Electronic supplementary materials *Mendeleev Commun.*, 2019, **29**, 346–348

Experimental study of X-ray charge density and the selection of reference points for a source function in η^6-(2-methyl-1,4-dihydro-2*H*-3,1-benzoxazine)tricarbonylchromium(0)

Georgy K. Fukin, Anton V. Cherkasov, Roman V. Rumyantcev, Natalia Yu. Grishina, Elena V. Sazonova, Alexander N. Artemov and Adam I. Stash

Contents

Table S1 Selected distances in independent molecules of **1**.

Atoms	Molecule **A**	Molecule **B**
Cr(1)-C(1)	1.8435(5)	1.8382(5)
Cr(1)-C(2)	1.8406(6)	1.8384(7)
Cr(1)-C(3)	1.8371(7)	1.8398(8)
Cr(1)-C(4)	2.3137(4)	2.3384(5)
Cr(1)-C(5)	2.2456(5)	2.2594(5)
Cr(1)-C(6)	2.2085(6)	2.2180(5)
Cr(1)-C(7)	2.2225(6)	2.2194(5)
Cr(1)-C(8)	2.2102(5)	2.2019(5)
Cr(1)-C(9)	2.2630(4)	2.2631(5)
C(1)-O(1)	1.1620(7)	1.1634(7)
C(2)-O(2)	1.1645(8)	1.1655(9)
C(3)-O(3)	1.1614(9)	1.1602(12)

Table S2 The main bond distances and topological parameters in **1** according to high resolution X–ray experiment*.

Bond	Distance Å	$\nu(r_{cp})$ a.u.	$\rho(r_{cp})$ a.u.	$\nabla^2\rho(r_{cp})$ a.u.	$h_e(r_{cp})$ a.u.
Cr(1A)-C(1A)	1.8435(5)	–0.216	0.122	0.531	–0.042
Cr(1A)-C(2A)	1.8406(6)	–0.221	0.122	0.585	–0.037
Cr(1A)-C(3A)	1.8371(7)	–0.256	0.137	0.547	–0.059
Cr(1A)-C(4A)	2.3137(4)	–	–	–	–
Cr(1A)-C(5A)	2.2456(5)	–0.073	0.054	0.239	–0.002
Cr(1A)-C(6A)	2.2085(6)	–	–	–	–
Cr(1A)-C(7A)	2.2225(6)	–	–	–	–
Cr(1A)-C(8A)	2.2102(5)	–0.080	0.066	0.213	–0.013
Cr(1A)-C(9A)	2.2630(4)	–	–	–	–
O(1A)-C(1A)	1.1620(7)	–1.679	0.500	–1.264	–0.997
O(2A)-C(2A)	1.1645(8)	–1.617	0.470	–0.150	–0.827
O(3A)-C(3A)	1.1614(9)	–1.646	0.481	–0.572	–0.895

* Data only for one independent molecule are presented.

Table S3 The source function percentage contributions in CP(3,-1) of the Cr–C_{arene} fragment.

Bonds	Source function in CP(3,-1), %						
	Cr(1A)	C(4A)	C(5A)	C(6A)	C(7A)	C(8A)	C(9A)
Cr(1A)–C(5A)	**10.47**	4.31	**2.76**	10.45	7.64	2.34	3.49
Cr(1A)–C(8A)	**14.07**	1.83	5.39	6.43	11.98	**2.78**	5.60

Table S4 The source function percentage contributions on the middle distances of the Cr–C_{arene} fragment.

Bonds	Source function on the middle distance, %						
	Cr(1A)	C(4A)	C(5A)	C(6A)	C(7A)	C(8A)	C(9A)
Cr(1A)–C(4A)	**3.78**	**-17.21**	11.85	7.96	7.57	4.16	7.14
Cr(1A)–C(5A)	**11.10**	4.64	3.54	11.02	7.44	2.28	3.58
Cr(1A)–C(6A)	**7.16**	3.08	14.60	**-11.65**	14.03	5.06	3.12
Cr(1A)–C(7A)	**10.61**	1.67	7.20	8.34	0.54	9.46	3.94
Cr(1A)–C(8A)	**11.80**	2.47	4.93	5.72	13.69	**-3.67**	6.71
Cr(1A)–C(9A)	**1.88**	4.94	7.38	5.71	10.54	7.33	**-13.22**

Table S5 The source function percentage contributions on the NCI index isosurface for Cr(1A)–C(4A, 6A, 7A, 9A) interactions.

