Reliable charge assessment on encapsulated fragment

for endohedral systems.

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Computational details.

Recently we have demonstrated that electronic properties of molecular endohedral borospherenes can be reliably described using DFT.¹ Geometrical structures of the endohedral complexes studied in present work were studied using density functional theory (DFT) with PBE1PBE (hereafter also termed as PBE0) hybrid functional in the ground state. Ahlrichs Def2-TZVP basis sets^{2, 3} triple- ξ quality basis set was employed in all cases. All calculations were carried out using Gaussian 09 (Rev. E.01).⁴ The population analysis performed within Mulliken^{5, 6}, Lowdin⁷, Hirshfeld^{8, 9} and CM5¹⁰ schemes were carried out using code implemented in Gaussian 09. Topological analyses of the electron distributions were conducted according to the "Quantum Theory of Atoms in Molecules" (QTAIM) proposed by Bader.^{11, 12} The QTAIM calculations were performed using the AIMALL suite of programs.¹³ Natural Population Analysis (NPA) was carried out with NBO 6.0 program.¹⁴

Table S1. Charge compensations schemes (CCS) used for verification of Cl 1s orbital energy dependence on compensation charge distribution method. Detailed description of particular CCS scheme provide in main text. Units are electrons.

Point	CCS1	CCS2	CCS3	CCS4	CCS5
charge			Cl ²⁻		
	0.05129	0.04562		0.20000	0 5 9 7 6 0
q 1	0.05128	-0.04502	0.05150	0.59999	0.56700
42 	0.05128	0.13307	-0.13840	0.20329	-0.23994
Ч ³	0.05128	-0 12873	0.21300	-0.02407	-0.13984
94 Q-	0.05128	-0.12873	-0 10389	-0.21854	-0 25040
4 5	0.05128	-0.03604	0.10303	0.43626	0.23040
4 ⁶	0.05128	-0.03602	-0.01656	0.43020	0.60335
ч ⁷	0.05128	0.00714	0.01050	0.28522	0.00333
	0.05128	0.08091	0.09396	-0 34974	-0 16209
Q 10	0.05128	-0.05192	-0.52281	0.44656	0.65451
Q11	0.05128	0.08773	0.40904	-0.14877	-0.15680
Q12	0.05128	0.08010	-0.09118	-0.12561	-0.08282
Q13	0.05128	0.07533	-0.20293	0.03466	0.11105
Q14	0.05128	0.18411	0.21150	0.05128	-0.12070
Q ₁₅	0.05128	-0.04991	-0.03019	0.56298	0.90852
Q 16	0.05128	-0.10511	0.36177	0.05110	0.41788
q ₁₇	0.05128	0.15151	-0.13516	-0.07971	-0.42133
q ₁₈	0.05128	-0.09485	0.34931	0.39922	0.66112
q ₁₉	0.05128	0.06707	-0.10362	-0.31363	-0.55948
q ₂₀	0.05128	0.17995	0.28964	0.01125	-0.11852
q ₂₁	0.05128	0.13477	0.12985	-0.05210	-0.17908
q ₂₂	0.05128	0.11394	0.10215	0.13658	-0.12492
q ₂₃	0.05128	-0.03320	0.14342	0.05511	0.14868
q ₂₄	0.05128	0.11163	-0.04345	-0.40100	-0.47046
q 25	0.05128	0.13210	-0.05152	-0.11750	-0.35273
q ₂₆	0.05128	0.15541	0.01344	-0.03770	-0.43480
q ₂₇	0.05128	0.12277	0.51709	0.14336	-0.10286
Q 28	0.05128	0.19329	0.20768	-0.00533	-0.51697
q ₂₉	0.05128	0.16975	0.25811	0.01566	-0.31878
q ₃₀	0.05128	0.06085	-0.19662	0.56713	0.34339
q ₃₁	0.05128	-0.02365	-0.44379	0.61305	0.72730
q ₃₂	0.05128	-0.04661	0.12142	0.39394	0.72918
q ₃₃	0.05128	0.13196	0.06513	-0.03567	-0.30795
q ₃₄	0.05128	0.07166	0.06034	-0.16396	0.09423
q ₃₅	0.05128	-0.11967	0.12839	-0.19129	0.32029
q ₃₆	0.05128	0.05424	-0.22468	0.00716	-0.06257
Q 37	0.05128	-0.09248	0.01488	0.22938	0.32371

