Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic supplementary material

Alternative (κ^1-N:η^6-arene vs κ^2-N,N) coordination of sterically demanding amidinate ligand: size or electronic structure of Ln ion is a decisive factor?

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Figure 1S. ^{1}H NMR spectrum of [C_6H_4-1,2-{NC(*t*Bu)N(2,6-*i*$Pr_2C_6H_3$)}$_2$]Yb(THF) (**1**).

Figure 2S. ^{13}C{^{1}H} NMR spectrum of [C_6H_4-1,2-{NC(*t*Bu)N(2,6-*i*$Pr_2C_6H_3$)}$_2$]Yb(THF) (**1**).

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Figure 4S. IR spectrum of [{(2,6-*i*$Pr_2C_6H_3$)=NC(*t*Bu)NH}-C_6H_4-1,2-{NC(*t*Bu)N(2,6-*i*$Pr_2C_6H_3$)}]YbI_2(THF)$_2$ (**2**).

Figure 5S. ^{1}H NMR spectrum of [C_6H_4-1,2-{NC(*t*Bu)N(2,6-*i*$Pr_2C_6H_3$)}$_2$]La(μ-Cl)Li(THF)(μ_2-Cl_2)Li(THF)$_2$ (**3**).

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Figure 10S. ^{13}C{^{1}H} NMR spectrum of [(C_6H_4-1,2-{NC(*t*Bu)N(2,6-$Me_2C_6H_3$)}$_2$)La)((*t*Bu)C(2,6-$Me_2C_6H_3$)$_2$)La$(THF)_2$(μ_2-Cl)$_3$(μ_3-Cl)$_2$] (**4**).

Figure 11S. IR spectrum of [(C_6H_4-1,2-{NC(*t*Bu)N(2,6-$Me_2C_6H_3$)}$_2$)La)((*t*Bu)C(2,6-$Me_2C_6H_3$)$_2$)La$(THF)_2$(μ_2-Cl)$_3$(μ_3-Cl)$_2$] (**4**).

Figure 12S. HPLC of the by-products of complex **4**.

Figure 13S. MS of the by-products of complex **4.**

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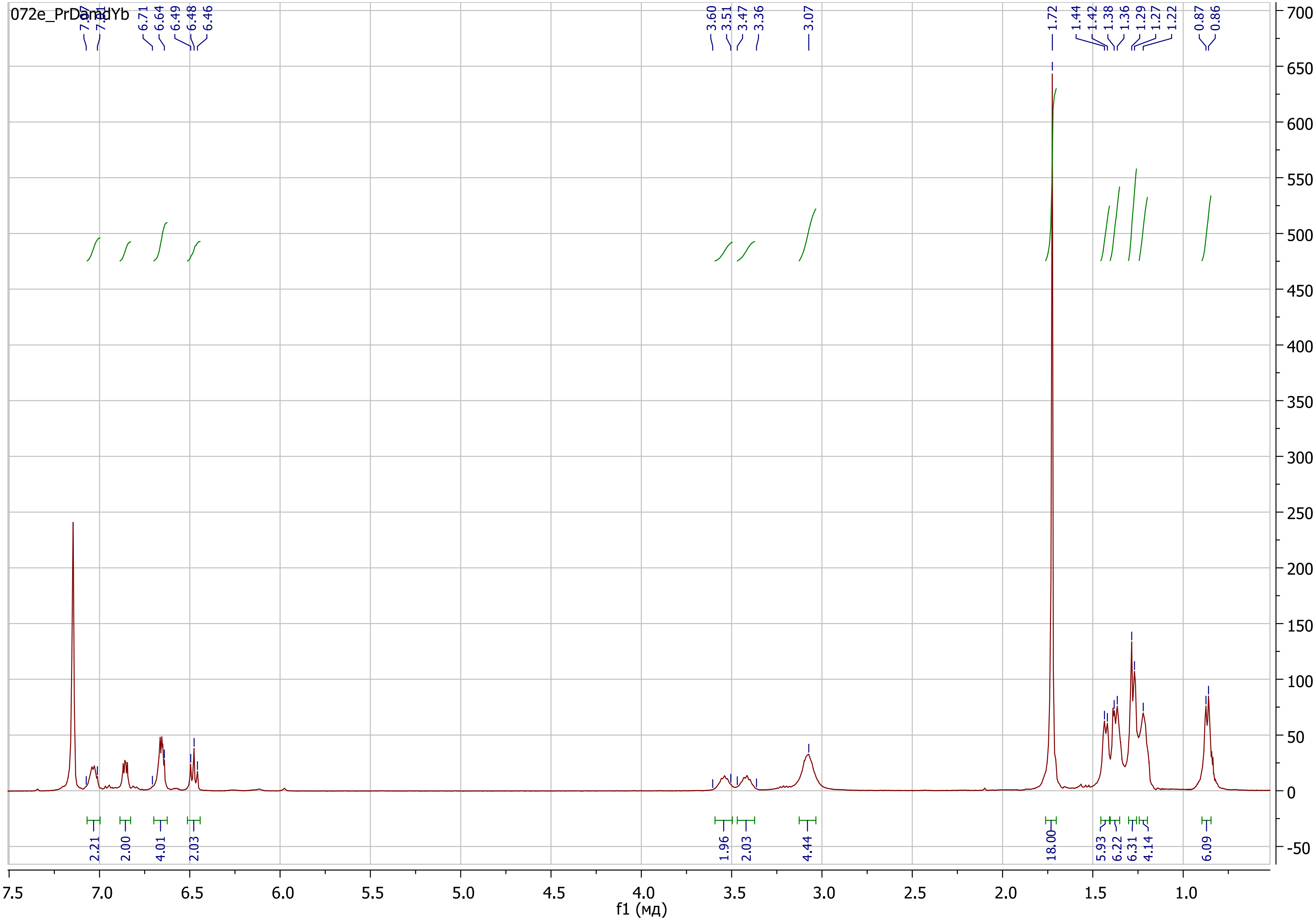
Table 1. Crystallographic data and structure refinement details for **1-4**.

Compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{44}H_{64}N_4OYb$	$C_{48}H_{73}I_2N_4O_2Yb$	$C_{52}H_{80}Cl_3LaLi_2N_4O_3$	$C_{82}H_{110}Cl_5La_3N_8O_2$, ½$C_7H_8$, 1½$C_4H_{10}O$
Formula weight	838.03	1164.94	1068.34	1991.00
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P–1*	$P2_1/n$	$P2_1/c$	$P2_1/c$
a [Å]	10.58550(10)	10.0868(7)	19.7507(9)	13.8933(7)
b [Å]	11.98560(10)	27.7319(18)	13.1135(6)	16.1925(9)
c [Å]	16.2221(2)	17.9352(12)	20.8949(10)	41.208(2)
α [°]	81.5750(10)	90	90	90
β [°]	87.1400(10)	90.1840(10)	99.2743(10)	92.2340(10)
γ [°]	77.4170(10)	90	90	90
V [Å^3]	1986.70(4)	5016.9(6)	5341.1(4)	9263.4(9)
Z	2	4	4	4
ρ_{calcd} [g cm^{-3}]	1.401	1.542	1.329	1.428
μ [mm^{-1}]	2.392	3.133	0.993	1.554
F_{000}	868	2324	2232	4072

Crystal sizes [mm]	0.39 × 0.27 ×0.21	0.23 × 0.20 ×0.18	0.45 × 0.36 × 0.31	0.24 × 0.19 × 0.18
θ range for data collection [°]	2.91–30.03	2.43–30.03	2.38–28.74	0.98–25.03
Index ranges	$-14 \leq h \leq 14$, $-16 \leq k \leq 16$, $-22 \leq l \leq 22$	$-14 \leq h \leq 14$, $-39 \leq k \leq 39$, $-25 \leq l \leq 25$	$-26 \leq h \leq 26$, $-17 \leq k \leq 17$, $-28 \leq l \leq 28$	$-16 \leq h \leq 16$, $-19 \leq k \leq 19$, $-49 \leq l \leq 49$
Reflections collected	39966	68901	68286	68555
Independent reflections	11595	14647	13798	16367
R_{int}	0.0355	0.0355	0.0209	0.1044
Completeness to θ [%]	99.8	99.7	99.9	99.9
Data / restraints / parameters	11595 / 7 / 472	14647 / 8 / 537	13798 / 18 / 593	16367 / 1458 / 1095
$S(F^2)$	1.040	1.055	1.004	1.135
Final R índices [$I > 2\sigma(I)$]	R_1 = 0.0232, wR_2 = 0.0503	R_1 = 0.0318, wR_2 = 0.0768	R_1 = 0.0213, wR_2 = 0.0528	R_1 = 0.0875, wR_2 = 0.1335
R indices (all data)	R_1 = 0.0272, wR_2 = 0.0521	R_1 = 0.0390, wR_2 = 0.0802	R_1 = 0.0238, wR_2 = 0.0541	R_1 = 0.1275, wR_2 = 0.1451
Largest diff. peak and hole [eÅ^{-3}]	1.11 / –1.05	2.87 / –0.53	0.86 / –0.27	1.79 / –0.85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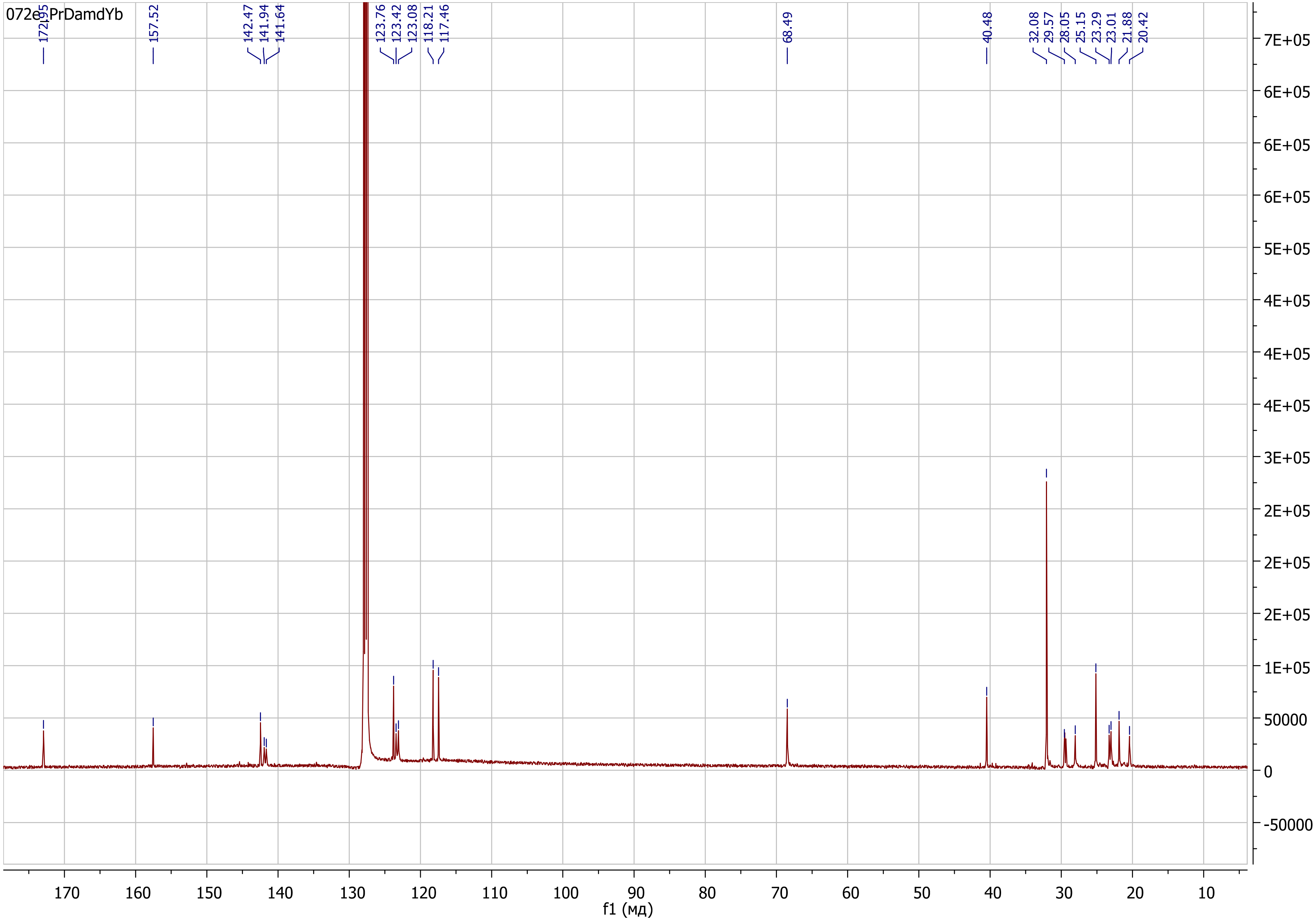
3.07
1.72
1.44
1.42
1.38
1.36
1.29
1.27
1.22
0.87
0.86
2.21
2.00
4.01
2.03
1.96
2.03
4.44
18.00
5.93
6.22
6.31
4.14
6.09
f1 (мд)