Bonds	Source function on NCI index isosurface, %						
	Cr(1A)	C(4A)	C(5A)	C(6A)	C(7A)	C(8A)	C(9A)
Cr(1A)–C(4A)	**9.33**	**3.58**	2.01	11.14	7.34	2.52	4.62
Cr(1A)–C(6A)	**9.71**	4.59	5.13	**11.02**	9.07	2.74	3.16
Cr(1A)–C(7A)	**11.22**	1.69	7.32	8.19	**4.31**	10.37	4.23
Cr(1A)–C(9A)	**10.87**	2.44	5.62	5.87	12.75	0.20	**5.64**

Table S6 Additional nine randomly selected rp's in regions of the concentrations ($\lambda_2 < 0$) of ED for the SF.

SOURCE FUNCTION REFERENCE POINT №1
label: Ref.Point x = 0.93380 y = 9.60680 z = 2.05130
RefPointRho = 0.43850 e/Å^3 (0.06498 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.05284	0.00783	12.051
2	C1A	48	64	0.00136	0.00020	0.310
3	O1A	48	64	0.02395	0.00355	5.461
4	C2A	48	64	0.00398	0.00059	0.908
5	O2A	48	64	0.02374	0.00352	5.415
6	C3A	48	64	0.00312	0.00046	0.712
7	O3A	48	64	0.03034	0.00450	6.918
8	N1A	48	64	0.01940	0.00287	4.424
9	H1AA	48	64	0.00254	0.00038	0.579
10	O4A	48	64	0.01063	0.00158	2.424
11	C4A	48	64	0.01014	0.00150	2.311
12	C5A	48	64	0.02257	0.00334	5.148
13	H5AA	48	64	0.01148	0.00170	2.618
14	C6A	48	64	0.02555	0.00379	5.827
15	H6AA	48	64	0.01313	0.00195	2.994
16	C7A	48	64	0.05910	0.00876	13.477
17	H7AA	48	64	0.01493	0.00221	3.406
18	C8A	48	64	0.00621	0.00092	1.417
19	H8AA	48	64	0.02194	0.00325	5.002
20	C9A	48	64	0.02849	0.00422	6.497
21	C10A	48	64	0.00937	0.00139	2.136
22	H10A	48	64	0.00662	0.00098	1.510
23	H10B	48	64	0.00505	0.00075	1.151
24	C11A	48	64	0.00022	0.00003	0.051
25	H11A	48	64	0.00200	0.00030	0.456
26	C12A	48	64	0.00344	0.00051	0.784
27	H12A	48	64	0.00206	0.00031	0.470
28	H12B	48	64	0.00168	0.00025	0.382
29	H12C	48	64	0.00145	0.00021	0.330
TOTAL				0.41732	0.06184	

SOURCE FUNCTION REFERENCE POINT №2
label: Ref.Point x = 0.92760 y = 9.57720 z = 2.04840
RefPointRho = 0.43821 e/Å^3 (0.06494 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%