Q 38	0.05128	0.09819	-0.01584	-0.48744	-0.19846
q ₃₉	0.05128	0.04190	0.23497	-0.41478	-0.31753
			Cl1-		
q ₁	0.02564	-0.02281	0.02575	0.19999	-0.02571
q ₂	0.02564	0.07653	-0.07920	0.10164	0.01691
Q3	0.02564	0.07372	0.10750	-0.01233	0.04183
q 4	0.02564	-0.06436	0.00698	-0.10927	0.01936
q 5	0.02564	0.02846	-0.05194	-0.22500	0.04913
q 6	0.02564	-0.01802	0.04741	0.21813	-0.02129
q 7	0.02564	-0.01801	-0.00828	0.28721	-0.01712
q 8	0.02564	0.00357	0.13443	0.14261	0.00325
q 9	0.02564	0.04045	0.04698	-0.17487	0.06531
q ₁₀	0.02564	-0.02596	-0.26140	0.22328	-0.02330
q 11	0.02564	0.04386	0.20452	-0.07438	0.05486
q ₁₂	0.02564	0.04005	-0.04559	-0.06280	0.06460
q ₁₃	0.02564	0.03766	-0.10146	0.01733	0.04599
q ₁₄	0.02564	0.09205	0.10575	0.02564	0.02424
q 15	0.02564	-0.02495	-0.01509	0.28149	-0.00071
q 16	0.02564	-0.05255	0.18088	0.02555	0.02385
q ₁₇	0.02564	0.07575	-0.06758	-0.03985	0.04134
q ₁₈	0.02564	-0.04742	0.17465	0.19961	-0.00638
q 19	0.02564	0.03353	-0.05181	-0.15681	0.06348
q ₂₀	0.02564	0.08997	0.14482	0.00562	0.02440
q ₂₁	0.02564	0.06738	0.06492	-0.02605	0.03970
q ₂₂	0.02564	0.05697	0.05107	0.06829	0.04306
q ₂₃	0.02564	-0.01660	0.07171	0.02755	0.00841
q ₂₄	0.02564	0.05581	-0.02172	-0.20050	0.06090
q ₂₅	0.02564	0.06605	-0.02576	-0.05875	0.03135
q ₂₆	0.02564	0.07770	0.00672	-0.01885	0.03621
q ₂₇	0.02564	0.06138	0.25854	0.07168	0.02972
q 28	0.02564	0.09664	0.10384	-0.00266	0.03351
q 29	0.02564	0.08487	0.12905	0.00783	0.02618
q ₃₀	0.02564	0.03042	-0.09831	0.28356	-0.02369
q ₃₁	0.02564	-0.01182	-0.22189	0.30652	-0.00504
q ₃₂	0.02564	-0.02330	0.06071	0.19697	-0.02297
q ₃₃	0.02564	0.06598	0.03256	-0.01783	0.04808
q ₃₄	0.02564	0.03583	0.03017	-0.08198	0.06231
q ₃₅	0.02564	-0.05983	0.06419	-0.09564	0.02918
q ₃₆	0.02564	0.02712	-0.11234	0.00358	0.03823
q ₃₇	0.02564	-0.04624	0.00744	0.11469	0.00511
q ₃₈	0.02564	0.04909	-0.00792	-0.24372	0.05097
q ₃₉	0.02564	0.02095	0.11748	-0.20739	0.06463
		Clc)		

Q1	n/a	0.02241	-0.01406	-0.12166	0.22284
Q2	n/a	-0.02268	0.07974	-0.06183	-0.15970
Q ₃	n/a	-0.02184	-0.05870	0.01165	-0.05419
Q 4	n/a	0.06324	-0.00381	0.10322	0.13034
Q5	n/a	-0.00843	0.05230	0.21256	-0.17984
q ₆	n/a	0.01770	-0.02589	-0.13269	0.37007
q ₇	n/a	0.01769	0.00833	-0.17471	0.30072
q ₈	n/a	-0.00105	-0.07341	-0.08675	0.04291
q ₉	n/a	-0.01199	-0.02565	0.16519	-0.14591
q ₁₀	n/a	0.02550	0.26321	-0.13582	0.26882
q ₁₁	n/a	-0.01300	-0.11169	0.07026	-0.07407
q ₁₂	n/a	-0.01186	0.04590	0.05933	-0.06338
q ₁₃	n/a	-0.01116	0.10216	-0.01054	0.05454
q ₁₄	n/a	-0.02728	-0.05775	-0.01559	-0.09940
q 15	n/a	0.02452	0.01519	-0.17123	0.22930
q ₁₆	n/a	0.05163	-0.09878	-0.01554	0.17128
q ₁₇	n/a	-0.02245	0.06804	0.03765	-0.19165
q ₁₈	n/a	0.04659	-0.09538	-0.12142	0.21863
q 19	n/a	-0.00993	0.05217	0.14814	-0.27054
q ₂₀	n/a	-0.02666	-0.07908	-0.00342	-0.08920
q ₂₁	n/a	-0.01997	-0.03545	0.02461	-0.06623
q ₂₂	n/a	-0.01688	-0.02789	-0.04154	-0.07513
q ₂₃	n/a	0.01631	-0.03916	-0.01676	0.05935
q ₂₄	n/a	-0.01654	0.02187	0.18940	-0.23557
q ₂₅	n/a	-0.01957	0.02593	0.05550	-0.16991
q ₂₆	n/a	-0.02302	-0.00367	0.01781	-0.18587
Q 27	n/a	-0.01819	-0.14119	-0.04360	-0.07406
Q 28	n/a	-0.02864	-0.05670	0.00251	-0.20717
q ₂₉	n/a	-0.02515	-0.07047	-0.00476	-0.13283
q 30	n/a	-0.00901	0.09899	-0.17250	0.08140
q ₃₁	n/a	0.01162	0.22342	-0.18646	0.27944
q ₃₂	n/a	0.02290	-0.03315	-0.11982	0.26538
q ₃₃	n/a	-0.01955	-0.01778	0.01684	-0.08966
q ₃₄	n/a	-0.01061	-0.01647	0.07744	-0.01237
q ₃₅	n/a	0.05879	-0.03505	0.09035	0.21882
q ₃₆	n/a	-0.00803	0.12419	-0.00217	-0.07277
Q ₃₇	n/a	0.04543	-0.00406	-0.06977	0.03810
Q ₃₈	n/a	-0.01455	0.00797	0.23023	-0.18478
q ₃₉	n/a	-0.00620	-0.06415	0.19591	-0.11768
		Cl ¹	+		
q ₁	-0.02564	0.02281	-0.02575	-0.20000	-0.09359
q ₂	-0.02564	-0.07653	0.07920	-0.10164	-0.03642
Q ₃	-0.02564	-0.07372	-0.10750	0.01233	0.00794