Figure 1S. ^{1}H NMR spectrum of $[C_6H_4\text{-}1,2\text{-}\{NC(t\text{Bu})N(2,6\text{-}i\text{Pr}_2C_6H_3)\}_2]Yb(THF)$ (**1**).



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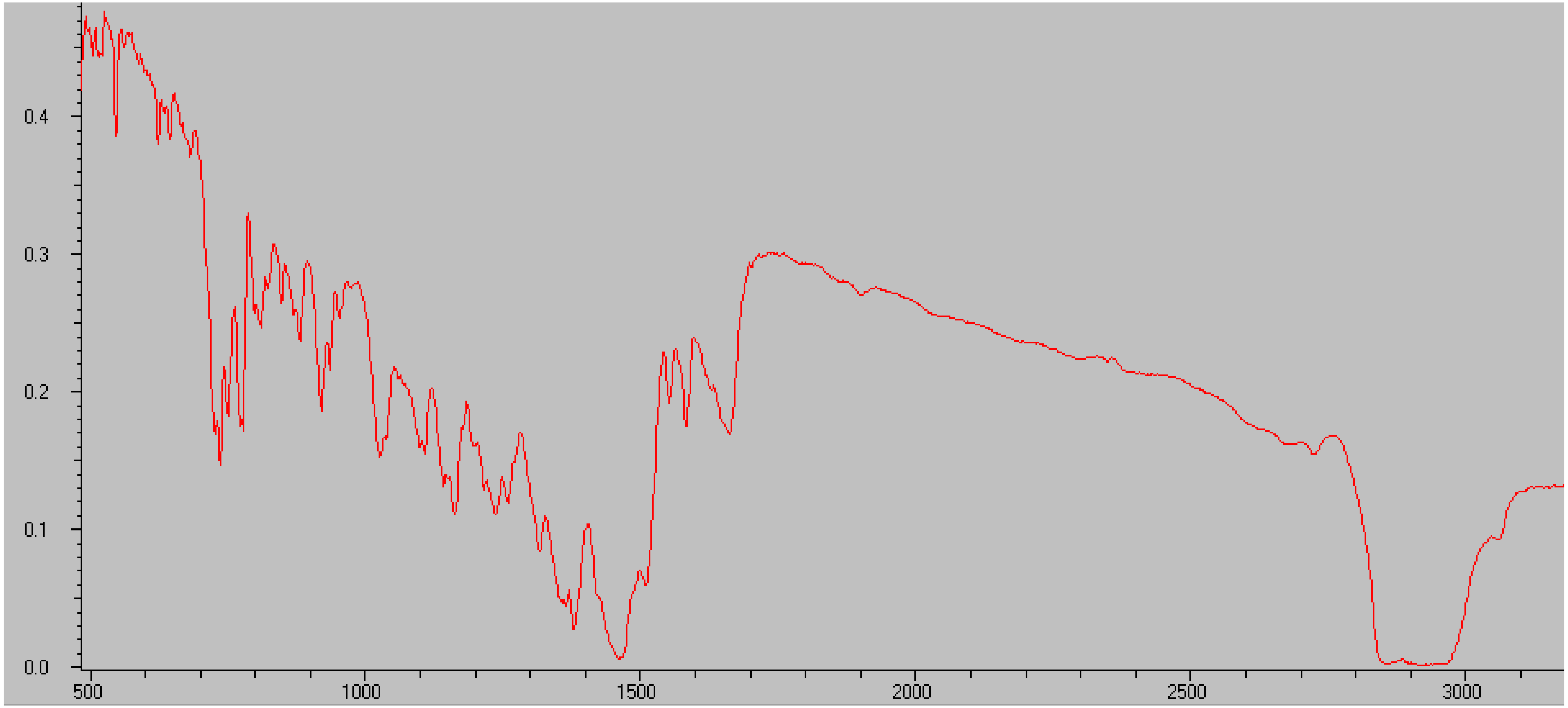

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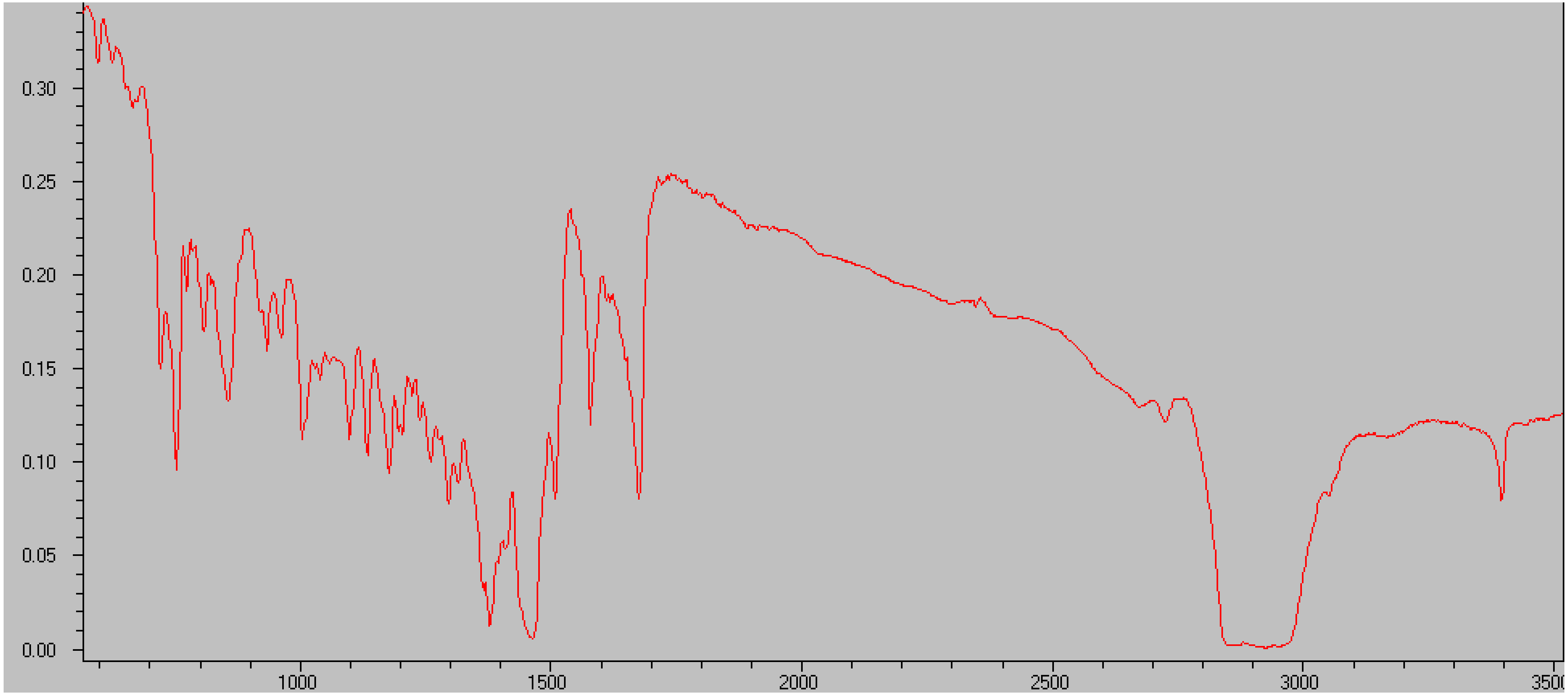

