Supporting Information

Cyclometallated platinum(II) complexes based on bidentate phosphines: Synthesis, structural properties and reactivity studies

Feng Zheng^{*a,c*}, Alan T. Hutton^{*a*}, Cornelia G.C.E. van Sittert^{*b*}, Wilhelmus J. Gerber^{*c*} and Selwyn F. Mapolie^{**c*}

^a Department of Chemistry, University of Cape Town, Private Bag, Rondebosch, 7700, South

Africa.

^b Catalysis and Synthesis Research Group, Chemical Resource Beneficiation Focus Area, North-

West University, Potchefstroom, 2520, South Africa

^c Department of Chemistry and Polymer Science, Stellenbosch University, Private Bag, Matieland, 7601, Stellenbosch, South Africa.

Corresponding author: Email smapolie@sun.ac.za



Figure S1. IR spectra for the mononuclear complexes as KBr pellet and in DCM.

Table S1. Molar conductivities (Ω^{-1} .cm².mol⁻¹) of mononuclear Pt(II) complexes with different bidentate phosphine in dichloromethane

Commlex	Concentration	k	Λ_{M}
Complex	(mM)	(mS.cm ⁻¹)	$(\Omega^{-1}.cm^2.mol^{-1})$
3a (dppf-mono)	1.10	0.32	0.3
3b (dppe-mono)	1.14	66.1	58.0
3c (dppm-mono)	1.18	58.0	49.2
2c (dppm-di)	0.98	0.16	0.2
DCM		0.01	

	2a	3a
τ (^o) ^a	143.5	39.2
θ (°) ^b	0.2	0.2
$X_A \cdots Fe \cdots X_B (^o)^c$	174.4	177.7
$P\cdots Fe\cdots P(^{o})$	154.6	62.4
$P\cdots P(Å)$	6.84	3.50
M–P (Å)	2.23, 2.23	2.23, 2.35
Fe…M (Å)	4.39	4.24

Table S2. The relevant structural parameters for complexes containing dppf ligand

^a The torsion angle CA-XA-XB-CB, where C is the carbon bonded to the P and X is the centroid.

^b The dihedral angle between the two Cp rings. c Centroid-Fe-centroid

	2a	2c	3a	3b
Empirical formula	$C_{72}H_{72}Cl_2FeN_2P_2Pt_2+CH_2Cl_2$	$C_{63}H_{66}Cl_2N_2P_2Pt_2$	C53H50ClFeNP2Pt	C ₄₈ H ₅₂ ClNOP ₂ Pt
Mr (g/mol)	1629.09	1374.20	1049.27	951.39
Crystal system	Orthorhombic	Monoclinic	monoclinic	Monoclinic
Space group	Ссса	P21/n	P21/c	P21/c
a (Å)	21.2184(18)	12.4432(5)	11.827(2)	9.8055(5)
b (Å)	37.581(3)	17.0241(7)	21.120(4)	39.311(2)
c (Å)	17.8803(14)	26.2651(11)	18.536(4)	11.2304(6)
α (°)	90	90	90	90
β (°)	90	96.9040(10)	103.533(3)	101.2840(10)
γ (°)	90	90	90	90
V (Å ³)	14258(2)	5523.5(4)	4501.6(15)	4245.3(4)
Z	8	4	4	4
Reflections collected/ Unique	145930/10069	35293/13187	29083 / 10803	92919/11079
R(int)	0.0869	0.0438	0.0754	0.0647
Data/restraints/parameters	10069/0/379	13187/0/648	10803/42/552	110790/0/493
Final R indices [l>2 σ (l)]	0.0362, 0.1015	0.0320, 0.0577	0.0477, 0.0850	0.0288, 0.0495
Largest diff. peak and hole (e.A ⁻³)	13.446, -1.065	0.888, -1.057	1.292, -0.764	0.494, -0.787

Table S3. Crystal data and structure refinement for complexes2a, 2c, 3a and 3b.



Figure S2. Variable-temperature ¹H NMR in *iso*-propyl methyl region of **3c** in CDCl₃.