q 4	-0.02564	0.06436	-0.00698	0.10927	-0.03223
q 5	-0.02564	-0.02846	0.05194	0.22500	0.03194
q 6	-0.02564	0.01802	-0.04741	-0.21813	-0.09084
q 7	-0.02564	0.01801	0.00828	-0.28721	-0.10364
q ₈	-0.02564	-0.00357	-0.13443	-0.14261	-0.05233
q 9	-0.02564	-0.04045	-0.04698	0.17487	0.03935
q ₁₀	-0.02564	0.02596	0.26140	-0.22328	-0.08111
q ₁₁	-0.02564	-0.04386	-0.20452	0.07438	0.01143
q ₁₂	-0.02564	-0.04005	0.04559	0.06280	0.01691
q ₁₃	-0.02564	-0.03766	0.10146	-0.01733	-0.01770
q ₁₄	-0.02564	-0.09205	-0.10575	-0.02564	-0.01542
q ₁₅	-0.02564	0.02495	0.01509	-0.28149	-0.09855
q ₁₆	-0.02564	0.05255	-0.18088	-0.02555	-0.03373
q ₁₇	-0.02564	-0.07575	0.06758	0.03985	0.00377
q ₁₈	-0.02564	0.04742	-0.17465	-0.19961	-0.09893
q 19	-0.02564	-0.03353	0.05181	0.15681	0.03043
q ₂₀	-0.02564	-0.08997	-0.14482	-0.00562	-0.01754
q ₂₁	-0.02564	-0.06738	-0.06492	0.02605	0.00471
q ₂₂	-0.02564	-0.05697	-0.05107	-0.06829	-0.01896
q ₂₃	-0.02564	0.01660	-0.07171	-0.02755	-0.07005
q ₂₄	-0.02564	-0.05581	0.02172	0.20050	0.02457
q ₂₅	-0.02564	-0.06605	0.02576	0.05875	-0.00850
q ₂₆	-0.02564	-0.07770	-0.00672	0.01885	0.00835
q ₂₇	-0.02564	-0.06138	-0.25854	-0.07168	-0.01112
q ₂₈	-0.02564	-0.09664	-0.10384	0.00266	0.00587
q 29	-0.02564	-0.08487	-0.12905	-0.00783	-0.01618
q ₃₀	-0.02564	-0.03042	0.09831	-0.28356	-0.09133
q ₃₁	-0.02564	0.01182	0.22189	-0.30652	-0.10467
q ₃₂	-0.02564	0.02330	-0.06071	-0.19697	-0.08405
q ₃₃	-0.02564	-0.06598	-0.03256	0.01783	0.00366
q ₃₄	-0.02564	-0.03583	-0.03017	0.08198	0.03067
q 35	-0.02564	0.05983	-0.06419	0.09564	-0.03639
q 36	-0.02564	-0.02712	0.11234	-0.00358	-0.00753
q ₃₇	-0.02564	0.04624	-0.00744	-0.11469	-0.08646
q ₃₈	-0.02564	-0.04909	0.00792	0.24372	0.04337
q ₃₉	-0.02564	-0.02095	-0.11748	0.20739	0.04439
		Cl ²	+		
q ₁	-0.05128	0.04562	-0.05150	-0.39999	0.33902
q ₂	-0.05128	-0.15307	0.15840	-0.20329	-0.22044
q ₃	-0.05128	-0.14744	-0.21500	0.02467	-0.07945
q ₄	-0.05128	0.12873	-0.01397	0.21854	0.19656
q 5	-0.05128	-0.05693	0.10389	0.45001	-0.28066
q 6	-0.05128	0.03604	-0.09483	-0.43626	0.52121