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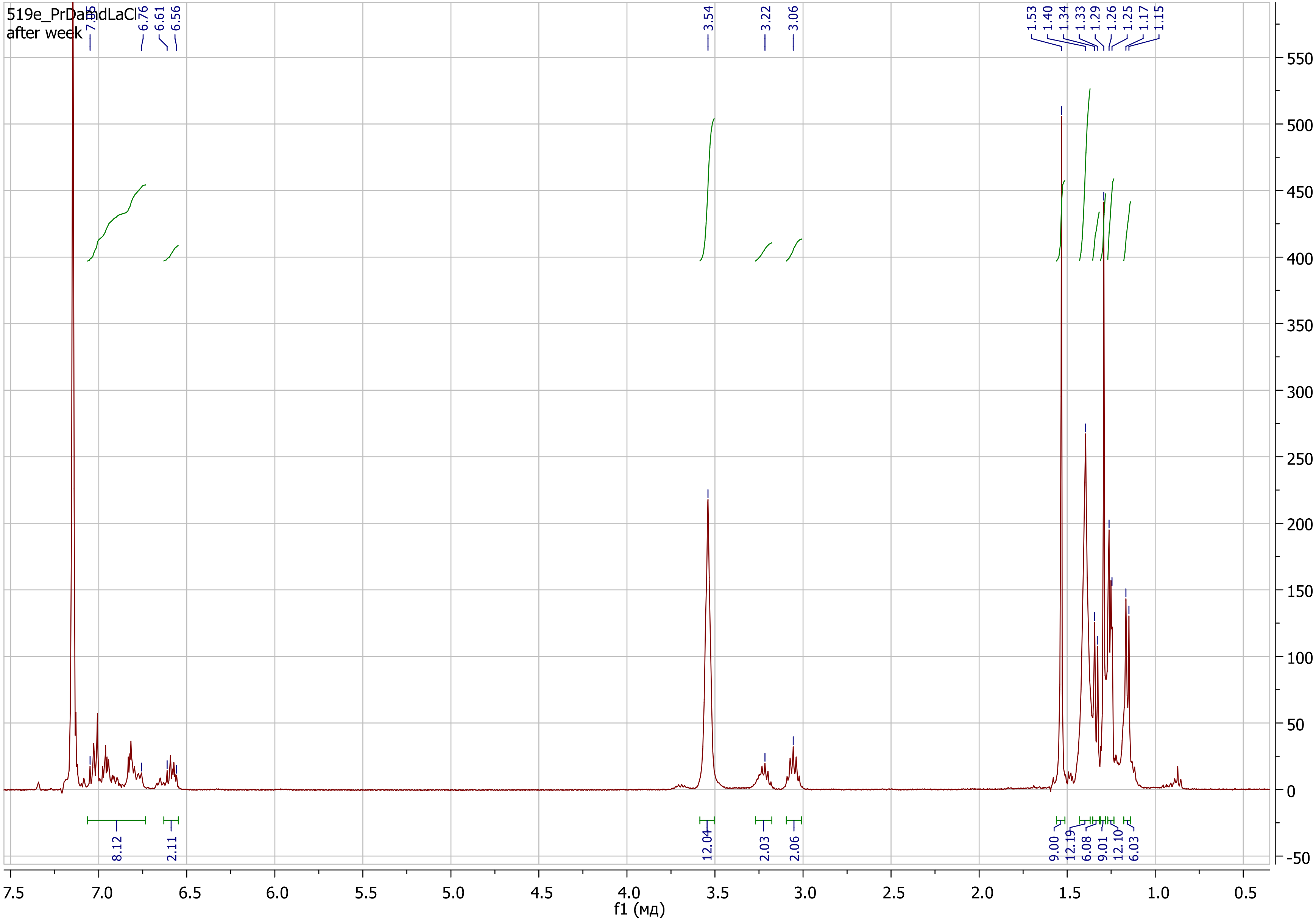

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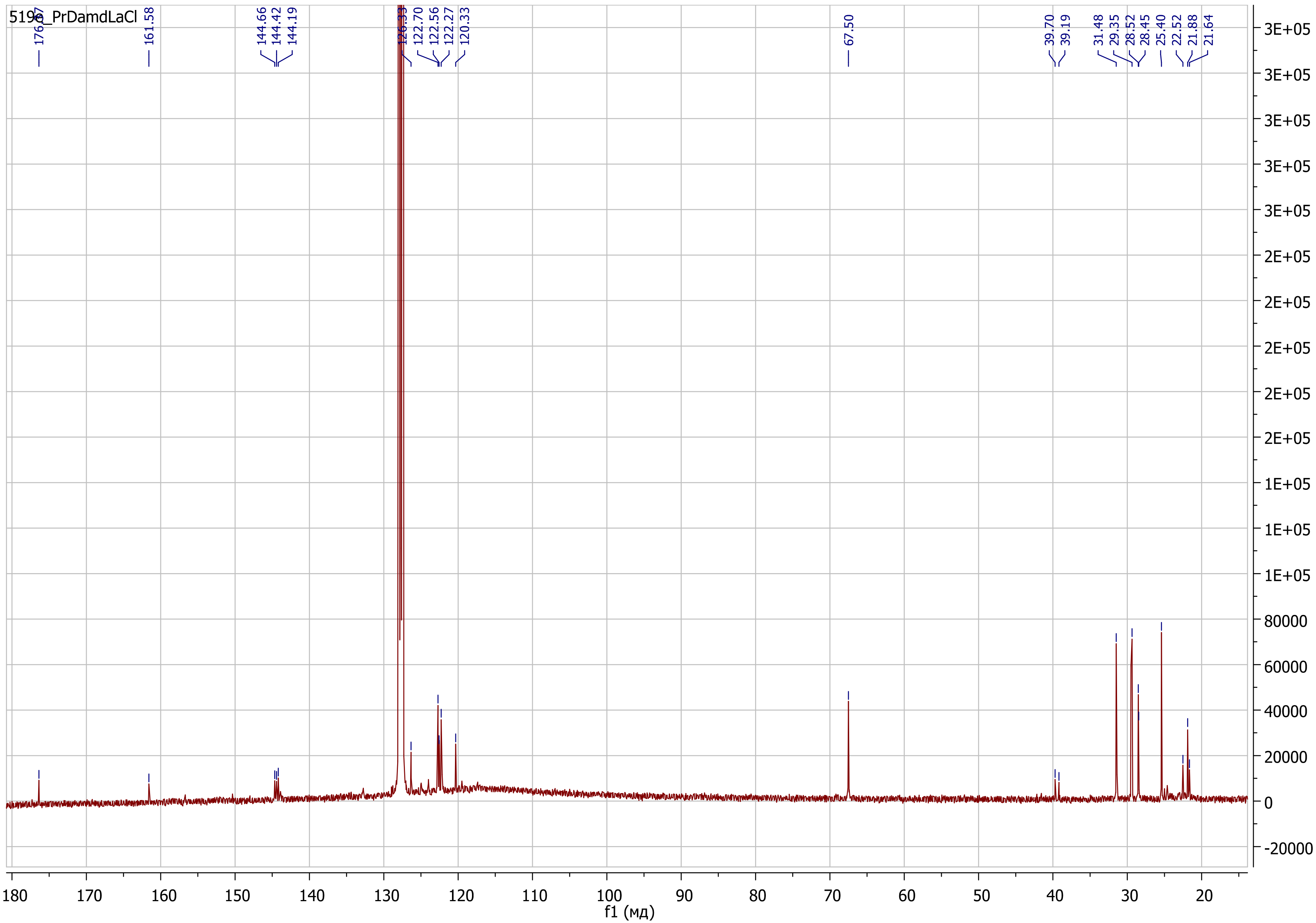

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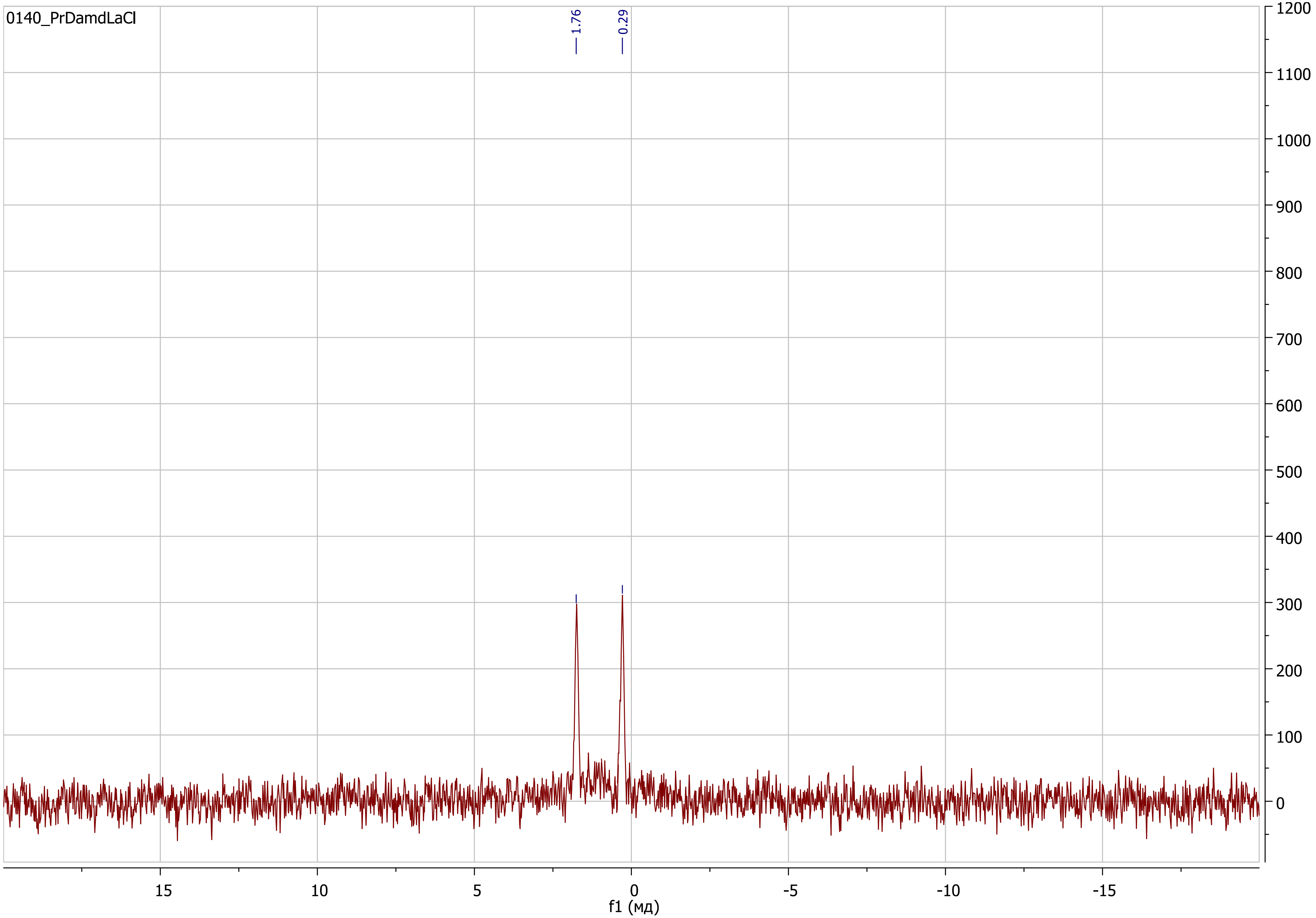