	$E^{I}_{\ pa}$	$E^{I}_{\ pc}$	E^2_{pa}	E^2_{pc}	$E^{1}_{1/2}$	$E^{2}_{1/2}$
dppf	0.487	0.433	1.10	0.980	0.460	1.04
2a	0.654	0.480			0.567	
3a	0.765	0.711	0.785	0.711	0.738	0.748

Table S4. cyclic voltammetry parameters in V for (dppf)PtL complexes



Figure S3. UV-Vis absorption spectra of the cyclometallated Pt complexes with bidentate phosphines, the dmso precursor and the free ligand in CH_2Cl_2 (10⁻⁴ M) at 298 K.

complex	c (10 ⁻⁵ M)	$\Box \Box (nm)$	А	$\Box (M^{-1}.cm^{-1})$
L	2.04	252	1.02731	50400
		340	0.0625149	3060
	• • •		0.01.610 .0	10.100
1	2.16	246	0.916192	42400
		320	0.26081	12100
		400	0.0888667	4110
2.9	1.06	310	0 374105	35300
24	1.00	412	0.116691	11000
		112	0.110091	11000
2b	1.12	264	0.764676	68300
		310	0.284136	25400
		412	0.12279495	11000
2c	0.98	268	0.74023	75500
		310	0.286552	29200
		414	0.10879	11100
3a	2.02	258	1 03554	51300
<i>ou</i>	2.02	314	0.239301	11800
		517	0.237301	11000
3b	2.28	242	2.57213	113000
		324	0.325564	14300
3c	2.36	324	0.272781	11600

Table S5. Absorption data for complexes 1 - 3 and the free ligand in CH₂Cl₂ (ca. 2 x 10⁻⁵ M in Pt concentration) at 298 K.

Complex	\square_{ex} (nm)	$\square_{\rm em}({\rm nm})$
1	334 _{max} , 400	530 _{max} , 568 (λ _{ex} 334)
2b	400 _{max} , 298	434, 532 _{max} , 568(sh)
2c	400	532 _{max} , 572(sh)
3b	282	310 _{max} , 568(sh)
3c	284	452 _{max} , 490(sh), 564

Table S6. Excitation and emission data for Pt complexes



Figure S4. ¹H NMR spectra of 1



Figure S5. ¹³C NMR spectra of 1



Figure S6. ¹H NMR spectra of 2a



Figure S7. ³¹P NMR spectra of 2a



Figure S8. ¹³C NMR spectra of 2a



Figure S9. ¹H NMR spectra of 2b



Figure S10. ³¹P NMR spectra of 2b



Figure S11. ¹³C NMR spectra of 2b



Figure S12. ¹H NMR spectra of 2c





Figure S14. ¹³C NMR spectra of 2c



Figure S15. ¹H NMR spectra of 3a



Figure S16. ³¹P NMR spectra of 3a



Figure S17. ¹³C NMR spectra of 3a



Figure S18. ¹H NMR spectra of 3b



Figure S19. ³¹P NMR spectra of 3b



Figure S20. ¹³C NMR spectra of 3b



Figure S21. ¹H NMR spectra of 3c



Figure S22. ³¹P NMR spectra of 3c



Figure S23. ¹³C NMR spectra of 3c

Table S7. Cartesian Coordinates (i	in Å)	A) of optimized structures
------------------------------------	-------	----------------------------

3aN-1

Pt	-16.8489	16.97936	2.55736
Fe	-14.4333	17.59301	-1.0453
Р	-17.606	17.49564	0.34193
Р	-14.6384	15.88912	1.92454
Cl	-16.2936	16.52069	4.92884
С	-18.6926	17.74211	3.31858
С	-13.2768	17.77966	3.47
Н	-14.1241	18.42553	3.24072
С	-16.0933	18.27139	-2.0625
Н	-16.6493	17.68264	-2.78378
С	-19.0297	18.6355	0.11238
С	-17.9374	14.73277	-0.02195
Н	-17.5085	14.65042	0.97791
С	-15.3116	19.17174	-0.06588
Н	-15.1958	19.39162	0.99095
Ν	-17.7229	21.13034	4.39279
С	-12.541	16.83825	-1.47585
Н	-11.7647	17.35871	-2.0286
С	-18.8254	19.97913	-0.23553
Н	-17.8171	20.35173	-0.41079
С	-19.7781	16.85972	3.39835
Н	-19.6828	15.83809	3.02681
С	-18.8362	19.04826	3.83337
С	-20.9969	17.26484	3.95207