q ₇	-0.05128	0.03602	0.01656	-0.57442	0.35827
q 8	-0.05128	-0.00714	-0.26886	-0.28522	-0.03233
q 9	-0.05128	-0.08091	-0.09396	0.34974	-0.37801
q ₁₀	-0.05128	0.05192	0.52281	-0.44656	0.29390
q ₁₁	-0.05128	-0.08773	-0.40904	0.14877	-0.10531
q ₁₂	-0.05128	-0.08010	0.09118	0.12561	-0.26825
q ₁₃	-0.05128	-0.07533	0.20293	-0.03466	0.03227
q ₁₄	-0.05128	-0.18411	-0.21150	-0.05128	-0.31749
q ₁₅	-0.05128	0.04991	0.03019	-0.56298	0.27189
q ₁₆	-0.05128	0.10511	-0.36177	-0.05110	0.31694
q ₁₇	-0.05128	-0.15151	0.13516	0.07971	-0.31097
q ₁₈	-0.05128	0.09485	-0.34931	-0.39922	0.23307
q 19	-0.05128	-0.06707	0.10362	0.31363	-0.38325
q ₂₀	-0.05128	-0.17995	-0.28964	-0.01125	-0.13421
q ₂₁	-0.05128	-0.13477	-0.12985	0.05210	-0.17795
q ₂₂	-0.05128	-0.11394	-0.10215	-0.13658	-0.05687
q ₂₃	-0.05128	0.03320	-0.14342	-0.05511	-0.29875
q ₂₄	-0.05128	-0.11163	0.04345	0.40100	-0.36550
q 25	-0.05128	-0.13210	0.05152	0.11750	-0.32154
q ₂₆	-0.05128	-0.15541	-0.01344	0.03770	-0.21742
q ₂₇	-0.05128	-0.12277	-0.51709	-0.14336	-0.21230
q ₂₈	-0.05128	-0.19329	-0.20768	0.00533	-0.38048
q ₂₉	-0.05128	-0.16975	-0.25811	-0.01566	-0.25043
q ₃₀	-0.05128	-0.06085	0.19662	-0.56713	0.00594
q ₃₁	-0.05128	0.02365	0.44379	-0.61305	0.33145
q ₃₂	-0.05128	0.04661	-0.12142	-0.39394	0.36638
q ₃₃	-0.05128	-0.13196	-0.06513	0.03567	-0.10962
q ₃₄	-0.05128	-0.07166	-0.06034	0.16396	-0.00949
q 35	-0.05128	0.11967	-0.12839	0.19129	0.29467
q ₃₆	-0.05128	-0.05424	0.22468	-0.00716	-0.12032
q ₃₇	-0.05128	0.09248	-0.01488	-0.22938	-0.03576
Q 38	-0.05128	-0.09819	0.01584	0.48744	-0.31500
Q 39	-0.05128	-0.04190	-0.23497	0.41478	-0.17971



Figure S1. Calibration curves and equations of approximating functions obtained for tested charge compensation schemes (CCS1 – CCS5).

Table S2. Values of Cl 1s orbital energies (ε_{1s}^{Cl}) accessed without (w/o CCS) and with various charge compensation schemes (CCS1-CCS5), corrections to electrostatic potentials (φ_{el}) as well as predicted charge (Q_{Cl}) on encapsulated fragment obtained within framework of different CCS for Cl@B₃₉ system.^a Energies in hartrees and charges in electrons.

Compe	nsation			Q_{Cl}			
scheme	5	-2	-1	0	1	2	predicted
w/o CCS	ε_{1s}^{Cl} , a. u.	-101.0261	-101.3441	-101.7538	-102.2460	-102.8180	-0.279
CCS1	ε_{1s}^{Cl} , a. u.	-101.3710	-101.5166	-101.7538	-102.0735	-102.4730	-0 475
CC31	φ_{el} , a. u.	0.3449	0.1725	0.0000	-0.1725	-0.3450	-0.475
ccsa	ε_{1s}^{Cl} , a. u.	-101.3956	-101.5291	-101.7472	-102.0620	-102.4377	0 506
CC32	φ_{el} , a. u.	0.3695	0.1850	-0.0065	-0.1840	-0.3803	-0.500
CC23	ε_{1s}^{Cl} , a. u.	-101.3019	-101.4828	-101.7824	-102.1112	-102.5479	0 492
CC35	φ_{el} , a. u.	0.2758	0.1387	0.0287	-0.1349	-0.2701	-0.465
CCSA	ε_{1s}^{Cl} , a. u.	-101.3618	-101.5135	-101.7605	-102.0818	-102.4879	0 505
CC34	φ_{el} , a. u.	0.3358	0.1695	0.0068	-0.1643	-0.3301	-0.505
0055	ε_{1s}^{Cl} , a. u.	-101.2566	-101.5237	-101.7055	-102.0873	-102.4057	0.440
CC35	φ_{el} , a. u.	0.2306	0.1796	-0.0483	-0.1587	-0.4123	-0.440

^aCl 1s orbital energy for Cl@B₃₉ complex is -101.62826 a.u.



