_5$) = 0.017x + 0.036y + z + 0.440 = 0
α_3 ($O_2N_4N_5$) = 0.023x + 0.030y + z + 0.442 = 0
α_4 ($O_3N_4N_5$) = 0.023x + 0.036y + z + 0.432 = 0

Coordination sphere of 6·py



Cartesian coordinates

Zn_1	0.0295	-0.5817	0.1175
O_2	-1.3902	-1.9682	0.0274
O_3	1.5753	-1.8476	0.0914
N_4	-1.3420	0.8593	-0.5014
N_5	1.2980	0.9583	-0.4722
N_6	-0.0199	-0.4207	2.2305

d	Å	∠	°
2-3	2.97	2-1-6	94.68
2-4	2.88	3-1-6	94.54
2-5	4.01	4-1-6	103.19
3-4	4.02	5-1-6	103.92
3-5	2.88	2-1-5	159.98
1-6	2.12	3-1-4	160.66
2-6	3.02		
3-6	3.03		
4-6	3.29		
5-6	3.31		

Equations of planes:

α_1 ($O_2O_3N_4$) = -0.028x + 0.189y + z + 0.301 = 0
α_2 ($O_2O_3N_5$) = -0.028x + 0.197y + z + 0.318 = 0
α_3 ($O_2N_4N_5$) = -0.018x + 0.188y + z + 0.314 = 0
α_4 ($O_3N_4N_5$) = -0.019x + 0.198y + z + 0.305 = 0

VII. Correlation between distortion parameters Φ and Ψ *vs*. ΔG of dimerization and ΔG for the formation of adducts with pyridine

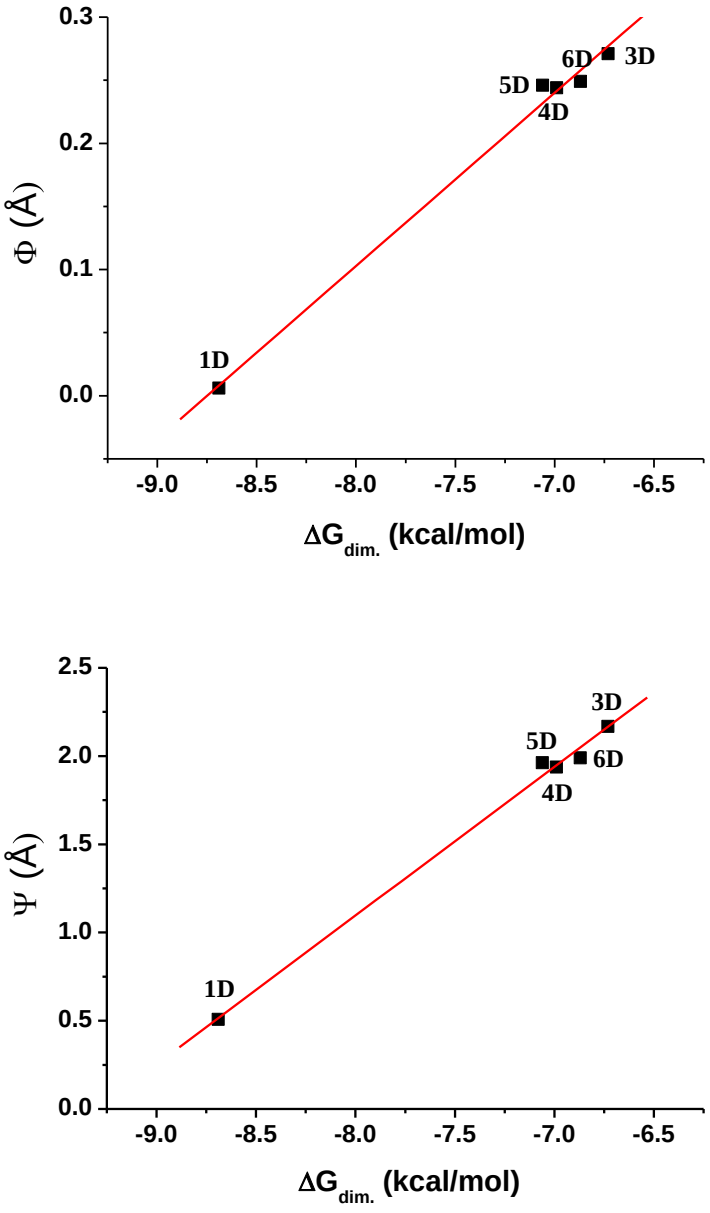


Fig. S4 Plot of distortion parameters Φ and Ψ *vs*. ΔG of dimerization for complexes **1** and **3-6**.