Н	-21.8291	16.56045	4.00002
С	-16.5773	21.95545	4.38304
С	-16.2569	22.73671	3.24071
С	-21.1479	18.57003	4.43867
Н	-22.0984	18.89264	4.86511
С	-19.9144	20.84426	-0.37956
Н	-19.742	21.8845	-0.65669
С	-17.1621	22.73244	2.01612
Н	-17.5506	21.71291	1.88755
С	-17.696	19.96977	3.84213
Н	-16.7799	19.57936	3.36296
С	-14.5036	19.67496	-1.12857
Н	-13.6445	20.32905	-1.01442
С	-16.3078	18.29274	-0.63658
С	-21.4239	19.03811	0.17039
Н	-22.4356	18.66476	0.33052
С	-13.5525	15.99461	-2.03436
Н	-13.685	15.7641	-3.08729
С	-14.3921	15.5413	-0.97075
Н	-15.2654	14.90583	-1.07823
С	-13.8955	16.09726	0.26575
С	-21.2147	20.37677	-0.17604
Н	-22.0629	21.05192	-0.29115
С	-12.7438	16.90249	-0.06385
Н	-12.1498	17.47449	0.64148
С	-20.34	18.1712	0.31541
Н	-20.5192	17.13082	0.58259

С	-15.8192	22.06523	5.57601
С	-18.1273	16.00086	-0.59079
С	-19.0783	14.94632	-2.56151
Н	-19.5329	15.03499	-3.54834
С	-18.8661	13.68442	-1.99568
Н	-19.1502	12.78607	-2.54397
С	-14.9829	19.12016	-2.3556
Н	-14.5469	19.27518	-3.33845
С	-18.3006	13.57932	-0.72288
Н	-18.1469	12.60125	-0.26638
С	-18.7206	16.09976	-1.86129
Н	-18.9166	17.07647	-2.30352
С	-13.2637	16.4557	3.00658
С	-14.6877	14.05868	2.12358
С	-20.0722	19.44889	4.38407
Н	-20.158	20.46431	4.77262
С	-12.196	15.6163	3.35563
Н	-12.1797	14.5791	3.02201
С	-15.5625	13.51776	3.08146
Н	-16.1653	14.18512	3.69905
С	-11.1625	17.42589	4.59501
Н	-10.3484	17.79842	5.2174
С	-12.2268	18.26496	4.2535
Н	-12.2527	19.29535	4.6081
С	-15.14	23.58024	3.30926
Н	-14.8741	24.18354	2.44168
С	-13.9847	11.8094	1.52845

Н	-13.3671	11.14764	0.92101
С	-14.7083	22.91745	5.58718
Н	-14.1073	22.99844	6.49333
С	-11.1526	16.1003	4.14993
Н	-10.333	15.43622	4.42574
С	-16.1952	21.24625	6.80101
Н	-17.2504	20.95933	6.67495
С	-13.8979	13.19304	1.34851
Н	-13.2164	13.59458	0.59953
С	-14.3605	23.66703	4.46367
Н	-13.4918	24.32654	4.48906
С	-15.6439	12.13434	3.25819
Н	-16.3266	11.72691	4.00431
С	-14.8593	11.27814	2.48033
Н	-14.9282	10.19837	2.61583
С	-16.0854	22.04148	8.11037
Н	-16.4675	21.43855	8.94655
Н	-16.6682	22.97193	8.06313
Н	-15.044	22.30348	8.34576
С	-15.3709	19.9487	6.87553
Н	-14.297	20.17674	6.95187
Н	-15.526	19.31622	5.99202
Н	-15.6574	19.36174	7.76036
С	-16.4531	23.11621	0.71167
Н	-17.139	22.98475	-0.13709
Н	-15.5667	22.49247	0.53207
Н	-16.1373	24.16911	0.71106

С	-18.3761	23.64932	2.26252
Н	-18.0456	24.68975	2.39963
Н	-18.9264	23.34206	3.16162
Н	-19.0675	23.61876	1.40795
3aN-2			
Pt	-16.9573	17.19864	2.65097
Fe	-14.5742	17.79428	-0.96688
Р	-17.7228	17.62047	0.42462
Р	-14.7293	16.20629	2.05879
Cl	-16.4279	16.636	5.02454
С	-18.8466	17.85091	3.37903
С	-13.4062	18.29843	3.32722
Н	-14.2863	18.87997	3.05704
С	-16.2346	18.4253	-2.00096
Н	-16.7664	17.82247	-2.72754
С	-19.2052	18.66812	0.13313
С	-17.9713	14.83933	0.1724
Н	-17.5871	14.82109	1.1933
С	-15.4948	19.35667	-0.00197
Н	-15.4071	19.58562	1.05449
Ν	-16.9233	20.22092	3.70751
С	-12.6756	17.0505	-1.39883
Н	-11.9146	17.55716	-1.98346
С	-19.0695	20.01123	-0.24823
Н	-18.0815	20.43778	-0.40617
С	-19.858	16.88379	3.4267