1	CR1A	48	64	0.05242	0.00777	11.963
2	C1A	48	64	0.00134	0.00020	0.305
3	O1A	48	64	0.02398	0.00355	5.472
4	C2A	48	64	0.00394	0.00058	0.900
5	O2A	48	64	0.02372	0.00352	5.414
6	C3A	48	64	0.00308	0.00046	0.703
7	O3A	48	64	0.02984	0.00442	6.810
8	N1A	48	64	0.01966	0.00291	4.487
9	H1AA	48	64	0.00255	0.00038	0.583
10	O4A	48	64	0.01057	0.00157	2.412
11	C4A	48	64	0.00992	0.00147	2.263
12	C5A	48	64	0.02293	0.00340	5.234
13	H5AA	48	64	0.01172	0.00174	2.675
14	C6A	48	64	0.02591	0.00384	5.913
15	H6AA	48	64	0.01338	0.00198	3.054
16	C7A	48	64	0.05890	0.00873	13.440
17	H7AA	48	64	0.01501	0.00222	3.425
18	C8A	48	64	0.00981	0.00145	2.238
19	H8AA	48	64	0.02161	0.00320	4.931
20	C9A	48	64	0.02812	0.00417	6.417
21	C10A	48	64	0.00938	0.00139	2.140
22	H10A	48	64	0.00659	0.00098	1.503
23	H10B	48	64	0.00506	0.00075	1.154
24	C11A	48	64	0.00025	0.00004	0.056
25	H11A	48	64	0.00204	0.00030	0.466
26	C12A	48	64	0.00344	0.00051	0.785
27	H12A	48	64	0.00208	0.00031	0.474
28	H12B	48	64	0.00167	0.00025	0.382
29	H12C	48	64	0.00144	0.00021	0.329
TOTAL				0.42036	0.06229	

SOURCE FUNCTION REFERENCE POINT №3

label: Ref.Point x = 0.91670 y = 9.51920 z = 2.07310

RefPointRho = 0.42929 e/Å^3 (0.06361 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.04945	0.00733	11.518
2	C1A	48	64	0.00133	0.00020	0.311
3	O1A	48	64	0.02393	0.00355	5.575
4	C2A	48	64	0.00391	0.00058	0.912
5	O2A	48	64	0.02394	0.00355	5.577
6	C3A	48	64	0.00308	0.00046	0.719
7	O3A	48	64	0.02899	0.00430	6.754
8	N1A	48	64	0.02054	0.00304	4.785
9	H1AA	48	64	0.00262	0.00039	0.610
10	O4A	48	64	0.01060	0.00157	2.469
11	C4A	48	64	0.00951	0.00141	2.214
12	C5A	48	64	0.02346	0.00348	5.465
13	H5AA	48	64	0.01223	0.00181	2.849

14	C6A	48	64	0.02589	0.00384	6.032
15	H6AA	48	64	0.01370	0.00203	3.190
16	C7A	48	64	0.05652	0.00838	13.167
17	H7AA	48	64	0.01477	0.00219	3.442
18	C8A	48	64	0.00706	0.00105	1.644
19	H8AA	48	64	0.02081	0.00308	4.848
20	C9A	48	64	0.02651	0.00393	6.175
21	C10A	48	64	0.00960	0.00142	2.237
22	H10A	48	64	0.00664	0.00098	1.546
23	H10B	48	64	0.00515	0.00076	1.200
24	C11A	48	64	0.00028	0.00004	0.064
25	H11A	48	64	0.00215	0.00032	0.500
26	C12A	48	64	0.00349	0.00052	0.812
27	H12A	48	64	0.00212	0.00031	0.495
28	H12B	48	64	0.00168	0.00025	0.392
29	H12C	48	64	0.00145	0.00022	0.339
TOTAL				0.41144	0.06097	