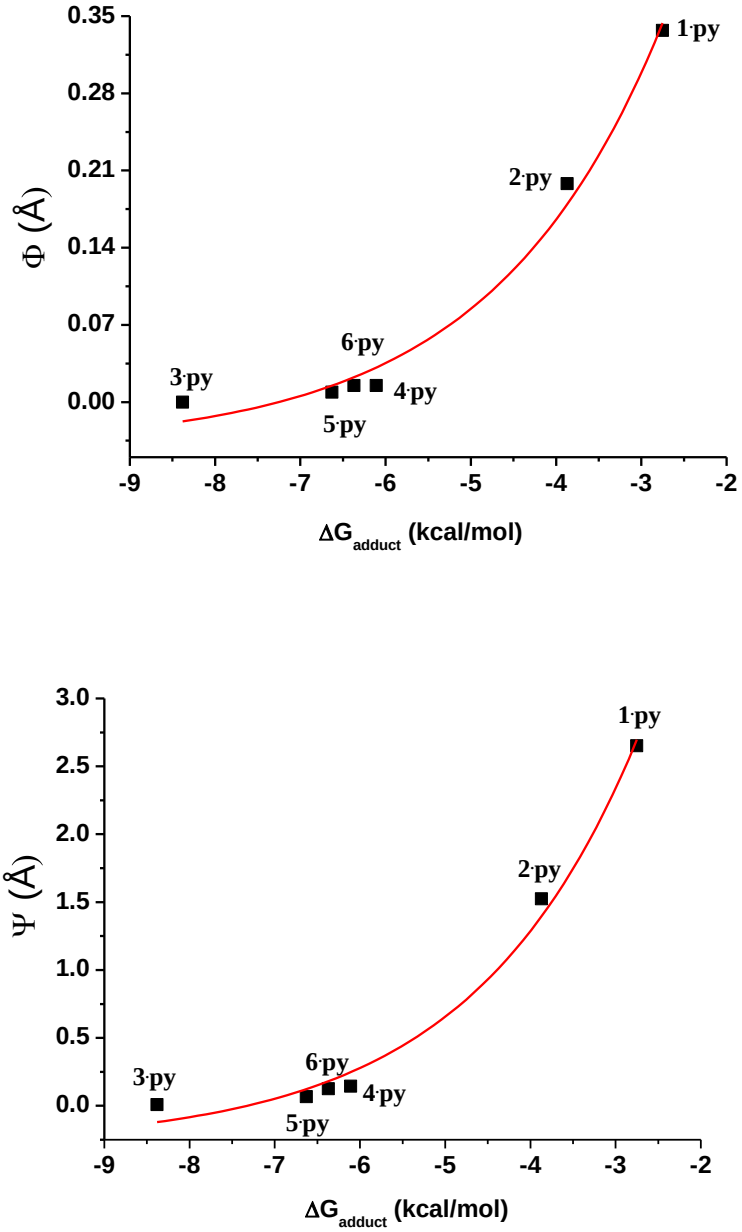


Fig. S5 Plot of distortion parameters Φ and Ψ *vs*. ΔG for the formation of **1**-**6**·py adducts.

VIII. Spectrophotometric titration of complex **4a** with pyridine

The optical absorption variations for titration of **4a** with pyridine and the relative binding isotherm are typical of conjugated complexes **3a-6a**.

