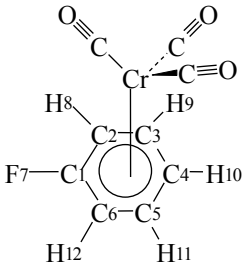
A successful DFT calculation of carbon-13 NMR chemical shifts and carbon-fluorine spin-spin coupling constants in (η^6-fluoroarene)tricarbonylchromium complexes

Adam Gryff-Keller[1] and Przemysław Szczeciński

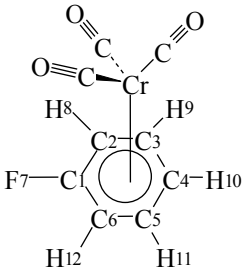
Department of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warszawa, Poland

Optimized molecular geometries of the minimum energy conformers of the investigated arenetricarbonylchromium complexes.

(η^6-Fluorobenzene)trikarbonylchromium (**4**)



Conformer A

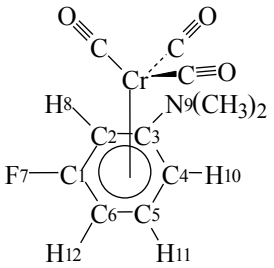


Conformer B

		Conformer A			Conformer B		
No.	Atom	x	y	z	x	y	z
1	C	-1.879266	0.091554	0.000024	-1.947437	-0.254290	0.001566
2	C	-1.488877	-0.442056	1.216994	-1.568093	0.317069	1.222120
3	C	-0.654557	-1.560171	1.201466	-0.872256	1.544902	1.224146
4	C	-0.266183	-2.147775	0.000337	-0.515819	2.138630	-0.002018
5	C	-0.654587	-1.560506	-1.200983	-0.873922	1.542343	-1.226374
6	C	-1.488857	-0.442401	-1.216824	-1.569168	0.314155	-1.220930
7	F	-2.631161	1.165653	-0.000147	-2.672305	-1.387800	0.002999
8	H	-1.799809	0.033413	2.133018	-1.826053	-0.185054	2.144367
9	H	-0.297396	-1.965123	2.136089	-0.577282	1.996522	2.159945
10	H	0.393648	-3.000001	0.000450	0.059985	3.054009	-0.003288
11	H	-0.297429	-1.965725	-2.135493	-0.580450	1.992291	-2.163468
12	H	-1.799760	0.032835	-2.132979	-1.829219	-0.190101	-2.141413
13	Cr	0.274003	-0.041046	0.000027	0.300450	0.049348	-0.000361
14	C	0.233208	1.803835	-0.001183	0.863989	-1.158252	1.300443
15	O	0.174093	2.930118	-0.001943	1.191179	-1.899425	2.117188
16	C	1.578331	-0.011000	1.298948	2.001369	0.812333	-0.002240
17	O	2.359465	-0.023143	2.114661	3.036982	1.312751	-0.002295
18	C	1.579168	-0.012788	-1.298075	0.861561	-1.161540	-1.299115
19	O	2.360798	-0.026140	-2.113297	1.185791	-1.905065	-2.114902

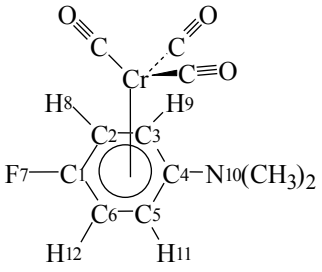
[1] E-mail: agryff@ch.pw.edu.pl

(η^6-1-Fluoro-3-dimetyloaminobenzene)tricarbonylchromium (**5**)