Н	-19.6542	15.87054	3.0814
С	-19.128	19.14347	3.88085
С	-21.1373	17.17761	3.91766
Н	-21.9008	16.39859	3.9383
С	-16.1051	21.32592	4.04574
С	-15.9744	22.41816	3.15166
С	-21.4315	18.46508	4.37592
Н	-22.4246	18.7105	4.75159
С	-20.2018	20.80615	-0.44991
Н	-20.0818	21.84614	-0.75107
С	-16.8103	22.48772	1.88466
Н	-17.1084	21.45938	1.64002
С	-18.1616	20.2328	4.04478
Н	-18.5854	21.11814	4.54846
С	-14.6912	19.87587	-1.05925
Н	-13.849	20.54977	-0.94038
С	-16.4625	18.44771	-0.57573
С	-21.6203	18.92948	0.10482
Н	-22.6123	18.4998	0.2386
С	-13.6811	16.1685	-1.90743
Н	-13.8226	15.89083	-2.9471
С	-14.4996	15.74828	-0.81364
Н	-15.361	15.09263	-0.87998
С	-13.998	16.36726	0.3894
С	-21.4795	20.26875	-0.27537
Н	-22.3615	20.88681	-0.4389
С	-12.8609	17.17083	0.01275

Н	-12.2646	17.77993	0.68402
С	-20.492	18.13399	0.31064
Н	-20.6187	17.09271	0.59902
С	-15.3618	21.2791	5.2554
С	-18.1616	16.07332	-0.46593
С	-18.9814	14.89964	-2.42886
Н	-19.3826	14.92688	-3.44191
С	-18.7674	13.67085	-1.79281
Н	-18.9928	12.74114	-2.3141
С	-15.1405	19.30036	-2.28828
Н	-14.7001	19.46455	-3.26654
С	-18.2717	13.64256	-0.4868
Н	-18.1135	12.69182	0.0211
С	-18.6901	16.09524	-1.76932
Н	-18.8933	17.04216	-2.26683
С	-13.3724	16.91899	3.07123
С	-14.6531	14.38302	2.30978
С	-20.4264	19.42896	4.36371
Н	-20.6311	20.42796	4.75329
С	-12.2777	16.16216	3.51181
Н	-12.2502	15.08637	3.34783
С	-15.5743	13.77239	3.17774
Н	-16.2838	14.38965	3.72856
С	-11.2276	18.1712	4.37434
Н	-10.3888	18.65784	4.87156
С	-12.328	18.92482	3.95549
Н	-12.359	19.99916	4.1309

С	-15.0889	23.45234	3.48627
Н	-14.9824	24.30322	2.81399
С	-13.7203	12.19365	1.80478
Н	-12.996	11.58382	1.26563
С	-14.4914	22.33917	5.5412
Н	-13.9154	22.31852	6.46531
С	-11.2142	16.78759	4.16897
Н	-10.3711	16.19045	4.51427
С	-15.5506	20.12561	6.22963
Н	-15.8447	19.2446	5.64166
С	-13.7255	13.57957	1.62309
Н	-13.0125	14.02958	0.9339
С	-14.3481	23.42026	4.66819
Н	-13.6663	24.23576	4.90959
С	-15.5657	12.38559	3.35536
Н	-16.2866	11.92737	4.03216
С	-14.6413	11.5923	2.6686
Н	-14.6375	10.51162	2.8062
С	-16.6941	20.42667	7.21874
Н	-16.8538	19.5679	7.88507
Н	-17.6392	20.63056	6.69997
Н	-16.4512	21.3031	7.83676
С	-14.2843	19.75106	7.01055
Н	-13.9822	20.53965	7.71479
Н	-13.4406	19.54747	6.34079
Н	-14.4738	18.84327	7.59924
С	-16.0473	23.05318	0.67796

Н	-16.6568	22.95916	-0.23131
Н	-15.1039	22.51795	0.51141
Н	-15.8144	24.11887	0.80733
С	-18.0999	23.29774	2.122
Н	-17.8548	24.33499	2.39095
Н	-18.6992	22.87276	2.93716
Н	-18.7213	23.31495	1.21619