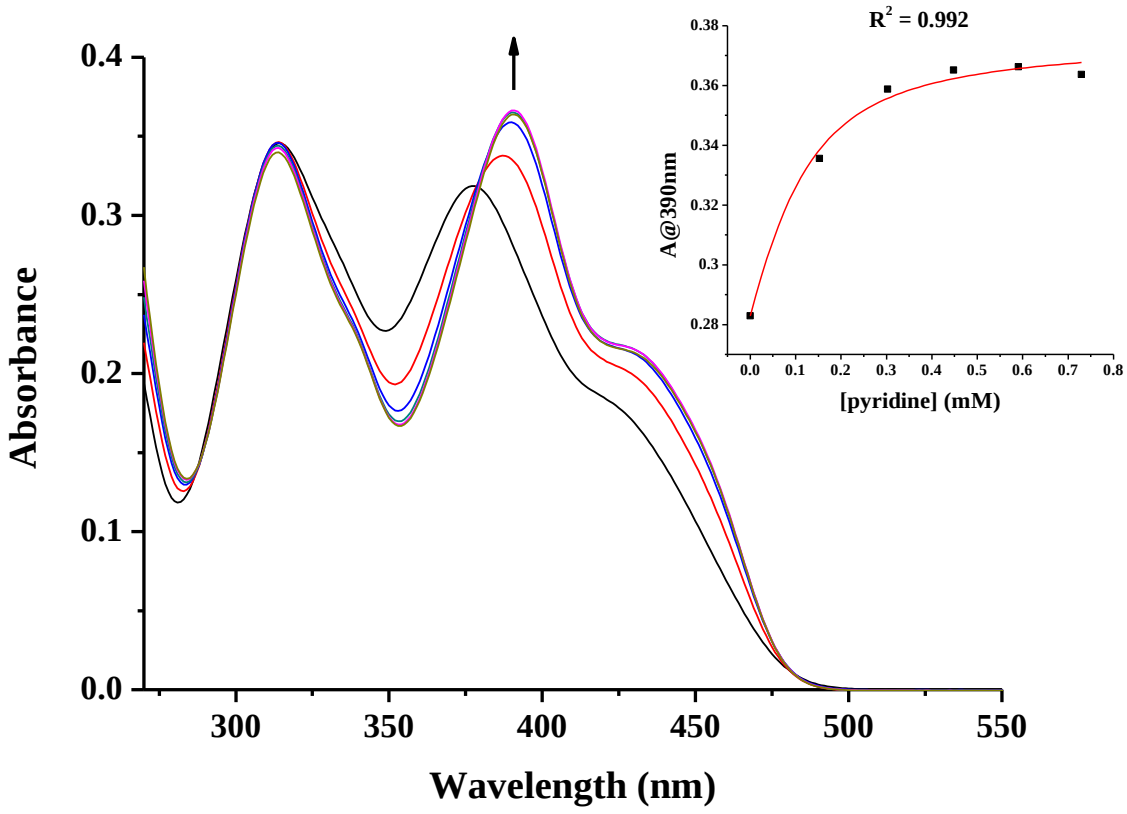


Fig. S6 UV-vis absorption titration curves of **4a** (100 μM solution in $CHCl_3$) with the addition of pyridine. The concentration of pyridine added varied from 0 to 0.73 mM. (Inset) Binding isotherm of **4a** with pyridine at 390nm.

IX. Binding isotherms of complexes **2**, **3a**, **5a**, and **6a** with pyridine

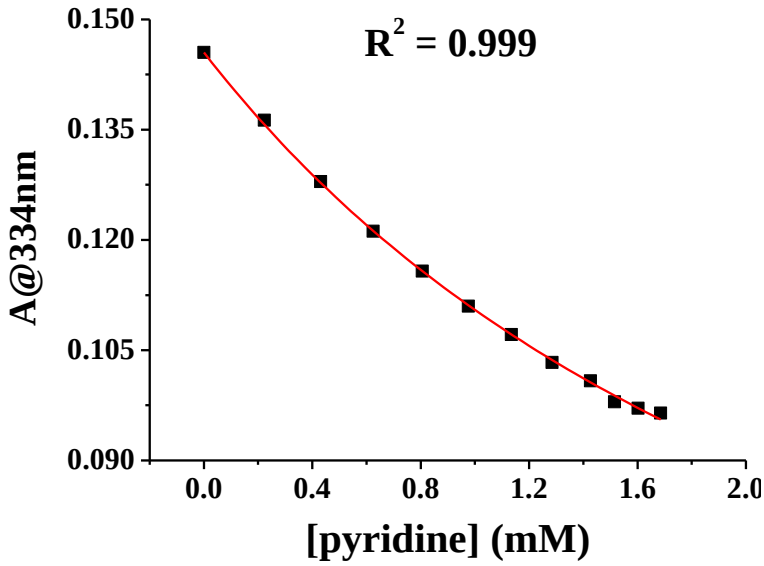


Fig. S7 Binding isotherm of **2** (100 μM solution in $CHCl_3$) with pyridine at 334nm. The concentration of pyridine added varied from 0 to 1.7 mM.

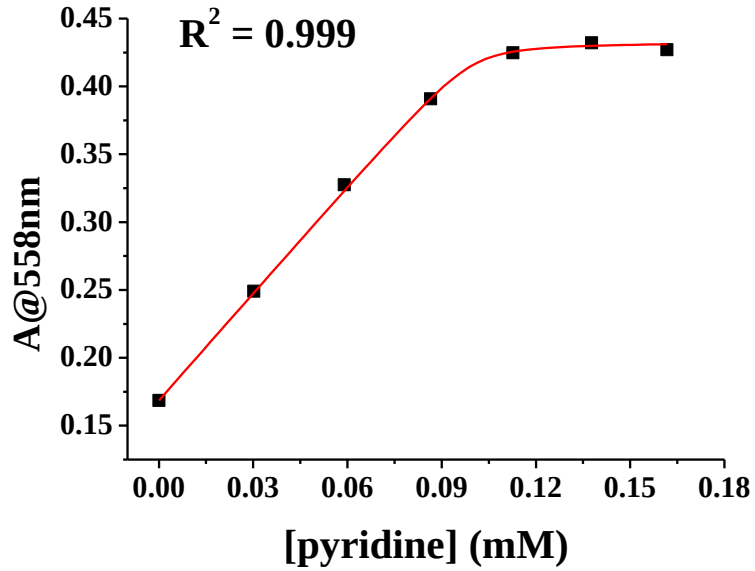


Fig. S8 Binding isotherm of **3a** (100 μM solution in $CHCl_3$) with pyridine at 558 nm. The concentration of pyridine added varied from 0 to 0.16 mM.