Figure S2. Calibration curves and equations of approximating functions constructed for charge prediction on central Cu fragment in Cu@B₃₉ complex based on 1s, 2s, and 3s orbital energies. (Cu 1s, 2s, and 3s orbital energy in complex of interest is -323.361 a.u., -38.947 a.u., and -4.376 a.u. correspondently).



Figure S3. Graphical representations X@B₃₉ type of systems investigated in present work.



Figure S4. Correlations of the Mulliken, Löwdin, Hirshfeld, CM5, NPA, and QTAIM charges (in electrons) with the results obtained by the proposed method.

Table S3. Slope (α), intercept (β), residual sum of squares (RSS) and R-square (R²) values for linear correlations of the Mulliken, Löwdin, Hirshfeld, CM5, NPA, and QTAIM charges with the results obtained by the proposed method.

Charge scheme	α	β	RSS	R ²
Mulliken	0.54163	-0.15564	0.86976	0.3875
Löwdin	0.38298	0.56413	1.32758	0.1716
Hirshfeld	0.67453	0.26404	0.08489	0.9094
CM5	0.93576	0.4627	0.19055	0.8960
NPA	1.46096	0.00891	0.21053	0.9500
QTAIM	1.26675	-0.06688	0.19125	0.9402

Cartesian coordinates (in Å) for the studied molecules.

CI@B₃₉

(B₃₉+Cl) VdW

Atom	Х	Y	Z	Atom	Х	Y	Z
В	-0.8525729	1.6461958	-2.7756007	В	-0.8525729	1.6461958	-2.7756007
В	-2.9197072	0.2090433	0.7349996	В	-2.9197072	0.2090433	0.7349996
В	-1.1690263	2.3266786	-1.3215332	В	-1.1690263	2.3266786	-1.3215332
В	1.2528336	-2.0567483	2.2331331	В	1.2528336	-2.0567483	2.2331331
В	2.3543614	-1.5620837	-0.2935620	В	2.3543614	-1.5620837	-0.2935620
В	-0.9993609	-1.5614477	-2.7756007	В	-0.9993609	-1.5614477	-2.7756007
В	1.7057430	2.5539606	-0.8683334	В	1.7057430	2.5539606	-0.8683334
В	-0.2877726	1.8503051	2.8335002	В	-0.2877726	1.8503051	2.8335002
В	0.1756234	2.8199786	-0.2935620	В	0.1756234	2.8199786	-0.2935620
В	-1.7079580	-2.5600143	0.2517388	В	-1.7079580	-2.5600143	0.2517388
В	-2.1823839	-1.5042932	1.3745563	В	-2.1823839	-1.5042932	1.3745563
В	0.1442372	-1.0279238	3.0668471	В	0.1442372	-1.0279238	3.0668471
В	1.2788167	-2.6330623	0.7349996	В	1.2788167	-2.6330623	0.7349996
В	0.5521702	0.8748793	-3.0344143	В	0.5521702	0.8748793	-3.0344143
В	1.3589233	-2.7541971	-0.8683334	В	1.3589233	-2.7541971	-0.8683334
В	-1.4585249	-1.1743710	2.8335002	В	-1.4585249	-1.1743710	2.8335002
В	-2.0849250	0.9518814	-1.9342788	В	-2.0849250	0.9518814	-1.9342788
В	-3.0646663	0.2002364	-0.8683334	В	-3.0646663	0.2002364	-0.8683334
В	-2.5299849	-1.2578949	-0.2935620	В	-2.5299849	-1.2578949	-0.2935620
В	-1.0337529	0.0407537	-3.0344143	В	-1.0337529	0.0407537	-3.0344143
В	-1.4304496	-2.1757458	-1.3215332	В	-1.4304496	-2.1757458	-1.3215332
В	-0.9623267	0.3890488	3.0668471	В	-0.9623267	0.3890488	3.0668471
В	-2.4076131	-0.0566116	2.2331331	В	-2.4076131	-0.0566116	2.2331331
В	-0.1763784	-2.7859879	-0.2670527	В	-0.1763784	-2.7859879	-0.2670527
В	0.2181090	-2.2815387	-1.9342788	В	0.2181090	-2.2815387	-1.9342788
В	1.8668160	1.3296573	-1.9342788	В	1.8668160	1.3296573	-1.9342788
В	-0.2115642	2.6421465	1.3745563	В	-0.2115642	2.6421465	1.3745563
В	-2.3245470	1.5457422	-0.2670527	В	-2.3245470	1.5457422	-0.2670527
В	0.4815826	-0.9156331	-3.0344143	В	0.4815826	-0.9156331	-3.0344143
В	-1.3630584	2.7591422	0.2517388	В	-1.3630584	2.7591422	0.2517388
В	3.0710164	-0.1991279	0.2517388	В	3.0710164	-0.1991279	0.2517388
В	1.8519339	-0.0847480	-2.7756007	В	1.8519339	-0.0847480	-2.7756007
В	2.5994759	-0.1509327	-1.3215332	В	2.5994759	-0.1509327	-1.3215332
В	0.8180895	0.6388750	3.0668471	В	0.8180895	0.6388750	3.0668471
В	1.1547794	2.1133599	2.2331331	В	1.1547794	2.1133599	2.2331331
В	1.6408905	2.4240189	0.7349996	В	1.6408905	2.4240189	0.7349996
В	1.7462975	-0.6759341	2.8335002	В	1.7462975	-0.6759341	2.8335002
В	2.5009255	1.2402456	-0.2670527	В	2.5009255	1.2402456	-0.2670527
В	2.3939481	-1.1378532	1.3745563	В	2.3939481	-1.1378532	1.3745563
Cl	0.0000000	0.0000000	0.0000000	Cl	0.0000000	-3.0000000	0.0000000