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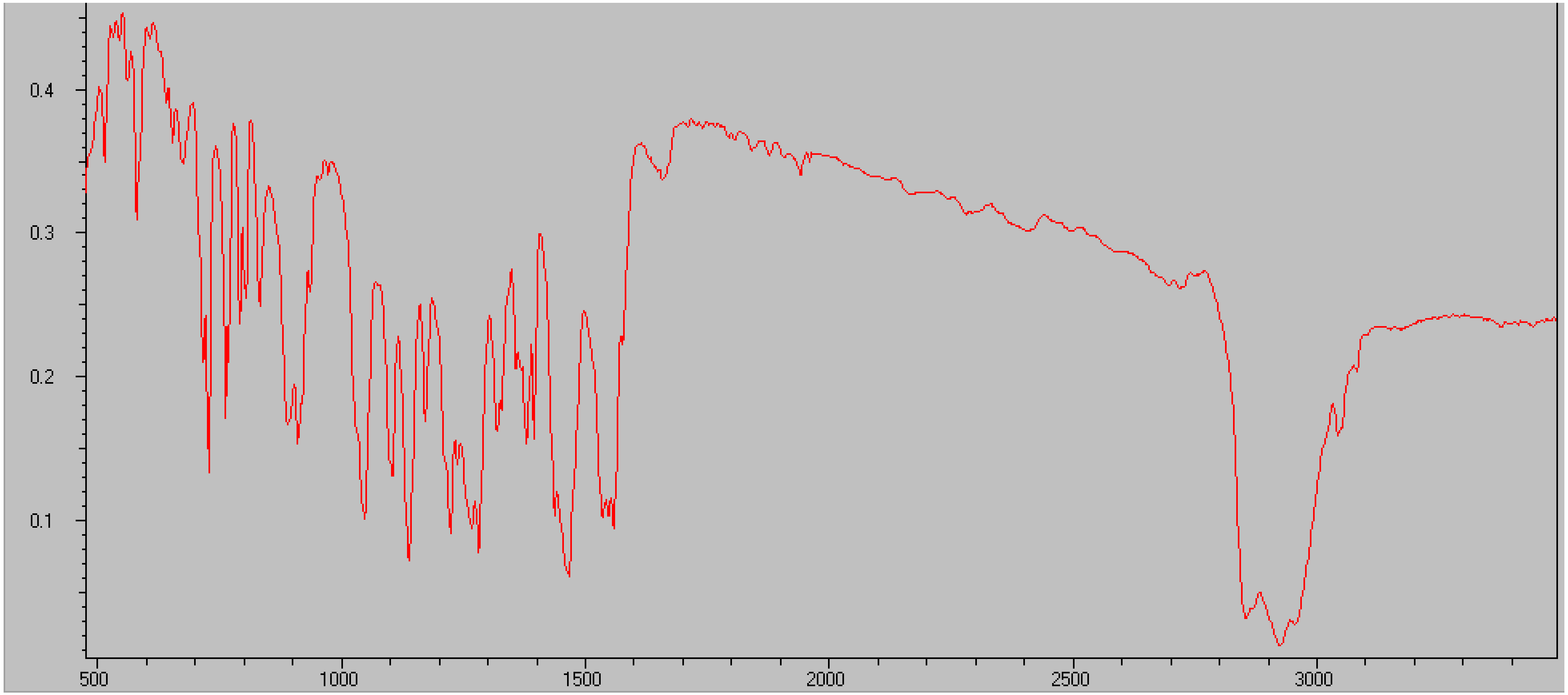

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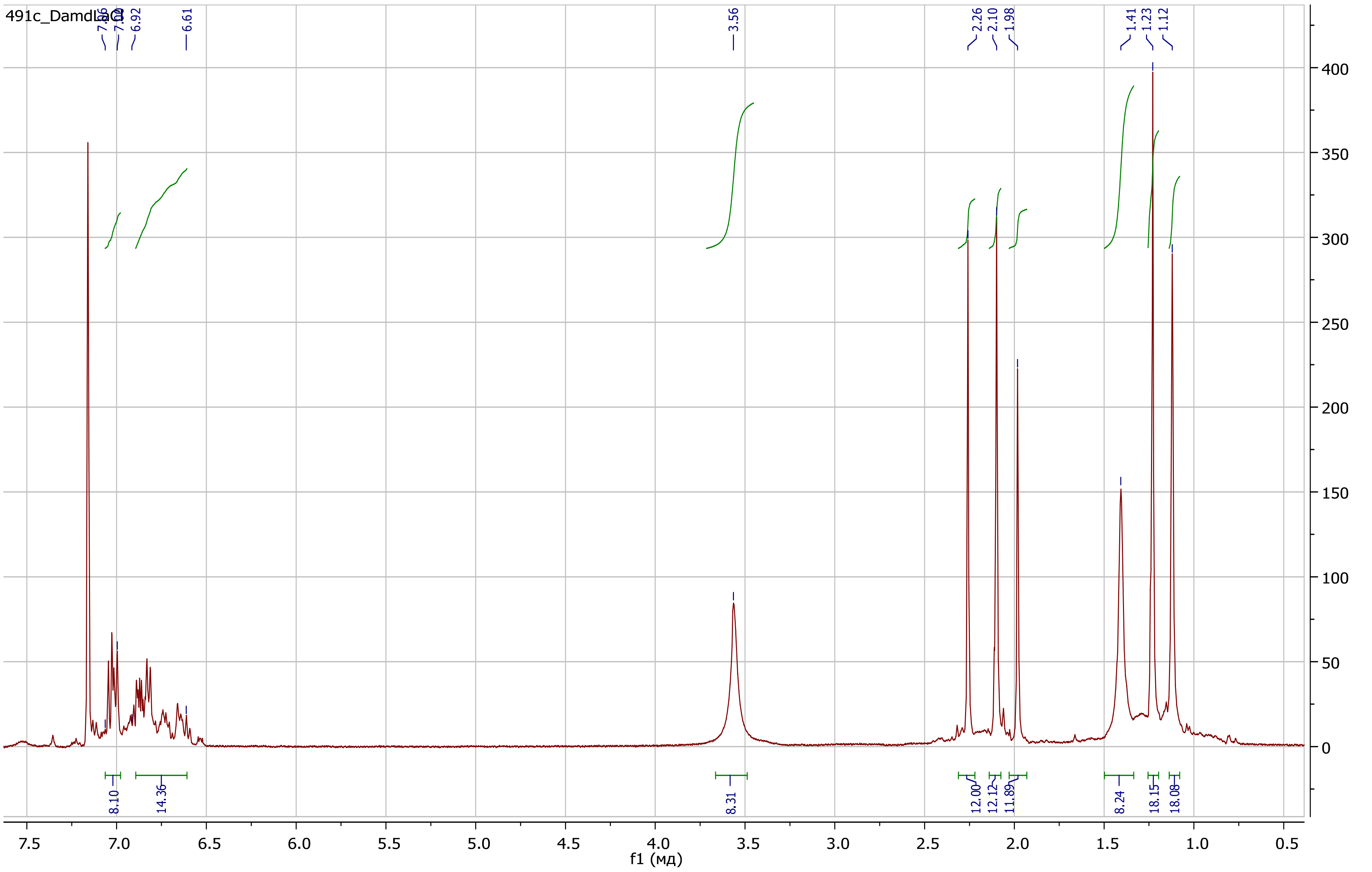

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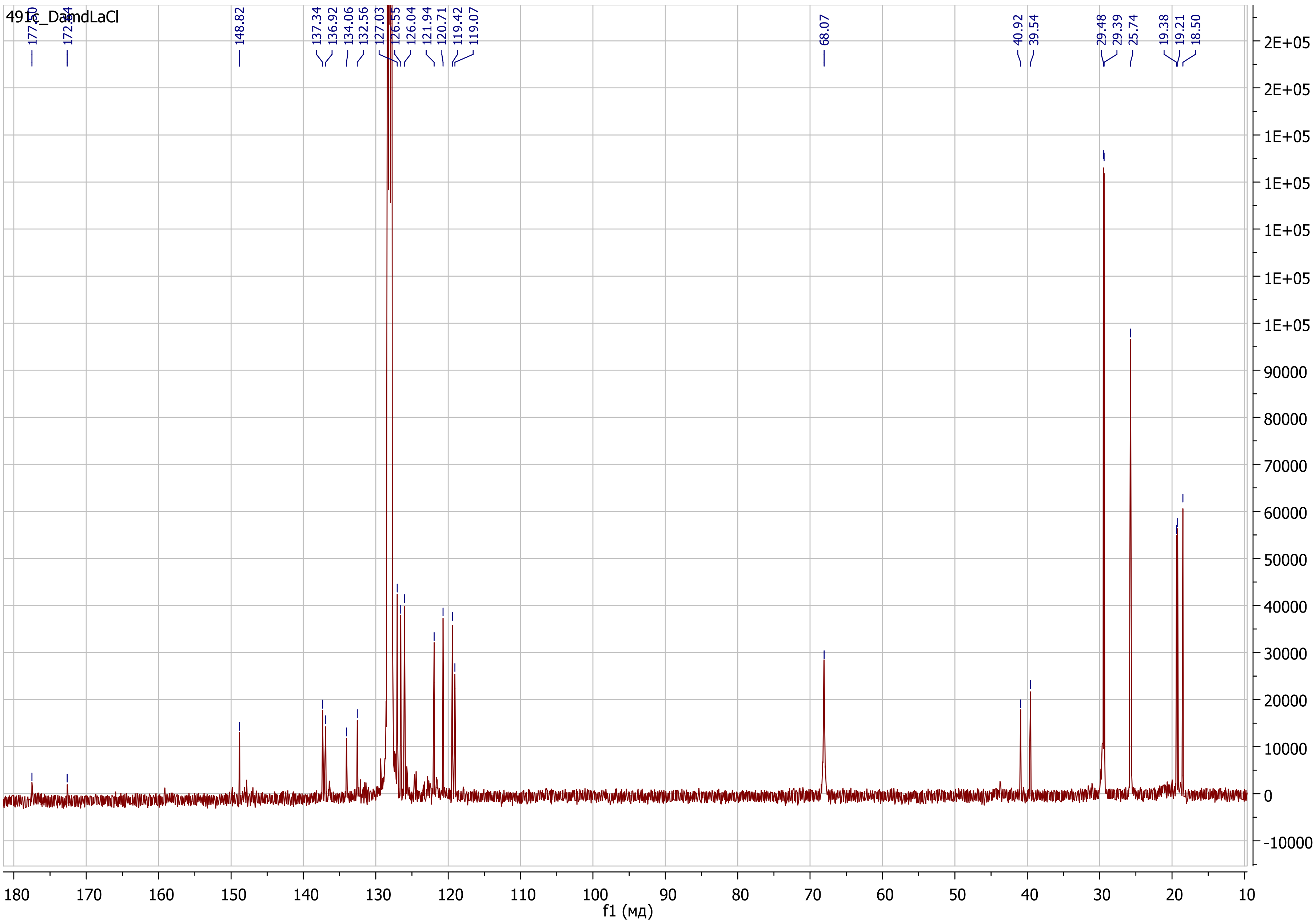