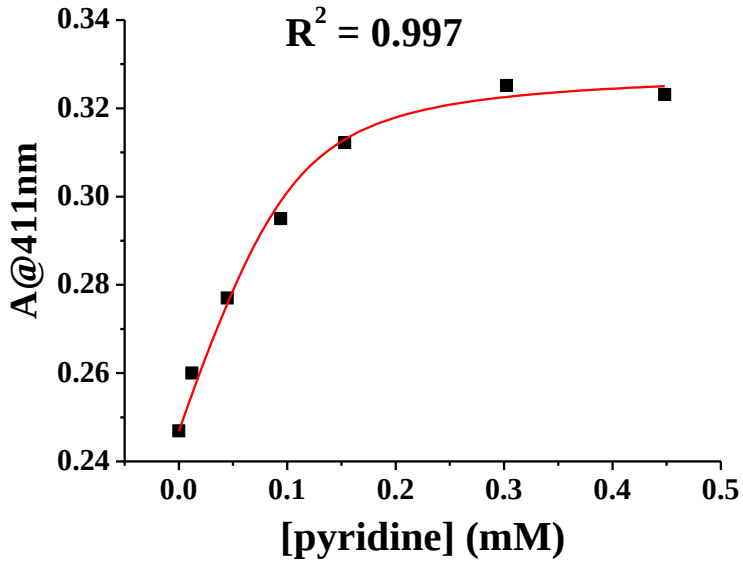


Fig. S9 Binding isotherm of **5a** (100 μM solution in $CHCl_3$) with pyridine at 411 nm. The concentration of pyridine added varied from 0 to 0.45 mM.

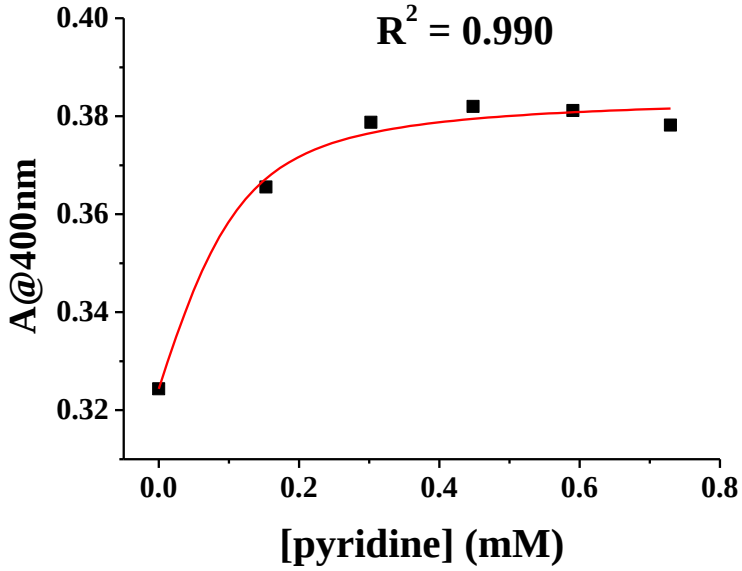


Fig. S10 Binding isotherm of **6a** (100 μM solution in $CHCl_3$) with pyridine at 400 nm. The concentration of pyridine added varied from 0 to 0.73 mM.

X. Experimental derived binding constants for the formation of **1-6**·py adducts

Table S6 Experimental derived binding constants, log *K*, and coefficients of determination, R^2, for replicate titrations of complexes **1a**, **2**, **3a-6a** with pyridine, and average log *K* values with relative standard deviations

Complex	log *K*	R^2	log *K* ± *σ*
1a	1.80	0.996	1.95 ± 0.17
	2.14	0.994	
	1.92	0.987	
2	3.06	0.997	2.93 ± 0.15
	2.96	0.998	
	2.76	0.999	
3a	6.35	0.999	6.17 ± 0.17
	6.15	0.999	
	6.01	0.999	
4a	4.20	0.992	4.27 ± 0.08
	4.26	0.999	
	4.36	0.998	
5a	4.64	0,999	4.70 ± 0.06
	4.71	0.996	
	4.75	0.998	
6a	4.46	0.993	4.47 ± 0.01
	4.47	0.999	
	4.48	0.990	