X@B₃₉⁺ (X = Cu, Ag, Au, F, Br)

NO@B₃₉

Atom	Х	Υ	Z	Atom	Х	Y	Z
В	-0.8525729	1.6461958	-2.7756007	В	-0.8525729	1.6461958	-2.7756007
В	-2.9197072	0.2090433	0.7349996	В	-2.9197072	0.2090433	0.7349996
В	-1.1690263	2.3266786	-1.3215332	В	-1.1690263	2.3266786	-1.3215332
В	1.2528336	-2.0567483	2.2331331	В	1.2528336	-2.0567483	2.2331331
В	2.3543614	-1.5620837	-0.2935620	В	2.3543614	-1.5620837	-0.2935620
В	-0.9993609	-1.5614477	-2.7756007	В	-0.9993609	-1.5614477	-2.7756007
В	1.7057430	2.5539606	-0.8683334	В	1.7057430	2.5539606	-0.8683334
В	-0.2877726	1.8503051	2.8335002	В	-0.2877726	1.8503051	2.8335002
В	0.1756234	2.8199786	-0.2935620	В	0.1756234	2.8199786	-0.2935620
В	-1.7079580	-2.5600143	0.2517388	В	-1.7079580	-2.5600143	0.2517388
В	-2.1823839	-1.5042932	1.3745563	В	-2.1823839	-1.5042932	1.3745563
В	0.1442372	-1.0279238	3.0668471	В	0.1442372	-1.0279238	3.0668471
В	1.2788167	-2.6330623	0.7349996	В	1.2788167	-2.6330623	0.7349996
В	0.5521702	0.8748793	-3.0344143	В	0.5521702	0.8748793	-3.0344143
В	1.3589233	-2.7541971	-0.8683334	В	1.3589233	-2.7541971	-0.8683334
В	-1.4585249	-1.1743710	2.8335002	В	-1.4585249	-1.1743710	2.8335002
В	-2.0849250	0.9518814	-1.9342788	В	-2.0849250	0.9518814	-1.9342788
В	-3.0646663	0.2002364	-0.8683334	В	-3.0646663	0.2002364	-0.8683334
В	-2.5299849	-1.2578949	-0.2935620	В	-2.5299849	-1.2578949	-0.2935620
В	-1.0337529	0.0407537	-3.0344143	В	-1.0337529	0.0407537	-3.0344143
В	-1.4304496	-2.1757458	-1.3215332	В	-1.4304496	-2.1757458	-1.3215332
В	-0.9623267	0.3890488	3.0668471	В	-0.9623267	0.3890488	3.0668471
В	-2.4076131	-0.0566116	2.2331331	В	-2.4076131	-0.0566116	2.2331331
В	-0.1763784	-2.7859879	-0.2670527	В	-0.1763784	-2.7859879	-0.2670527
В	0.2181090	-2.2815387	-1.9342788	В	0.2181090	-2.2815387	-1.9342788
В	1.8668160	1.3296573	-1.9342788	В	1.8668160	1.3296573	-1.9342788
В	-0.2115642	2.6421465	1.3745563	В	-0.2115642	2.6421465	1.3745563
В	-2.3245470	1.5457422	-0.2670527	В	-2.3245470	1.5457422	-0.2670527
В	0.4815826	-0.9156331	-3.0344143	В	0.4815826	-0.9156331	-3.0344143
В	-1.3630584	2.7591422	0.2517388	В	-1.3630584	2.7591422	0.2517388
В	3.0710164	-0.1991279	0.2517388	В	3.0710164	-0.1991279	0.2517388
В	1.8519339	-0.0847480	-2.7756007	В	1.8519339	-0.0847480	-2.7756007
В	2.5994759	-0.1509327	-1.3215332	В	2.5994759	-0.1509327	-1.3215332
В	0.8180895	0.6388750	3.0668471	В	0.8180895	0.6388750	3.0668471
В	1.1547794	2.1133599	2.2331331	В	1.1547794	2.1133599	2.2331331
В	1.6408905	2.4240189	0.7349996	В	1.6408905	2.4240189	0.7349996
В	1.7462975	-0.6759341	2.8335002	В	1.7462975	-0.6759341	2.8335002
В	2.5009255	1.2402456	-0.2670527	В	2.5009255	1.2402456	-0.2670527
В	2.3939481	-1.1378532	1.3745563	В	2.3939481	-1.1378532	1.3745563
х	0.0000000	0.0000000	0.0000000	Ν	0.0000000	0.0000000	0.5698790
				0	0.0000000	0.0000000	-0.5698790