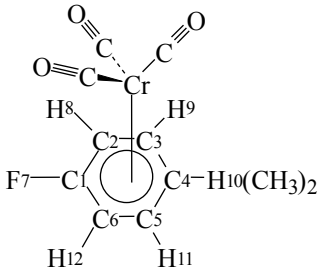


No.	Atom	x	y	z
1	C	-0.697154	1.834676	-0.336841
2	C	0.567194	1.535694	0.144602
3	C	1.368000	0.608552	-0.545571
4	C	0.800035	-0.055039	-1.647515
5	C	-0.486100	0.257550	-2.079936
6	C	-1.250041	1.237949	-1.453088
7	F	-1.402032	2.727076	0.318394
8	H	0.900675	2.033635	1.037950
9	N	2.619971	0.324798	-0.121210
10	H	1.344103	-0.834642	-2.150056
11	H	-0.900689	-0.283550	-2.916699
12	H	-2.248792	1.491419	-1.767945
13	C	3.019925	0.776189	1.175613
14	C	3.269598	-0.838720	-0.639991
15	H	4.052215	0.487008	1.343793
16	H	2.408245	0.345859	1.974881
17	H	2.972608	1.861880	1.241273
18	H	4.267219	-0.899474	-0.217295
19	H	3.378613	-0.774151	-1.721215
20	H	2.734628	-1.760839	-0.391911
21	Cr	-0.642025	-0.291167	-0.015813
22	C	-1.850360	-0.003563	1.338184
23	O	-2.596329	0.197390	2.162683
24	C	-1.635152	-1.726206	-0.575210
25	O	-2.247346	-2.600276	-0.951607
26	C	0.374051	-1.363710	1.061945
27	O	1.080959	-1.981694	1.698487

(η^6-1-Fluoro-4-dimetyloaminobenzene)tricarbonylchromium (**6**)



Conformer A



Conformer B

		Conformer A			Conformer B		
No.	Atom	x	y	z	x	y	z
1	C	-1.391358	-1.687583	0.000156	-1.356236	-1.727979	-0.000379
2	C	-0.747961	-1.497104	1.206906	-0.713795	-1.479005	1.195679
3	C	0.593128	-1.108394	1.193036	0.624613	-1.083372	1.203227
4	C	1.320973	-0.990303	-0.000129	1.335934	-0.937154	-0.000178
5	C	0.592671	-1.108233	-1.193378	0.624630	-1.082788	-1.203678
6	C	-0.748106	-1.496989	-1.206957	-0.713781	-1.478430	-1.196331
7	F	-2.661030	-2.017402	0.000104	-2.602303	-2.147143	-0.000481
8	H	-1.293439	-1.611635	2.129502	-1.259681	-1.594602	2.119808
9	H	1.073100	-0.909605	2.136131	1.100545	-0.886180	2.147035
10	N	2.656945	-0.693835	-0.000195	2.643154	-0.583412	0.000001
11	H	1.072346	-0.909191	-2.136561	1.100547	-0.885076	-2.147378
12	H	-1.293876	-1.611241	-2.129418	-1.259666	-1.593590	-2.120514
13	C	3.190300	-0.135928	1.202867	3.226848	-0.122467	1.220812
14	C	3.191026	-0.137287	-1.203607	3.227246-	0.122093	-1.220478
15	H	4.247581	0.063598	1.058629	4.277363	0.088147	1.048312
16	H	2.692415	0.801170	1.483433	2.751456	0.790038	1.595051
17	H	3.107062	-0.836967	2.030601	3.172865	-0.889129	1.992054
18	H	4.248476	0.061295	-1.059264	4.277868	0.087801	-1.047737
19	H	2.694252	0.800080	-1.485067	2.752426	0.790895	-1.594278
20	H	3.107381	-0.838924	-2.030777	3.172939	-0.888294	-1.992143
21	Cr	-0.515061	0.303111	-0.000094	-0.561839	0.306228	0.000061
22	C	-2.253149	0.911875	-0.008034	-1.583746	1.125025	1.281543
23	O	-3.328050	1.255532	-0.012864	-2.218099	1.602802	2.087385
24	C	-0.092779	1.521565	1.300277	0.627377	1.696347	0.000109
25	O	0.192176	2.239743	2.128713	1.439312	2.487917	-0.000029
26	C	-0.080297	1.526158	-1.291729	-1.583900	1.125583	-1.280912
27	O	0.212142	2.247669	-2.114722	-2.218090	1.603869	-2.086584