SOURCE FUNCTION REFERENCE POINT №4

label: Ref.Point x = 0.67430 y = 9.54060 z = 1.60620

RefPointRho = 0.42269 e/Å^3 (0.06264 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.04893	0.00725	11.576
2	C1A	48	64	0.00107	0.00016	0.253
3	O1A	48	64	0.02855	0.00423	6.754
4	C2A	48	64	0.00388	0.00057	0.917
5	O2A	48	64	0.02162	0.00320	5.115
6	C3A	48	64	0.00299	0.00044	0.708
7	O3A	48	64	0.02889	0.00428	6.834
8	N1A	48	64	0.01477	0.00219	3.494
9	H1AA	48	64	0.00204	0.00030	0.483
10	O4A	48	64	0.00818	0.00121	1.935
11	C4A	48	64	0.00695	0.00103	1.645
12	C5A	48	64	0.02780	0.00412	6.576
13	H5AA	48	64	0.01168	0.00173	2.763
14	C6A	48	64	0.03530	0.00523	8.351
15	H6AA	48	64	0.01737	0.00257	4.109
16	C7A	48	64	0.01572	0.00233	3.719
17	H7AA	48	64	0.02075	0.00307	4.908
18	C8A	48	64	0.04219	0.00625	9.981
19	H8AA	48	64	0.01867	0.00277	4.418
20	C9A	48	64	0.01840	0.00273	4.354
21	C10A	48	64	0.00592	0.00088	1.401
22	H10A	48	64	0.00466	0.00069	1.103
23	H10B	48	64	0.00343	0.00051	0.811
24	C11A	48	64	0.00044	0.00007	0.104
25	H11A	48	64	0.00149	0.00022	0.352
26	C12A	48	64	0.00286	0.00042	0.677

27	H12A	48	64	0.00184	0.00027	0.435
28	H12B	48	64	0.00130	0.00019	0.308
29	H12C	48	64	0.00118	0.00017	0.279
TOTAL				0.39886	0.05911	

SOURCE FUNCTION REFERENCE POINT №5
label: Ref.Point x = 0.66220 y = 9.44740 z = 1.62300
RefPointRho = 0.42947 e/Å^3 (0.06364 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.04855	0.00719	11.305
2	C1A	48	64	0.00093	0.00014	0.217
3	O1A	48	64	0.02840	0.00421	6.612
4	C2A	48	64	0.00374	0.00055	0.870
5	O2A	48	64	0.02167	0.00321	5.046
6	C3A	48	64	0.00285	0.00042	0.665
7	O3A	48	64	0.02753	0.00408	6.409
8	N1A	48	64	0.01540	0.00228	3.585
9	H1AA	48	64	0.00209	0.00031	0.486
10	O4A	48	64	0.00814	0.00121	1.896
11	C4A	48	64	0.00718	0.00106	1.671
12	C5A	48	64	0.03037	0.00450	7.071
13	H5AA	48	64	0.01250	0.00185	2.910
14	C6A	48	64	0.03580	0.00530	8.335
15	H6AA	48	64	0.01854	0.00275	4.318
16	C7A	48	64	0.01921	0.00285	4.472
17	H7AA	48	64	0.02046	0.00303	4.765
18	C8A	48	64	0.04478	0.00664	10.426
19	H8AA	48	64	0.01793	0.00266	4.176
20	C9A	48	64	0.01828	0.00271	4.257
21	C10A	48	64	0.00607	0.00090	1.413
22	H10A	48	64	0.00468	0.00069	1.089
23	H10B	48	64	0.00353	0.00052	0.822
24	C11A	48	64	0.00049	0.00007	0.114
25	H11A	48	64	0.00160	0.00024	0.371
26	C12A	48	64	0.00289	0.00043	0.673
27	H12A	48	64	0.00189	0.00028	0.439
28	H12B	48	64	0.00130	0.00019	0.303
29	H12C	48	64	0.00117	0.00017	0.273
TOTAL				0.40796	0.06045	

SOURCE FUNCTION REFERENCE POINT №6
label: Ref.Point x = 0.62300 y = 9.48630 z = 1.57880
RefPointRho = 0.41804 e/Å^3 (0.06195 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%