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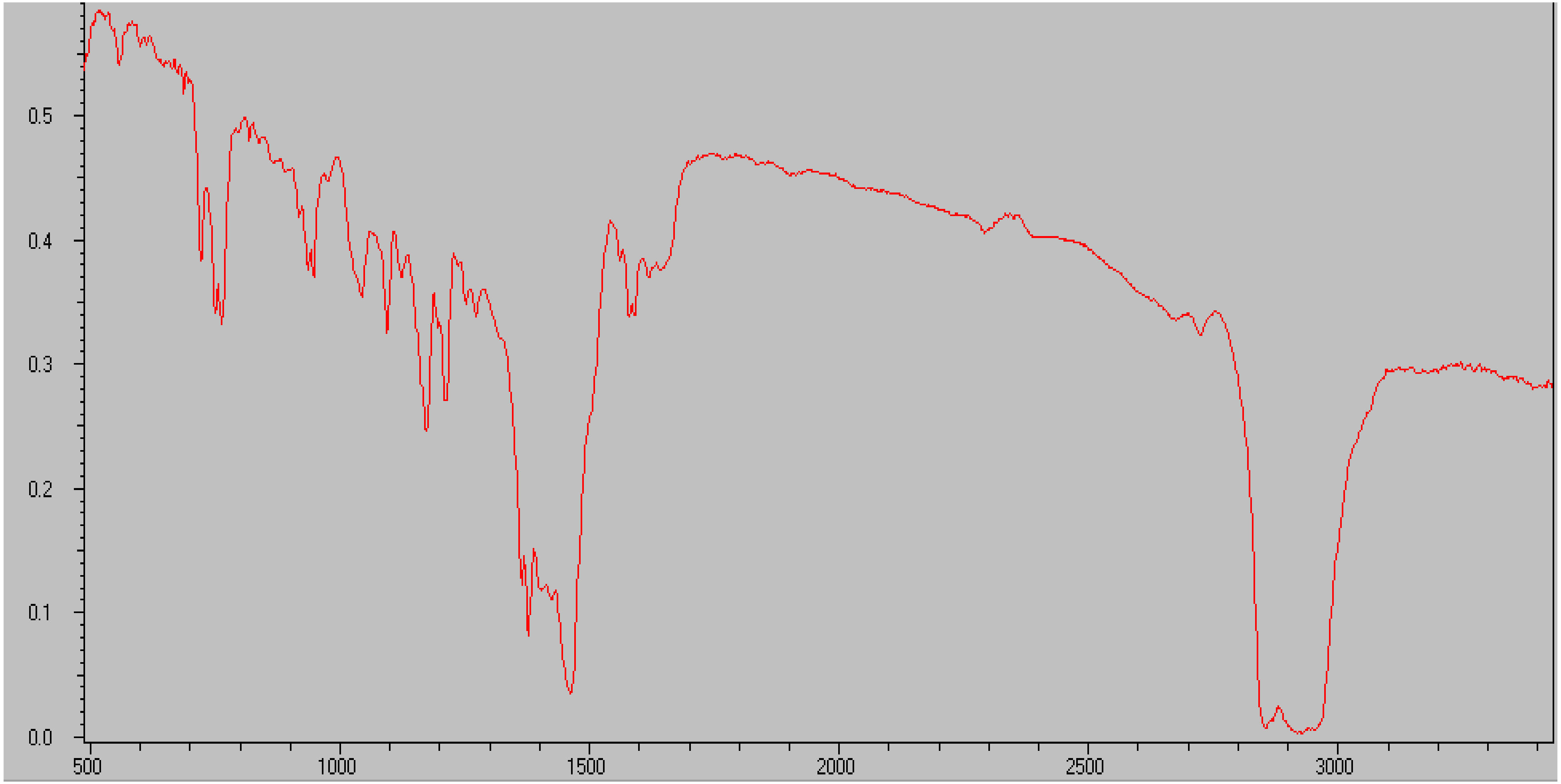

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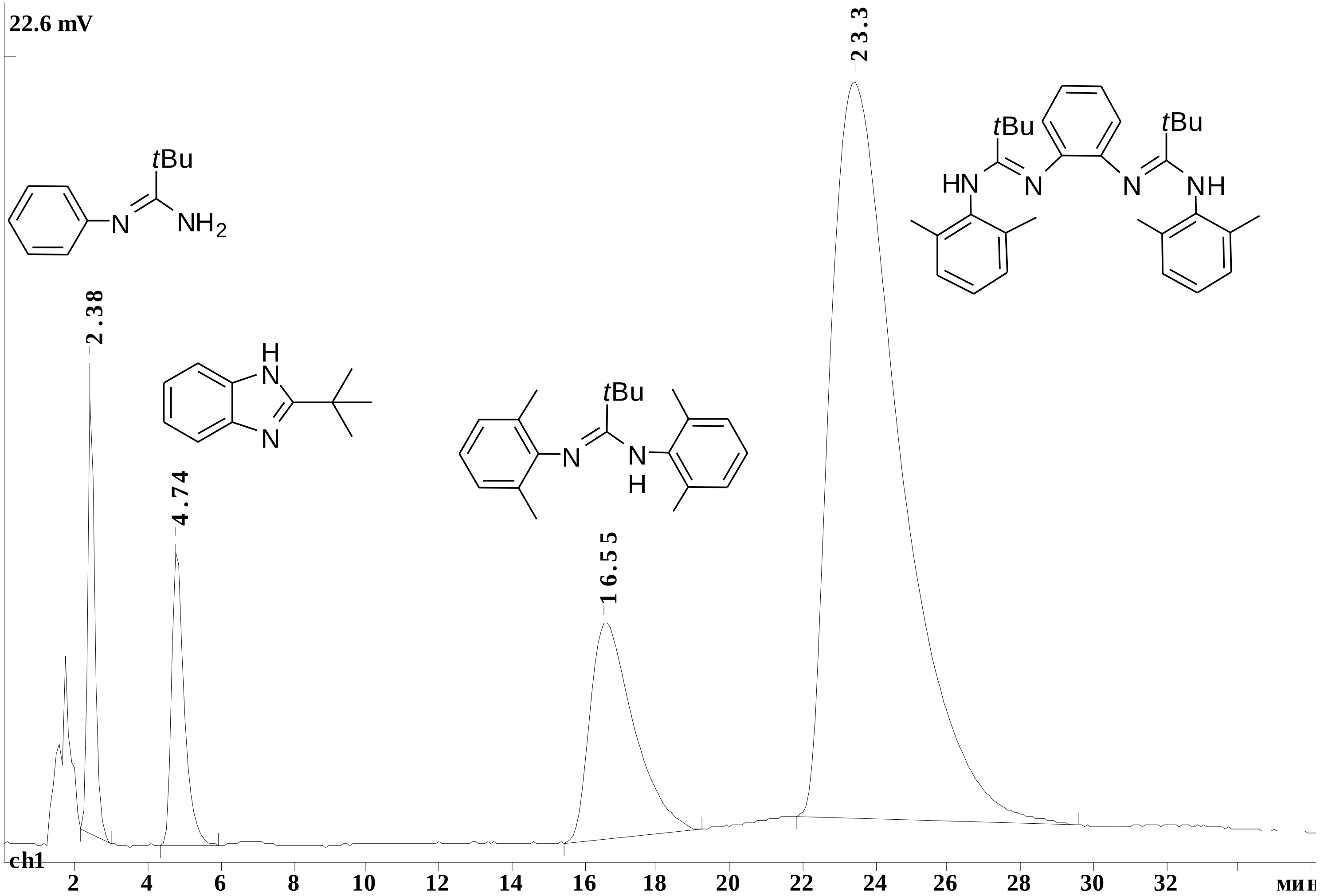

Figure 12S. HPLC of the by-products of complex **4**.

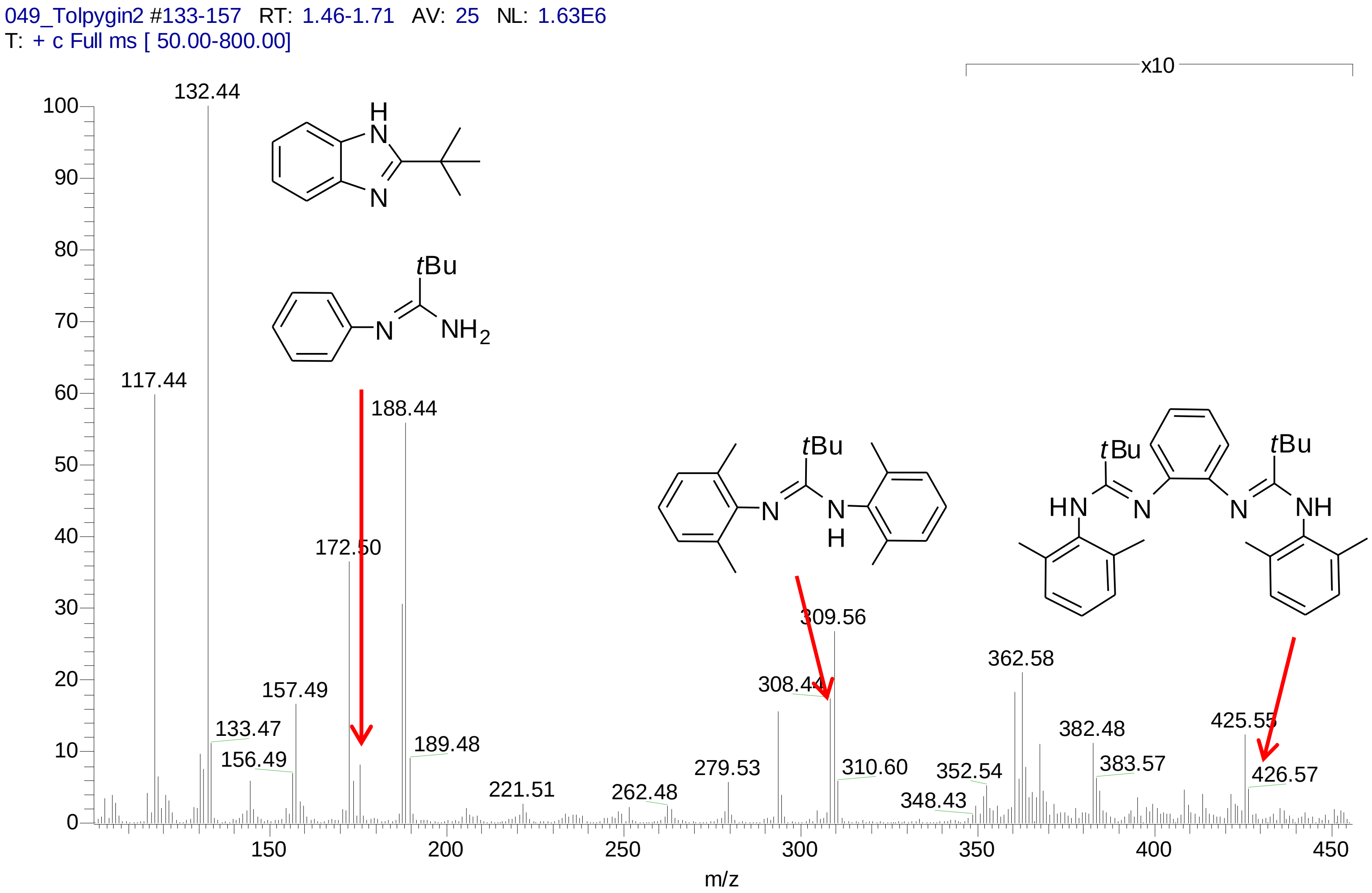

Figure 13S. MS of the by-products of complex **4**.