3bN

Pt	-21.4899	35.70039	8.51353
Cl	-23.0073	35.64349	6.5528
Р	-20.0045	35.8199	10.3741
Р	-19.687	36.91071	7.31094
Ν	-22.8126	31.25511	8.46822
С	-22.9901	34.72349	9.70736
С	-23.681	35.47252	10.67206
Н	-23.4701	36.53542	10.79419
С	-24.6364	34.88289	11.50983
Н	-25.1596	35.4928	12.24806
С	-24.9096	33.51342	11.40066
Н	-25.6486	33.04414	12.05129
С	-24.244	32.75838	10.441
Н	-24.4574	31.69628	10.31994
С	-23.2928	33.34795	9.58102
С	-22.6788	32.53372	8.52475
Н	-22.149	33.09916	7.74205
С	-22.2979	30.52204	7.3821

С	-23.2407	29.76238	6.63405
С	-22.7926	29.0224	5.53749
Н	-23.5084	28.4535	4.94422
С	-21.4395	28.9968	5.18976
Н	-21.105	28.41936	4.32715
С	-20.5184	29.69717	5.96569
Н	-19.4598	29.64983	5.70636
С	-20.9142	30.46348	7.07268
С	-24.7125	29.80985	7.01451
Н	-24.7404	30.03823	8.09058
С	-25.4471	28.48121	6.79441
Н	-25.5513	28.24022	5.72714
Н	-24.9236	27.64812	7.28343
Н	-26.4605	28.54243	7.21496
C	-25.4363	30.95981	6.29006
Н	-25.4436	30.78625	5.20397
Н	-26.479	31.03245	6.63141
Н	-24.946	31.9238	6.47729
С	-19.8471	31.14829	7.9182
Н	-20.3396	31.60706	8.78533
С	-18.8257	30.1349	8.46513
Н	-18.2592	29.65938	7.65223
Н	-18.106	30.64241	9.12332
Н	-19.3212	29.34282	9.04206
С	-19.1372	32.26872	7.14335
Н	-19.8442	33.0364	6.80558
Н	-18.3826	32.75613	7.77662

Н	-18.6248	31.87369	6.2551
С	-19.6484	34.37675	11.44027
С	-20.7272	33.70646	12.05617
Н	-21.7475	34.05741	11.90187
С	-20.4967	32.59208	12.86308
Н	-21.343	32.07821	13.32758
С	-19.1923	32.12325	13.05713
Н	-19.0158	31.24663	13.68045
С	-18.1148	32.78673	12.45512
Н	-17.0936	32.43176	12.60534
С	-18.3394	33.90382	11.64456
Н	-17.481	34.40236	11.19001
С	-20.4375	37.17699	11.53092
С	-19.9561	37.20136	12.84952
Н	-19.3505	36.37745	13.22728
С	-20.2594	38.27786	13.68642
Н	-19.8867	38.28639	14.71041
С	-21.0412	39.33711	13.21497
Н	-21.2775	40.17415	13.87179
С	-21.5252	39.31749	11.90449
Н	-22.1426	40.13604	11.53504
С	-21.2312	38.23804	11.06754
Н	-21.6344	38.20739	10.054
С	-18.3504	36.33624	9.70186
Н	-17.8853	35.44306	9.26249
Н	-17.7111	36.68297	10.52506
С	-18.5085	37.43329	8.64449

Н	-18.9452	38.33824	9.0908
Н	-17.5339	37.72599	8.2313
С	-20.0813	38.46395	6.42904
С	-21.3591	39.02319	6.57682
Н	-22.1134	38.49804	7.16314
С	-21.6723	40.23101	5.94704
Н	-22.6696	40.6554	6.06096
С	-20.7158	40.88241	5.16438
Н	-20.9626	41.82137	4.66912
С	-19.4428	40.32299	5.00653
Н	-18.6956	40.82362	4.39043
С	-19.1256	39.11639	5.63264
Н	-18.137	38.67852	5.49118
С	-18.7042	35.9449	6.10707
С	-17.3358	35.67674	6.26232
Н	-16.7835	36.06062	7.11882
С	-16.6573	34.90757	5.31176
Н	-15.5953	34.70187	5.4455
С	-17.335	34.40726	4.19792
Н	-16.8042	33.80632	3.45936
С	-18.7003	34.67007	4.03887
Н	-19.2375	34.27429	3.17743
С	-19.3843	35.42733	4.98984
Н	-20.4546	35.60617	4.87727