1	CR1A	48	64	0.04720	0.00699	11.291
2	C1A	48	64	0.00106	0.00016	0.253
3	O1A	48	64	0.02932	0.00434	7.013
4	C2A	48	64	0.00385	0.00057	0.920
5	O2A	48	64	0.02161	0.00320	5.170
6	C3A	48	64	0.00301	0.00045	0.719
7	O3A	48	64	0.02811	0.00417	6.724
8	N1A	48	64	0.01465	0.00217	3.504
9	H1AA	48	64	0.00202	0.00030	0.483
10	O4A	48	64	0.00797	0.00118	1.906
11	C4A	48	64	0.00694	0.00103	1.661
12	C5A	48	64	0.02978	0.00441	7.124
13	H5AA	48	64	0.01209	0.00179	2.891
14	C6A	48	64	0.03507	0.00520	8.388
15	H6AA	48	64	0.01848	0.00274	4.420
16	C7A	48	64	0.01454	0.00216	3.479
17	H7AA	48	64	0.02095	0.00310	5.010
18	C8A	48	64	0.04253	0.00630	10.174
19	H8AA	48	64	0.01766	0.00262	4.224
20	C9A	48	64	0.01710	0.00253	4.091
21	C10A	48	64	0.00573	0.00085	1.371
22	H10A	48	64	0.00452	0.00067	1.081
23	H10B	48	64	0.00333	0.00049	0.796
24	C11A	48	64	0.00047	0.00007	0.112
25	H11A	48	64	0.00148	0.00022	0.354
26	C12A	48	64	0.00283	0.00042	0.676
27	H12A	48	64	0.00184	0.00027	0.441
28	H12B	48	64	0.00126	0.00019	0.301
29	H12C	48	64	0.00116	0.00017	0.278
TOTAL				0.39654	0.05876	

SOURCE FUNCTION REFERENCE POINT №7

label: Ref.Point x = 0.18270 y = 8.78020 z = 2.17720

RefPointRho = 0.40689 e/Å^3 (0.06029 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.04167	0.00617	10.241
2	C1A	48	64	0.00077	0.00011	0.190
3	O1A	48	64	0.03023	0.00448	7.430
4	C2A	48	64	0.00332	0.00049	0.815
5	O2A	48	64	0.02839	0.00421	6.976
6	C3A	48	64	0.00349	0.00052	0.859
7	O3A	48	64	0.02148	0.00318	5.279
8	N1A	48	64	0.02215	0.00328	5.444
9	H1AA	48	64	0.00280	0.00042	0.689
10	O4A	48	64	0.00841	0.00125	2.068
11	C4A	48	64	0.01928	0.00286	4.739
12	C5A	48	64	0.01155	0.00171	2.837
13	H5AA	48	64	0.02537	0.00376	6.235

14	C6A	48	64	0.04382	0.00649	10.770
15	H6AA	48	64	0.02006	0.00297	4.930
16	C7A	48	64	0.03489	0.00517	8.574
17	H7AA	48	64	0.01086	0.00161	2.669
18	C8A	48	64	0.01094	0.00162	2.689
19	H8AA	48	64	0.01036	0.00154	2.547
20	C9A	48	64	0.01425	0.00211	3.502
21	C10A	48	64	0.00593	0.00088	1.458
22	H10A	48	64	0.00493	0.00073	1.212
23	H10B	48	64	0.00341	0.00051	0.838
24	C11A	48	64	0.00082	0.00012	0.202
25	H11A	48	64	0.00204	0.00030	0.502
26	C12A	48	64	0.00331	0.00049	0.814
27	H12A	48	64	0.00246	0.00036	0.605
28	H12B	48	64	0.00110	0.00016	0.270
29	H12C	48	64	0.00149	0.00022	0.367
TOTAL				0.38960	0.05773	