Computational details.

All DFT calculations were carried out with the Gaussian 09 suite of programs.[1] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[2] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Yb atoms were treated with stuttgart effective core potential (ECP28MWB), associated with its adapted basis set.[3] The basis sets were augmented by a set of polarization functions ($\zeta f = 1.000$). For the other elements (H, C, O and N), Pople's double-ζ basis set 6-31G(d,p) was used.[4]

1. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheesman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian Inc., 2009, Wallingford CT.

2. (a) A. D. Becke, Density-Functional Thermochemistry. III. The Role of Exact Exchange., *J. Chem. Phys.*, 1993, **98**, 5648 and references therein; (b) K. Burke, J. P. Perdew and W. Yang, Electronic Density Functional Theory: Recent Progress and New Directions; Plenum: New York, 1998.

3. (a) M. Dolg, H. Stoll and H. Preuss, Energy-adjusted *ab initio* pseudopotentials for the rare earth elements, *J. Chem. Phys.*, 1989, **90**, 1730; (b) X. Cao and M. Dolg, Segmented contraction scheme for small-core lanthanide pseudopotential basis sets, *J. Molec. Struct. Theochem.*, 2002, **581**, 139.

4. (a) P. C. Hariharan and J. A. Pople, The Influence of Polarization Functions on Molecular Orbital Hydrogenation Energies, *Theor. Chem. Acc.*, 1973, **28**, 213; (b) W. J. Hehre, R. Ditchfield, J. A. Pople, Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules, *J. Chem. Phys.*, 1972, **56**, 2257.

Structures

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κ^2-N,N complex

C	9.20381	0.09839	3.76860
O	8.45022	0.66527	4.86750
C	8.10997	-0.37993	5.81504
C	8.66733	-1.68062	5.23230
C	8.79003	-1.36246	3.73880
Yb	6.87276	2.39928	4.24944
N	7.07078	2.57124	1.87175
C	7.96323	3.02623	0.90987
C	8.67543	4.22587	1.16724
C	9.65652	4.66019	0.27726
C	9.97415	3.92404	-0.86089
C	9.30845	2.72406	-1.09150
C	8.31804	2.25275	-0.22634
C	8.36964	5.02285	2.40370
C	7.67031	0.92075	-0.49095
C	4.68409	2.97293	6.04269
N	5.86091	3.60801	6.12191
C	6.31423	4.62314	6.97386
C	6.25622	5.97435	6.55846
C	6.82667	6.96282	7.36325
C	7.46815	6.64336	8.55641
C	7.55845	5.30931	8.94225
C	7.00276	4.29103	8.16435
C	5.59166	6.34255	5.26083
C	7.14899	2.85222	8.57635
N	4.70130	2.02220	5.09191
C	3.85655	1.09976	4.48794
C	4.29186	0.69812	3.17307
C	3.64600	-0.35507	2.51786
C	2.53061	-0.98498	3.06840
C	2.06729	-0.57155	4.31116

C	2.72459	0.44261	5.00872
N	5.50227	1.22375	2.70805
C	5.79976	2.11063	1.76489
C	4.73753	2.77785	0.83646
C	3.75686	3.53335	1.75992
C	3.44444	3.28299	6.92656
C	3.24338	2.09860	7.90172
C	3.54274	4.54076	7.80629
C	2.22683	3.51268	6.00687
C	5.33698	3.81054	-0.12894
C	3.94492	1.75436	0.00439
H	4.05314	-0.69569	1.57062
H	2.04385	-1.79606	2.53397
H	1.20098	-1.04802	4.76269
H	2.34753	0.70431	5.98696
H	2.03604	2.70052	5.30715
H	2.37173	4.42776	5.42250
H	1.32799	3.65188	6.61824
H	3.93106	2.19190	8.74833
H	3.42299	1.12331	7.44878
H	2.22487	2.10980	8.30655
H	4.35106	4.49179	8.53709
H	2.60126	4.63465	8.36101
H	3.66840	5.45484	7.22226
H	6.76604	8.00063	7.04232
H	7.90540	7.42452	9.17180
H	8.07671	5.04506	9.86176
H	5.63974	7.42119	5.08735
H	4.53802	6.04296	5.23240
H	6.07279	5.84510	4.40997
H	6.18160	2.36815	8.74736
H	7.73629	2.76475	9.49486
H	7.65028	2.26767	7.79462
H	3.30493	2.29053	-0.70574
H	3.30244	1.13118	0.62554

H	4.60328	1.10050	-0.57616
H	4.27616	4.31135	2.33085
H	3.25529	2.86531	2.46295
H	2.98919	4.02530	1.15174
H	5.91311	4.57938	0.39128
H	4.51446	4.30869	-0.65453
H	5.98620	3.35993	-0.88269
H	10.17949	5.59155	0.48483
H	10.74055	4.27125	-1.54774
H	9.56957	2.12155	-1.95960
H	8.88931	5.98517	2.39917
H	8.69574	4.50187	3.31954
H	7.29557	5.21956	2.50526
H	6.69265	1.02102	-0.97775
H	7.50193	0.36615	0.43771
H	8.29422	0.31142	-1.15177
H	7.01883	-0.40230	5.90902
H	8.54393	-0.12305	6.78616
H	8.01441	-2.53235	5.43774
H	9.65268	-1.90037	5.65675
H	7.82219	-1.46379	3.23737
H	9.51792	-1.99441	3.22360
H	10.27549	0.21833	3.97521
H	8.94311	0.65835	2.86594

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TS κ^2-N,N → η^1-N:η^6-arene

C	1.46069	-3.17751	0.69334
O	1.86888	-1.91100	0.11867
C	2.87985	-2.12503	-0.89749
C	2.80291	-3.60869	-1.22324
C	2.43267	-4.21112	0.13478
Yb	0.50558	0.08260	0.14589
N	-0.03644	0.53409	2.56966
C	0.95642	1.47602	2.60316
C	0.95797	2.70819	1.87255

C	2.11555	3.50224	1.87135
C	3.26677	3.13966	2.55437
C	3.26762	1.93953	3.27007
C	2.15307	1.11252	3.30537
C	-0.26315	3.24158	1.15832
C	2.16524	-0.17068	4.08523
N	-1.67981	-0.01934	1.17423
C	-2.78240	-0.53096	0.50252
C	-2.54773	-0.72479	-0.90396
C	-3.48853	-1.44537	-1.65082
C	-4.68171	-1.89317	-1.08600
C	-4.93823	-1.65462	0.25984
C	-3.99138	-0.99617	1.04319
N	-1.27730	-0.39904	-1.37862
C	-0.81676	0.45815	-2.28252
C	-1.72297	1.40321	-3.13445
C	-0.91567	2.34567	-4.03883
C	-1.36510	0.57608	2.31435
C	-2.31847	1.14869	3.38783
C	-3.51990	1.87476	2.76355
N	0.52807	0.61440	-2.21232
C	1.45590	0.84972	-3.22265
C	2.42800	1.86753	-3.04246
C	3.43438	2.04246	-3.99211
C	3.52167	1.22491	-5.11566
C	2.59073	0.20392	-5.27593
C	1.56665	-0.00856	-4.34923
C	2.36868	2.75976	-1.83526
C	0.61757	-1.16007	-4.54529
C	-2.76431	-0.03448	4.27683
C	-1.58752	2.13427	4.31364
C	-2.50915	2.28146	-2.13819
C	-2.73251	0.65220	-4.02329
H	-4.18735	-0.87463	2.10043
H	-5.86007	-2.00439	0.71650

H	-5.39305	-2.44474	-1.69464
H	-3.25234	-1.69333	-2.67973
H	-3.54814	0.22276	-3.44269
H	-2.26144	-0.14767	-4.60266
H	-0.39438	1.81755	-4.84053
H	-0.17437	2.92066	-3.47945
H	-1.60807	3.05702	-4.50337
H	-3.17225	1.35749	-4.73761
H	-3.12342	1.68299	-1.46094
H	-1.83039	2.89952	-1.54143
H	-3.17365	2.95552	-2.69072
H	-0.74059	1.66249	4.81711
H	-1.21398	3.00965	3.77742
H	-2.28530	2.48855	5.08069
H	-3.19181	2.76675	2.22012
H	-4.20372	2.20368	3.55407
H	-4.08476	1.25352	2.06794
H	-3.44989	0.32414	5.05314
H	-3.26823	-0.82739	3.72129
H	-1.89354	-0.47950	4.76807
H	1.49119	-3.08440	1.78227
H	0.42879	-3.37835	0.38235
H	1.97961	-5.20286	0.06004
H	3.31941	-4.28934	0.77321
H	3.74315	-3.99345	-1.62612
H	2.01246	-3.79630	-1.95746
H	2.65531	-1.46959	-1.74344
H	3.85598	-1.85238	-0.47701
H	2.66095	-0.46036	-6.13536
H	4.31035	1.37361	-5.84764
H	4.16056	2.83926	-3.84397
H	1.05139	-1.90936	-5.21472
H	-0.33205	-0.84518	-4.99489
H	0.36817	-1.64188	-3.59459
H	2.61606	2.22690	-0.90586