3bC

D	01 50/7	24 (2041	0 10 (00
Pt	-21.5267	34.63841	9.10689

Cl	-23.9874	35.90205	8.65038
Р	-20.0083	35.66434	10.62844
Р	-20.078	35.73777	7.34777
Ν	-22.3156	32.65437	8.13262
С	-22.7208	33.79159	10.6489
С	-23.0509	34.34201	11.88899
Н	-22.6111	35.28438	12.21373
С	-23.9654	33.70632	12.73996
Н	-24.1971	34.15952	13.70517
С	-24.5813	32.5059	12.36667
Н	-25.2943	32.02009	13.03261
С	-24.2829	31.9498	11.12662
Н	-24.7663	31.02641	10.80239
С	-23.3628	32.58433	10.26754
С	-23.0981	32.0363	8.9619
Н	-23.5697	31.08743	8.67529
С	-22.0169	32.04052	6.8806
С	-22.7757	32.38608	5.73778
С	-22.4483	31.76201	4.52667
Н	-23.021	32.00331	3.63128
С	-21.4091	30.83231	4.44707
Н	-21.1783	30.35376	3.49454
С	-20.6654	30.52003	5.58488
Н	-19.8474	29.80296	5.51154
С	-20.9416	31.12342	6.81857
С	-23.9406	33.36039	5.84013
Н	-23.7724	33.99399	6.72326

С	-25.2633	32.60374	6.0648
Н	-25.4977	31.96414	5.2007
Н	-25.2189	31.96363	6.9562
Н	-26.0889	33.3164	6.2014
С	-24.0598	34.29391	4.62774
Н	-24.3374	33.75087	3.71286
Н	-24.8415	35.04157	4.81855
Н	-23.1204	34.83096	4.44239
С	-20.1268	30.78575	8.06042
Н	-20.3098	31.58741	8.79014
С	-20.5945	29.46137	8.69034
Н	-20.4266	28.62248	7.99932
Н	-20.0354	29.25963	9.61554
Н	-21.6648	29.48289	8.93609
С	-18.6133	30.75425	7.80105
Н	-18.2665	31.69668	7.35891
Н	-18.0804	30.59887	8.74981
Н	-18.3288	29.93464	7.12603
С	-19.0663	34.66215	11.84704
С	-19.5726	33.42374	12.27073
Н	-20.5208	33.06858	11.86865
С	-18.8656	32.64417	13.18986
Н	-19.2747	31.68608	13.5106
С	-17.6367	33.08644	13.68693
Н	-17.082	32.47595	14.39974
С	-17.1165	34.31093	13.2598
Н	-16.1545	34.6593	13.63621

С	-17.8243	35.09644	12.34669
Н	-17.3946	36.04462	12.02594
С	-20.744	37.06015	11.57724
С	-20.2033	37.53472	12.7838
Н	-19.3521	37.03389	13.24369
С	-20.7625	38.64888	13.41447
Н	-20.3373	39.00416	14.35342
С	-21.8645	39.29852	12.84909
Н	-22.3	40.1667	13.3437
С	-22.4153	38.82049	11.6578
Н	-23.2881	39.30593	11.22106
С	-21.8655	37.7023	11.0251
Н	-22.34	37.29952	10.12547
С	-18.6527	36.49122	9.657
Н	-17.8738	35.73207	9.50939
Н	-18.2196	37.30603	10.25279
С	-19.1676	37.02829	8.32396
Н	-19.8987	37.8328	8.48952
Н	-18.3521	37.45808	7.72516
С	-20.7826	36.74188	5.97739
С	-22.0929	37.22738	6.10288
Н	-22.7081	36.92884	6.9577
С	-22.6233	38.06458	5.11681
Н	-23.6445	38.43234	5.22084
С	-21.8604	38.41436	4.00035
Н	-22.281	39.06278	3.23119
С	-20.5567	37.92407	3.86772