CN@B₃₉

FO@B₃₉

Atom	х	Υ	Z	Atom	Х	Υ	Z
В	-0.8525729	1.6461958	-2.7756007	В	-0.8525729	1.6461958	-2.7756007
В	-2.9197072	0.2090433	0.7349996	В	-2.9197072	0.2090433	0.7349996
В	-1.1690263	2.3266786	-1.3215332	В	-1.1690263	2.3266786	-1.3215332
В	1.2528336	-2.0567483	2.2331331	В	1.2528336	-2.0567483	2.2331331
В	2.3543614	-1.5620837	-0.2935620	В	2.3543614	-1.5620837	-0.2935620
В	-0.9993609	-1.5614477	-2.7756007	В	-0.9993609	-1.5614477	-2.7756007
В	1.7057430	2.5539606	-0.8683334	В	1.7057430	2.5539606	-0.8683334
В	-0.2877726	1.8503051	2.8335002	В	-0.2877726	1.8503051	2.8335002
В	0.1756234	2.8199786	-0.2935620	В	0.1756234	2.8199786	-0.2935620
В	-1.7079580	-2.5600143	0.2517388	В	-1.7079580	-2.5600143	0.2517388
В	-2.1823839	-1.5042932	1.3745563	В	-2.1823839	-1.5042932	1.3745563
В	0.1442372	-1.0279238	3.0668471	В	0.1442372	-1.0279238	3.0668471
В	1.2788167	-2.6330623	0.7349996	В	1.2788167	-2.6330623	0.7349996
В	0.5521702	0.8748793	-3.0344143	В	0.5521702	0.8748793	-3.0344143
В	1.3589233	-2.7541971	-0.8683334	В	1.3589233	-2.7541971	-0.8683334
В	-1.4585249	-1.1743710	2.8335002	В	-1.4585249	-1.1743710	2.8335002
В	-2.0849250	0.9518814	-1.9342788	В	-2.0849250	0.9518814	-1.9342788
В	-3.0646663	0.2002364	-0.8683334	В	-3.0646663	0.2002364	-0.8683334
В	-2.5299849	-1.2578949	-0.2935620	В	-2.5299849	-1.2578949	-0.2935620
В	-1.0337529	0.0407537	-3.0344143	В	-1.0337529	0.0407537	-3.0344143
В	-1.4304496	-2.1757458	-1.3215332	В	-1.4304496	-2.1757458	-1.3215332
В	-0.9623267	0.3890488	3.0668471	В	-0.9623267	0.3890488	3.0668471
В	-2.4076131	-0.0566116	2.2331331	В	-2.4076131	-0.0566116	2.2331331
В	-0.1763784	-2.7859879	-0.2670527	В	-0.1763784	-2.7859879	-0.2670527
В	0.2181090	-2.2815387	-1.9342788	В	0.2181090	-2.2815387	-1.9342788
В	1.8668160	1.3296573	-1.9342788	В	1.8668160	1.3296573	-1.9342788
В	-0.2115642	2.6421465	1.3745563	В	-0.2115642	2.6421465	1.3745563
В	-2.3245470	1.5457422	-0.2670527	В	-2.3245470	1.5457422	-0.2670527
В	0.4815826	-0.9156331	-3.0344143	В	0.4815826	-0.9156331	-3.0344143
В	-1.3630584	2.7591422	0.2517388	В	-1.3630584	2.7591422	0.2517388
В	3.0710164	-0.1991279	0.2517388	В	3.0710164	-0.1991279	0.2517388
В	1.8519339	-0.0847480	-2.7756007	В	1.8519339	-0.0847480	-2.7756007
В	2.5994759	-0.1509327	-1.3215332	В	2.5994759	-0.1509327	-1.3215332
В	0.8180895	0.6388750	3.0668471	В	0.8180895	0.6388750	3.0668471
В	1.1547794	2.1133599	2.2331331	В	1.1547794	2.1133599	2.2331331
В	1.6408905	2.4240189	0.7349996	В	1.6408905	2.4240189	0.7349996
В	1.7462975	-0.6759341	2.8335002	В	1.7462975	-0.6759341	2.8335002
В	2.5009255	1.2402456	-0.2670527	В	2.5009255	1.2402456	-0.2670527
В	2.3939481	-1.1378532	1.3745563	В	2.3939481	-1.1378532	1.3745563
С	0.0000000	0.0000000	0.5811170	F	0.0000000	0.0000000	-0.6743775
Ν	0.0000000	0.0000000	-0.5811170	0	0.0000000	0.0000000	0.6743775