H	1.36839	3.18383	-1.69322
H	3.08101	3.58542	-1.92105
H	4.15736	1.63919	3.82022
H	4.14720	3.77458	2.53291
H	2.09352	4.43640	1.31299
H	-0.89483	2.46929	0.70642
H	-0.92445	3.79738	1.83604
H	0.03206	3.93679	0.36694
H	2.00633	-1.03899	3.43337
H	3.11456	-0.30348	4.61242
H	1.35076	-0.19807	4.81818

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η^1-N:η^6-arene compex

C	2.23875	2.44120	-2.46160
C	1.57494	1.21626	-2.71161
C	1.95183	0.44928	-3.84319
C	2.93257	0.93809	-4.70926
C	3.56544	2.15561	-4.47741
C	3.21662	2.89246	-3.34924
Yb	0.69447	-0.25378	0.46713
N	0.67701	0.70811	-1.76925
C	-0.61838	0.35842	-1.93019
C	-1.63151	1.15750	-2.79718
C	-0.98437	2.20371	-3.71423
C	1.32620	-0.89500	-4.09552
C	1.87863	3.25512	-1.25218
O	1.45149	-2.54429	0.03216
C	2.79965	-3.00893	-0.18123
C	2.67339	-4.24453	-1.06471
C	1.31567	-4.80514	-0.63459
C	0.49949	-3.53604	-0.43689
C	0.43788	0.72205	3.03701
C	1.35662	1.66685	2.49452
C	2.64467	1.24881	2.13210
C	3.05679	-0.07446	2.32262

C	2.18344	-0.97644	2.94123
C	0.88428	-0.60472	3.30560
N	-0.84049	1.14002	3.32374
C	-1.82276	0.77165	2.52734
N	-1.56070	0.03264	1.41702
C	-2.44247	-0.83321	0.76940
C	-2.18627	-1.12210	-0.61312
C	-2.95554	-2.09645	-1.26184
C	-3.98183	-2.77988	-0.60869
C	-4.21195	-2.53072	0.74077
C	-3.43483	-1.59166	1.41671
C	0.92514	3.09865	2.33753
C	-0.04483	-1.58036	3.97082
N	-0.98188	-0.64527	-1.14152
C	-3.18769	1.41114	2.93449
C	-4.27452	1.39578	1.85027
C	-3.70515	0.75181	4.22673
C	-2.91469	2.89812	3.25451
C	-2.55773	1.90282	-1.81407
C	-2.48476	0.22469	-3.67289
H	-3.57588	-1.45454	2.48380
H	-4.97595	-3.08350	1.28147
H	-4.56475	-3.52469	-1.14343
H	-2.70752	-2.34592	-2.28952
H	-3.13325	-0.41552	-3.07558
H	-1.86559	-0.41087	-4.31490
H	-0.35475	1.75460	-4.48582
H	-0.37564	2.92241	-3.16231
H	-1.78234	2.76156	-4.21802
H	-3.12373	0.82875	-4.32700
H	-3.09273	1.21000	-1.16085
H	-1.98710	2.59750	-1.18860
H	-3.29834	2.48489	-2.37468
H	-2.16694	2.99853	4.04189
H	-2.55152	3.42925	2.36777

H	-3.84493	3.38083	3.57593
H	-3.89449	1.79590	0.90585
H	-5.10034	2.04000	2.17329
H	-4.68566	0.40632	1.65293
H	-4.59718	1.28006	4.58309
H	-3.98380	-0.29667	4.08225
H	-2.94078	0.79884	5.00754
H	-0.29293	-3.62335	0.31051
H	0.05761	-3.16921	-1.36839
H	0.86846	-5.47099	-1.37693
H	1.40873	-5.35792	0.30692
H	3.50065	-4.94412	-0.91966
H	2.65052	-3.95647	-2.12098
H	3.37800	-2.20215	-0.64206
H	3.24398	-3.25046	0.79278
H	3.33699	1.97302	1.70936
H	4.06061	-0.38180	2.04515
H	2.51318	-1.99329	3.14155
H	1.75391	3.72617	1.99962
H	0.55303	3.48221	3.29250
H	0.09965	3.20330	1.62595
H	-0.50523	-1.12391	4.85267
H	0.48653	-2.48601	4.27646
H	-0.86439	-1.86706	3.30297
H	3.21058	0.34059	-5.57554
H	4.32704	2.52021	-5.16093
H	3.70703	3.84322	-3.14993
H	1.89416	-1.45471	-4.84485
H	0.29537	-0.81613	-4.46147
H	1.27898	-1.48436	-3.17316
H	2.12512	2.72464	-0.32441
H	0.80407	3.46572	-1.20718
H	2.41518	4.20846	-1.24282

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TS η^1-N:η^6-arene → η^6-arene:η^6-arene

C	1.49368	2.32089	-1.70465
C	1.73796	1.04931	-2.33062
C	3.09776	0.72649	-2.67434
C	4.12197	1.63111	-2.42967
C	3.87766	2.87600	-1.84320
C	2.57094	3.19573	-1.49952
Yb	1.13476	-0.24845	0.04319
N	0.81174	0.08309	-2.57407
C	-0.53439	0.02604	-2.38164
C	-1.42901	0.24853	-3.62605
C	-0.73851	1.20092	-4.61644
C	3.36902	-0.58708	-3.34972
C	0.10381	2.80191	-1.35492
O	1.46272	-2.63248	-0.52689
C	2.53951	-3.55094	-0.25202
C	2.49598	-4.57892	-1.37321
C	0.99422	-4.67274	-1.64673
C	0.54648	-3.22479	-1.49262
C	1.36474	0.61015	2.69681
C	2.28069	1.47158	2.02781
C	3.43369	0.93343	1.43979
C	3.72931	-0.42818	1.55003
C	2.88117	-1.25232	2.29936
C	1.70160	-0.76254	2.87066
N	0.19809	1.15266	3.19001
C	-0.92055	0.91059	2.54258
N	-0.90795	0.17324	1.39941
C	-1.96512	-0.58692	0.91408
C	-2.01595	-0.83555	-0.50070
C	-3.01138	-1.67912	-1.01189
C	-3.95110	-2.29145	-0.18179
C	-3.87837	-2.09207	1.19323
C	-2.88802	-1.26991	1.72611
C	2.00699	2.94892	1.99098
C	0.79326	-1.65699	3.66603

N	-0.90182	-0.35964	-1.18516
C	-2.13866	1.69814	3.11911
C	-3.35626	1.79069	2.18710
C	-2.54314	1.11152	4.48357
C	-1.66298	3.14800	3.36219
C	-2.79512	0.84349	-3.25487
C	-1.58555	-1.10650	-4.34861
H	-2.80533	-1.16338	2.80277
H	-4.57637	-2.59223	1.85967
H	-4.70875	-2.94134	-0.61031
H	-3.03410	-1.88556	-2.07531
H	-2.05558	-1.87133	-3.72559
H	-0.60561	-1.48081	-4.66138
H	0.24408	0.82418	-4.90763
H	-0.60271	2.20269	-4.19897
H	-1.35736	1.29915	-5.51544
H	-2.20341	-0.97989	-5.24493
H	-3.36821	0.21634	-2.57132
H	-2.67590	1.82383	-2.78208
H	-3.39160	0.98488	-4.16321
H	-0.80050	3.17057	4.02918
H	-1.37991	3.62996	2.41985
H	-2.47827	3.73257	3.80422
H	-3.06178	2.09106	1.17651
H	-4.03814	2.55595	2.57525
H	-3.91727	0.85983	2.10662
H	-3.31557	1.73707	4.94608
H	-2.95020	0.09912	4.40005
H	-1.67828	1.07959	5.15232
H	-0.47007	-3.11553	-1.10845
H	0.64343	-2.65468	-2.42173
H	0.75882	-5.07086	-2.63705
H	0.50846	-5.31063	-0.90014
H	2.94784	-5.53062	-1.08125
H	3.02516	-4.20400	-2.25597

H	3.47336	-2.98465	-0.21029
H	2.36514	-4.01941	0.72531
H	4.09688	1.58964	0.88230
H	4.63333	-0.82848	1.10078
H	3.13731	-2.29896	2.44493
H	2.79280	3.47742	1.44741
H	1.95122	3.33958	3.01268
H	1.04477	3.17787	1.52522
H	0.49246	-1.16194	4.59439
H	1.28554	-2.60237	3.91119
H	-0.12718	-1.87922	3.11545
H	5.13533	1.35995	-2.72078
H	4.68524	3.58244	-1.67695
H	2.35642	4.16858	-1.06130
H	4.43206	-0.69956	-3.58319
H	2.79339	-0.67586	-4.27875
H	3.05623	-1.43473	-2.72691
H	-0.41508	2.18506	-0.61080
H	-0.55270	2.83097	-2.23182
H	0.15322	3.82019	-0.95857

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η^6-arene:η^6-arene complex

C	2.17428	1.74946	-2.11043
C	1.32474	0.83445	-2.79017
C	1.79916	-0.47880	-3.06334
C	3.07613	-0.84962	-2.63631
C	3.90127	0.03861	-1.94262
C	3.44753	1.33351	-1.69761
Yb	0.87119	0.12317	0.10526
N	0.10926	1.27563	-3.27604
C	-0.99187	0.94657	-2.64401
C	-2.28438	1.50625	-3.30469
C	-2.01722	2.98861	-3.64162
C	0.94513	-1.41900	-3.86511
C	1.72167	3.17505	-1.93777

O	1.30492	-2.29057	0.14042
C	2.57486	-2.92439	0.40425
C	2.45360	-4.33829	-0.14888
C	0.96491	-4.62716	0.05485
C	0.33395	-3.28690	-0.28885
C	0.66901	1.14857	2.76281
C	1.28929	2.20772	2.03978
C	2.60924	2.05802	1.59748
C	3.33411	0.89137	1.85812
C	2.73999	-0.12417	2.61192
C	1.42039	-0.02022	3.06524
N	-0.62878	1.29896	3.18987
C	-1.57760	0.81121	2.41772
N	-1.24302	0.20680	1.25449
C	-2.01043	-0.67029	0.48755
C	-1.86411	-0.59760	-0.93817
C	-2.51837	-1.56639	-1.72254
C	-3.30885	-2.56767	-1.16295
C	-3.42445	-2.65770	0.22330
C	-2.75890	-1.73213	1.02638
C	0.51549	3.47330	1.79226
C	0.78236	-1.10973	3.87849
N	-0.93662	0.30577	-1.45055
C	-3.01262	1.11792	2.93714
C	-4.11679	1.02927	1.87336
C	-3.33650	0.19342	4.12575
C	-3.01600	2.56884	3.46360
C	-3.52560	1.46106	-2.40433
C	-2.55631	0.76617	-4.62662
H	-2.81147	-1.82326	2.10709
H	-4.01023	-3.45042	0.68108
H	-3.80659	-3.28725	-1.80781
H	-2.38259	-1.52905	-2.79960
H	-2.81104	-0.28617	-4.46589
H	-1.67831	0.81391	-5.27698