Н	-19.9571	38.18935	2.9966
С	-20.0167	37.093	4.8514
Н	-19.0009	36.716	4.73632
С	-18.7591	34.77935	6.49596
С	-17.393	34.952	6.77296
Н	-17.0614	35.65917	7.53034
С	-16.4251	34.23181	6.06602
Н	-15.3701	34.38232	6.2968
С	-16.8079	33.33893	5.0628
Н	-16.0527	32.78438	4.50502
С	-18.1657	33.15837	4.78185
Н	-18.4785	32.45832	4.0078
С	-19.1348	33.86311	5.49779
Н	-20.1882	33.70273	5.26699
3cN			
Pt	-21.9719	35.53101	8.31085
Cl	-23.5003	35.37464	6.37873
Р	-20.312	35.80647	10.00353
Р	-19.9135	36.5612	7.29375
Ν	-22.9459	31.07095	8.51637
С	-23.3833	34.57001	9.58632
С	-24.0555	35.32512	10.55705
Н	-23.9131	36.40561	10.60869
С	-24.9124	34.71417	11.48038
Н	-25.4304	35.3242	12.22244
С	-25.0972	33.3256	11.45524

Н	-25.7581	32.84604	12.17828
С	-24.4384	32.56412	10.49552
Н	-24.5767	31.48357	10.44616
С	-23.5844	33.17134	9.55043
С	-22.9411	32.3579	8.5122
Н	-22.4808	32.93008	7.69081
С	-22.3455	30.35941	7.45773
С	-23.1913	29.49873	6.70411
С	-22.6435	28.77547	5.64172
Н	-23.2881	28.13146	5.04344
С	-21.2837	28.86482	5.3328
Н	-20.8717	28.30012	4.49574
С	-20.4555	29.66855	6.1128
Н	-19.3895	29.71511	5.88446
С	-20.9547	30.42496	7.18382
С	-24.6729	29.42251	7.03795
Н	-24.7584	29.67539	8.10577
С	-25.2751	28.02612	6.83314
Н	-25.3137	27.74788	5.77006
Н	-24.6953	27.25785	7.36373
Н	-26.3059	28.0036	7.21416
С	-25.4732	30.48238	6.25799
Н	-25.4273	30.28452	5.17691
Н	-26.5295	30.4674	6.56386
Н	-25.0805	31.49231	6.43542
С	-19.9794	31.2418	8.02389
Н	-20.5336	31.68522	8.86086

С	-18.8735	30.36193	8.63211
Н	-18.2304	29.92819	7.8531
Н	-18.2366	30.96371	9.29658
Н	-19.2998	29.53724	9.21918
С	-19.368	32.39416	7.21304
Н	-20.1405	33.08576	6.85413
Н	-18.6571	32.9605	7.8317
Н	-18.8198	32.02281	6.33574
С	-19.7624	34.4961	11.14466
С	-20.7315	33.8494	11.93175
Н	-21.783	34.12053	11.83968
С	-20.3513	32.85018	12.82841
Н	-21.1105	32.35461	13.43337
С	-19.0077	32.48124	12.94323
Н	-18.7136	31.69551	13.63892
С	-18.0416	33.1193	12.16124
Н	-16.9922	32.83743	12.24668
С	-18.4141	34.12477	11.26495
Н	-17.6458	34.61672	10.66941
С	-20.5053	37.30809	11.03149
С	-19.7739	37.491	12.21603
Н	-19.0981	36.71381	12.57166
С	-19.912	38.67472	12.94447
Н	-19.3436	38.81039	13.86449
С	-20.7796	39.67813	12.5012
Н	-20.8881	40.5975	13.07622
С	-21.5143	39.49684	11.32632

Н	-22.1986	40.27109	10.9807
С	-21.3855	38.31215	10.59864
Н	-21.9735	38.15977	9.69211
С	-18.9142	36.15997	8.82456
Н	-18.3786	35.22083	8.63454
Н	-18.1976	36.91874	9.16128
С	-19.7501	38.36724	7.0465
С	-20.8938	39.08937	6.67238
Н	-21.8477	38.57335	6.55461
С	-20.8097	40.46548	6.44284
Н	-21.7013	41.0189	6.14935
С	-19.5895	41.12794	6.59502
Н	-19.5264	42.20241	6.42287
С	-18.4472	40.41193	6.96869
Н	-17.493	40.92464	7.09084
С	-18.5242	39.03629	7.18928
Н	-17.6243	38.49177	7.47579
С	-19.0308	35.78958	5.89033
С	-17.6369	35.62496	5.86251
Н	-17.0178	35.96949	6.69216
С	-17.0305	34.99586	4.77259
Н	-15.9491	34.8583	4.76101
С	-17.8091	34.53628	3.70487
Н	-17.3333	34.04026	2.85817
С	-19.1964	34.70474	3.72668
Н	-19.8071	34.33815	2.90088
С	-19.8106	35.32532	4.81805