SOURCE FUNCTION REFERENCE POINT №8
label: Ref.Point x = 0.06700 y = 8.74520 z = 2.29510
RefPointRho = 0.40650 e/Å^3 (0.06024 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.04455	0.00660	10.960
2	C1A	48	64	0.00075	0.00011	0.184
3	O1A	48	64	0.03096	0.00459	7.616
4	C2A	48	64	0.00334	0.00049	0.821
5	O2A	48	64	0.03077	0.00456	7.569
6	C3A	48	64	0.00363	0.00054	0.892
7	O3A	48	64	0.02125	0.00315	5.228
8	N1A	48	64	0.02200	0.00326	5.413
9	H1AA	48	64	0.00291	0.00043	0.716
10	O4A	48	64	0.00853	0.00126	2.098
11	C4A	48	64	0.01952	0.00289	4.801
12	C5A	48	64	0.01544	0.00229	3.797
13	H5AA	48	64	0.02647	0.00392	6.513
14	C6A	48	64	0.04486	0.00665	11.035
15	H6AA	48	64	0.01813	0.00269	4.459
16	C7A	48	64	0.03046	0.00451	7.493
17	H7AA	48	64	0.00973	0.00144	2.395
18	C8A	48	64	0.00896	0.00133	2.204
19	H8AA	48	64	0.00956	0.00142	2.353
20	C9A	48	64	0.01364	0.00202	3.356
21	C10A	48	64	0.00565	0.00084	1.390
22	H10A	48	64	0.00493	0.00073	1.212
23	H10B	48	64	0.00322	0.00048	0.793
24	C11A	48	64	0.00080	0.00012	0.198
25	H11A	48	64	0.00192	0.00029	0.474
26	C12A	48	64	0.00337	0.00050	0.829

27	H12A	48	64	0.00253	0.00038	0.623
28	H12B	48	64	0.00102	0.00015	0.251
29	H12C	48	64	0.00160	0.00024	0.393
TOTAL				0.39050	0.05787	

SOURCE FUNCTION REFERENCE POINT №9
label: Ref.Point x = 0.16670 y = 8.74990 z = 2.45960
RefPointRho = 0.39960 e/Å^3 (0.05922 a.u.) is taken as 100%

num	atom	nTheta	nPhi	SF, e/Å^3	SF,a.u.	S%
1	CR1A	48	64	0.04066	0.00603	10.175
2	C1A	48	64	0.00062	0.00009	0.154
3	O1A	48	64	0.02827	0.00419	7.073
4	C2A	48	64	0.00310	0.00046	0.777
5	O2A	48	64	0.03217	0.00477	8.051
6	C3A	48	64	0.00348	0.00052	0.871
7	O3A	48	64	0.02121	0.00314	5.308
8	N1A	48	64	0.02657	0.00394	6.649
9	H1AA	48	64	0.00332	0.00049	0.831
10	O4A	48	64	0.00928	0.00138	2.323
11	C4A	48	64	0.01723	0.00255	4.311
12	C5A	48	64	0.00525	0.00078	1.313
13	H5AA	48	64	0.02627	0.00389	6.575
14	C6A	48	64	0.04402	0.00652	11.017
15	H6AA	48	64	0.01600	0.00237	4.005
16	C7A	48	64	0.02796	0.00414	6.996
17	H7AA	48	64	0.00922	0.00137	2.308
18	C8A	48	64	0.00900	0.00133	2.253
19	H8AA	48	64	0.00973	0.00144	2.435
20	C9A	48	64	0.01644	0.00244	4.114
21	C10A	48	64	0.00629	0.00093	1.573
22	H10A	48	64	0.00540	0.00080	1.353
23	H10B	48	64	0.00362	0.00054	0.905
24	C11A	48	64	0.00083	0.00012	0.208
25	H11A	48	64	0.00225	0.00033	0.563
26	C12A	48	64	0.00366	0.00054	0.917
27	H12A	48	64	0.00270	0.00040	0.675
28	H12B	48	64	0.00116	0.00017	0.291
29	H12C	48	64	0.00174	0.00026	0.436
TOTAL				0.37747	0.05593	

Synthesis of 1.

A mixture of 1.5 g (0.006 mol) of (η^6-o-aminobenzyl alcohol)tricarbonylchromium(0),0.32 g (0.4 ml, 0.007 mol) of acetaldehyde, 30 ml of tetrahydrofuran and 1.44 g of (0.012 mol) anhydrous $MgSO_4$ was placed in a two-neck flask and stirred for 8 hours at room temperature. Then solvent was removed. The product was purified by column chromatography (eluent – hexane : ethyl acetate = 4:1) and recrystallized from a mixture of hexane and ethyl acetate (6:1). The obtained yellow crystals were filtered and dried in vacuum. M.p. = 111–112°C. The yield was 0.49 g (29 %).