H	-1.14409	3.08844	-4.28817
H	-1.83643	3.57121	-2.73143
H	-2.89145	3.41668	-4.14605
H	-3.40052	1.23067	-5.14978
H	-3.90558	0.45125	-2.24476
H	-3.31567	1.89918	-1.42371
H	-4.32531	2.04861	-2.86951
H	-2.25769	2.70875	4.23498
H	-2.81378	3.27949	2.65490
H	-4.00261	2.80557	3.87889
H	-3.84698	1.59016	0.97336
H	-5.03325	1.47349	2.27858
H	-4.34975	0.00845	1.57112
H	-4.30124	0.47294	4.56513
H	-3.40443	-0.85811	3.83054
H	-2.56653	0.28438	4.89736
H	-0.61033	-3.08405	0.22019
H	0.18354	-3.17522	-1.36735
H	0.58844	-5.43333	-0.57986
H	0.76361	-4.89298	1.09856
H	3.11147	-5.04195	0.36800
H	2.70388	-4.35647	-1.21521
H	3.35966	-2.32910	-0.07117
H	2.73972	-2.93304	1.48826
H	3.07666	2.87291	1.05110
H	4.35726	0.79173	1.51024
H	3.31487	-1.01265	2.86276
H	1.12568	4.21667	1.27244
H	0.17249	3.89493	2.74236
H	-0.38585	3.28492	1.19927
H	0.37198	-0.69993	4.80697
H	1.50233	-1.89512	4.12598
H	-0.05677	-1.56279	3.34022
H	3.43814	-1.84858	-2.87226
H	4.89818	-0.26245	-1.63330

H	4.09910	2.04904	-1.20150
H	1.48579	-2.33920	-4.10574
H	0.62966	-0.94253	-4.79941
H	0.02827	-1.68443	-3.32916
H	0.76701	3.24841	-1.40636
H	1.55327	3.63546	-2.91729
H	2.46753	3.76597	-1.39836

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κ^2-N,N Cl complex

C	7.57243	1.18372	6.54039
C	7.80874	1.83227	5.27556
C	8.92940	1.40469	4.53972
C	9.73698	0.35031	4.96753
C	9.44128	-0.32917	6.14232
C	8.35882	0.08637	6.91295
N	6.83547	2.78196	4.96924
C	6.47670	3.58267	3.93961
C	7.32922	3.79405	2.66872
C	6.78441	4.81348	1.65464
N	6.43521	1.60692	7.20731
Yb	5.15018	3.28851	6.42804
Cl	6.12780	5.28072	7.63873
N	4.71153	2.07550	8.48770
C	5.99891	1.68906	8.47545
C	6.88773	1.59645	9.74915
C	6.34691	2.52358	10.85379
C	3.74697	1.81612	9.47760
C	3.06311	2.86720	10.14240
C	2.02473	2.56414	11.02627
C	1.63595	1.25403	11.28001
C	2.29288	0.22439	10.61889
C	3.32756	0.47666	9.71271
C	3.44371	4.31256	9.96874
C	3.90708	-0.71045	8.98004
C	6.93227	0.16458	10.31567

C	8.31214	2.10146	9.44129
O	2.87444	4.15225	6.53477
C	1.85737	3.39580	5.88664
C	2.20094	1.93104	6.01888
O	3.51533	1.74390	5.49523
C	3.85928	0.37276	5.28860
N	5.30793	4.16920	4.20239
C	4.50819	5.03941	3.43512
C	3.50699	4.50372	2.58909
C	2.60176	5.36774	1.96546
C	2.66862	6.74379	2.15695
C	3.66527	7.26617	2.97521
C	4.59042	6.44018	3.62182
C	3.43304	3.02464	2.32170
C	5.66950	7.04945	4.47201
C	2.58886	5.55530	6.56906
C	8.70362	4.34376	3.11682
C	7.40992	2.44864	1.90771
H	9.19394	1.88373	3.60998
H	10.58927	0.05820	4.36024
H	10.04215	-1.17534	6.46331
H	8.10936	-0.45169	7.82005
H	7.23284	-0.58342	9.57739
H	5.95943	-0.12784	10.71868
H	7.65738	0.12856	11.13643
H	8.27964	3.10506	9.00631
H	8.87220	1.45692	8.76572
H	8.86950	2.16102	10.38232
H	6.27500	3.55523	10.49893
H	7.04734	2.50474	11.69601
H	5.37136	2.21279	11.22900
H	1.99295	-0.80781	10.79078
H	0.83272	1.03954	11.97939
H	1.52426	3.38513	11.53633
H	3.13206	-1.20068	8.37667

H	4.27788	-1.46842	9.67864
H	4.72966	-0.44349	8.31692
H	3.72092	4.75500	10.93273
H	2.59881	4.89697	9.58602
H	4.28799	4.44983	9.29387
H	9.40647	4.32056	2.27636
H	9.14777	3.80686	3.95367
H	8.59463	5.38730	3.42891
H	6.48245	2.28685	1.34921
H	7.55786	1.58095	2.54988
H	8.22800	2.47809	1.17917
H	5.81565	4.52983	1.24006
H	7.49555	4.86436	0.82134
H	6.69686	5.81906	2.06914
H	1.83734	4.94670	1.31565
H	1.95630	7.40276	1.66830
H	3.73726	8.34173	3.12077
H	2.49444	2.76502	1.82265
H	3.51863	2.44577	3.24453
H	4.24909	2.69499	1.66672
H	6.66339	6.88278	4.03914
H	5.70536	6.61931	5.47720
H	5.52856	8.13028	4.56069
H	2.17529	1.61168	7.06868
H	1.48061	1.33668	5.44087
H	1.79833	3.69625	4.83224
H	0.88785	3.58558	6.36744
H	4.89946	0.35054	4.96418
H	3.75573	-0.19407	6.21780
H	3.21412	-0.05504	4.51170
H	3.42601	6.03128	7.08056
H	2.49751	5.95054	5.55177
H	1.66182	5.72779	7.12823

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η^1-N Cl Complex

C	-2.99327	-1.59993	1.04908
C	-2.14057	-0.62232	0.49082
C	-1.96175	-0.61092	-0.94099
C	-2.71832	-1.52329	-1.70932
C	-3.59120	-2.43168	-1.13062
C	-3.71898	-2.48183	0.26255
Yb	0.46674	0.83799	0.10915
N	-1.01285	0.23216	-1.49411
C	-1.11388	0.66414	-2.81962
C	-2.33990	1.50441	-3.28984
C	-2.97259	0.85868	-4.53340
N	-1.40139	0.26195	1.25677
C	-1.78745	0.69132	2.51832
C	-3.19703	1.28622	2.81859
C	-2.96020	2.76293	3.20736
C	1.05783	-0.07223	-3.59349
C	2.22289	0.73143	-3.50529
C	3.47879	0.12657	-3.60352
C	3.61047	-1.24396	-3.81511
C	2.46112	-2.02287	-3.93563
C	1.18399	-1.46380	-3.83227
C	2.09612	2.22676	-3.41283
N	-0.17480	0.56692	-3.69086
C	-0.03508	-2.31425	-4.05765
O	1.48998	-1.36392	0.17041
C	2.84619	-1.44747	-0.27648
C	0.37915	0.40020	3.47939
C	1.38375	1.39899	3.58995
C	2.71535	1.00797	3.76704
C	3.06961	-0.33547	3.86967
C	2.07528	-1.30880	3.79318
C	0.73470	-0.96891	3.60135
N	-0.95094	0.81366	3.49418
C	0.99595	2.85184	3.64382
C	-0.32743	-2.03157	3.62384

C	-1.78829	2.89189	-3.68316
C	-3.40469	1.72290	-2.21097
C	-4.18231	1.28266	1.64438
C	-3.81582	0.55866	4.02390
H	-3.08251	-1.64065	2.13057
H	-4.37586	-3.20957	0.73033
H	-4.15380	-3.11536	-1.76002
H	-2.59341	-1.50796	-2.78716
H	-3.45053	-0.09813	-4.29753
H	-2.21621	0.69029	-5.30445
H	-1.05814	2.80193	-4.49004
H	-1.30613	3.37902	-2.82922
H	-2.61049	3.53290	-4.02108
H	-3.74523	1.51936	-4.94265
H	-3.91725	0.80253	-1.92394
H	-2.96605	2.17026	-1.31460
H	-4.16010	2.41729	-2.59459
H	-2.30077	2.83366	4.07402
H	-2.50598	3.31900	2.38040
H	-3.91778	3.23765	3.44914
H	-3.74200	1.73007	0.75002
H	-5.05465	1.88556	1.92022
H	-4.54144	0.28589	1.38423
H	-4.75001	1.05111	4.31664
H	-4.05421	-0.48528	3.79194
H	-3.12992	0.57609	4.87454
H	3.47416	1.77977	3.87926
H	4.10360	-0.61926	4.04860
H	2.33568	-2.35847	3.91327
H	1.87084	3.48107	3.83046
H	0.27232	3.01134	4.45073
H	0.52316	3.20221	2.72114
H	-1.12394	-1.76575	4.32764
H	0.09071	-2.99577	3.92649
H	-0.80157	-2.16080	2.64625

H	2.54879	-3.08823	-4.13931
H	4.59386	-1.69524	-3.91537
H	4.36560	0.75506	-3.55103
H	0.24192	-3.29895	-4.44494
H	-0.70963	-1.83853	-4.77822
H	-0.61161	-2.46486	-3.13902
H	1.56782	2.56573	-2.51483
H	1.51938	2.60689	-4.26354
H	3.08013	2.70435	-3.42285
Cl	0.44471	3.36188	-0.04485
C	3.61151	-0.28581	0.30075
O	2.89679	0.91771	0.01311
C	3.70583	2.08446	0.20849
H	3.07351	2.94939	0.01114
H	4.07340	2.11813	1.23967
H	4.55065	2.06212	-0.48918
C	0.77117	-2.57372	-0.08610
H	-0.26581	-2.40978	0.20485
H	0.82022	-2.82151	-1.15091
H	1.20020	-3.38747	0.50974
H	2.86991	-1.43822	-1.37201
H	3.29442	-2.38283	0.08469
H	3.72359	-0.37943	1.38752
H	4.60287	-0.24785	-0.16903