Н	-20.8972	35.42222	4.85509
3cC			
Pt	-21.8619	34.49158	9.09588
Cl	-24.1526	35.99527	8.52525
Р	-20.3428	35.8324	10.36954
Р	-20.2363	35.61464	7.5104
Ν	-22.5508	32.52069	8.15402
С	-22.934	33.59168	10.66754
С	-23.1787	34.0956	11.946
Н	-22.7565	35.05159	12.25666
С	-23.9836	33.38857	12.85144
Н	-24.1495	33.7971	13.84956
С	-24.5743	32.17106	12.49035
Н	-25.1992	31.63017	13.20082
С	-24.3618	31.66273	11.21204
Н	-24.8259	30.72384	10.90446
С	-23.5465	32.36269	10.30074
С	-23.2957	31.84721	8.97862
Н	-23.721	30.88156	8.67927
С	-22.1868	31.95729	6.89513
С	-22.8541	32.39376	5.72676
С	-22.4603	31.83846	4.50304
Н	-22.966	32.14901	3.58864
С	-21.4351	30.89291	4.43354
Н	-21.1437	30.47157	3.47056
С	-20.7816	30.48965	5.5969

Н	-19.9761	29.75751	5.53373
С	-21.1336	31.01312	6.84813
С	-24.0065	33.3814	5.82025
Н	-23.8553	33.98989	6.7243
С	-25.3429	32.63465	5.99146
Н	-25.5614	32.0211	5.10457
Н	-25.3265	31.97024	6.86599
Н	-26.1641	33.35236	6.12724
С	-24.0829	34.34987	4.63287
Н	-24.3632	33.84049	3.6993
Н	-24.846	35.11343	4.83525
Н	-23.1267	34.86533	4.47309
С	-20.4077	30.55768	8.10791
Н	-20.6404	31.28187	8.90025
С	-20.9066	29.1758	8.56897
Н	-20.6874	28.41152	7.80945
Н	-20.409	28.87996	9.50379
Н	-21.991	29.17109	8.74291
С	-18.8802	30.55059	7.9449
Н	-18.5132	31.52549	7.59979
Н	-18.406	30.32489	8.91081
Н	-18.5487	29.78621	7.22793
С	-18.9775	35.04003	11.29138
С	-19.2081	33.78477	11.87655
Н	-20.1716	33.29489	11.73216
С	-18.2077	33.16343	12.6275
Н	-18.3983	32.19171	13.08363

С	-16.965	33.78224	12.78785
Н	-16.1834	33.2946	13.37058
С	-16.7221	35.0242	12.1932
Н	-15.7536	35.50935	12.31437
С	-17.7245	35.65587	11.45269
Н	-17.526	36.63117	11.00692
С	-20.9765	37.16006	11.46234
С	-20.3082	37.60649	12.61309
Н	-19.3669	37.15122	12.91885
С	-20.8548	38.63842	13.38181
Н	-20.3302	38.97878	14.27495
С	-22.0677	39.22736	13.01062
Н	-22.4917	40.03101	13.61311
С	-22.7429	38.77168	11.87344
Н	-23.6994	39.21079	11.58872
С	-22.2073	37.73665	11.10457
Н	-22.7601	37.34103	10.24817
С	-19.5952	36.68808	8.89637
Н	-20.0953	37.66095	8.79273
Н	-18.5132	36.87027	8.9246
С	-20.6265	36.79597	6.16066
С	-21.9489	37.25148	6.03786
Н	-22.7204	36.87326	6.71568
С	-22.2711	38.18927	5.05172
Н	-23.2998	38.5385	4.95882
С	-21.2861	38.67135	4.18641
Н	-21.5429	39.39789	3.41532

С	-19.968	38.21607	4.3069
Н	-19.1956	38.5866	3.63273
С	-19.6361	37.2822	5.28997
Н	-18.6086	36.92754	5.37108
С	-18.8183	34.66723	6.84763
C	-17.5786	34.57111	7.50183
Н	-17.4096	35.07113	8.45553
C	-16.5373	33.82656	6.93641
Н	-15.5748	33.77085	7.44965
C	-16.725	33.16935	5.71695
Н	-15.91	32.59907	5.26986
С	-17.9666	33.24017	5.07258
Н	-18.1265	32.72088	4.12666
С	-19.0095	33.97662	5.63526
Н	-19.9759	34.01323	5.12777