CF@B₃₉

Sc₃N@I_h-C₈₀

Atom	х	Υ	Z	Atom	х	Υ	Z
В	-0.8525729	1.6461958	-2.7756007	С	2.0969437	0.3049768	0.3301716
В	-2.9197072	0.2090433	0.7349996	С	-0.8556314	-1.4574183	0.8355135
В	-1.1690263	2.3266786	-1.3215332	С	-0.7048720	1.0165015	-1.5965134
В	1.2528336	-2.0567483	2.2331331	С	0.1854454	-0.0588864	-0.1565573
В	2.3543614	-1.5620837	-0.2935620	С	-3.1511421	2.3855960	-0.2307880
В	-0.9993609	-1.5614477	-2.7756007	С	-3.5857610	1.2805242	-1.0062417
В	1.7057430	2.5539606	-0.8683334	С	-3.0672152	1.1729197	-2.3481687
В	-0.2877726	1.8503051	2.8335002	С	4.0701106	-0.0254233	-1.3119469
В	0.1756234	2.8199786	-0.2935620	С	-2.9799369	2.2907628	1.1869176
В	-1.7079580	-2.5600143	0.2517388	С	-2.4053564	0.7393536	2.9755701
В	-2.1823839	-1.5042932	1.3745563	С	-3.2258515	1.0592857	1.8601897
В	0.1442372	-1.0279238	3.0668471	С	-3.7390658	-0.0268086	1.0955989
В	1.2788167	-2.6330623	0.7349996	С	-3.6741027	-1.2097291	-0.9055681
В	0.5521702	0.8748793	-3.0344143	С	-3.0688530	-1.3421964	-2.1836253
В	1.3589233	-2.7541971	-0.8683334	С	-2.7809651	-0.1274230	-2.8896550
В	-1.4585249	-1.1743710	2.8335002	С	-2.2112803	-2.4448714	-2.4182447
В	-2.0849250	0.9518814	-1.9342788	С	-3.3385882	-2.1208759	0.1539609
В	-3.0646663	0.2002364	-0.8683334	С	-1.6347107	-3.6221916	1.0894725
В	-2.5299849	-1.2578949	-0.2935620	С	-2.4312531	-3.2092200	-0.0470873
В	-1.0337529	0.0407537	-3.0344143	С	-1.8804602	-3.3585724	-1.3575576
В	-1.4304496	-2.1757458	-1.3215332	С	-2.0478336	-0.6242847	3.2702823
В	-0.9623267	0.3890488	3.0668471	С	-2.5461376	-1.7328926	2.5135159
В	-2.4076131	-0.0566116	2.2331331	С	-3.3856440	-1.3898260	1.4023644
В	-0.1763784	-2.7859879	-0.2670527	С	-1.6950898	-2.9047558	2.3714562
В	0.2181090	-2.2815387	-1.9342788	С	0.6440761	2.7548889	-3.0946401
В	1.8668160	1.3296573	-1.9342788	С	0.1649084	1.6554899	-3.8751922
В	-0.2115642	2.6421465	1.3745563	С	-1.6567153	-0.0122449	-3.7672458
В	-2.3245470	1.5457422	-0.2670527	С	-1.2546842	1.3762374	-3.8186689
В	0.4815826	-0.9156331	-3.0344143	С	-0.2260727	3.4906334	-2.2018242
В	-1.3630584	2.7591422	0.2517388	С	-2.1522638	3.2921474	-0.7480052
В	3.0710164	-0.1991279	0.2517388	С	-1.6197680	3.1772077	-2.0723874
В	1.8519339	-0.0847480	-2.7756007	С	-2.1539380	2.1364213	-2.9382857
В	2.5994759	-0.1509327	-1.3215332	С	0.8747517	3.7700913	1.3296367
В	0.8180895	0.6388750	3.0668471	С	0.0188951	4.0374702	0.2221900
В	1.1547794	2.1133599	2.2331331	С	0.5710388	3.9350967	-1.0863159
В	1.6408905	2.4240189	0.7349996	С	-1.3642488	3.7460370	0.3689252
В	1.7462975	-0.6759341	2.8335002	С	2.0129806	-0.0143059	3.5353222
В	2.5009255	1.2402456	-0.2670527	С	0.1759922	-1.6790262	3.6004766
В	2.3939481	-1.1378532	1.3745563	С	1.5640734	-1.3754742	3.4915507
С	0.0000000	0.0000000	0.6341220	С	-0.3294687	-2.8067019	2.8562794
F	0.0000000	0.0000000	-0.6341220	С	3.1668938	0.1049220	2.6796571
				С	4.1497468	1.2010457	0.6981333
				С	3.4877624	1.3204794	1.9888808
				С	2.5550775	2.3918263	2.1715929
				С	3.4914920	-2.4364242	-0.0040667

С	3.9609163	-1.3375940	0.7799342
С	3.4117622	-1.1959540	2.0936077
С	4.3646248	-0.1248302	0.1003711
С	0.5381600	-3.4895613	1.9361370
С	1.9235526	-3.1528399	1.7814525
С	2.4206992	-2.1043079	2.6005526
С	2.4957439	-3.3437242	0.4999793
С	-0.2513414	-3.9651280	0.8414437
С	-0.5301694	-3.8123505	-1.5761533
С	0.3237184	-4.0796165	-0.4744508
С	1.7095703	-3.8005934	-0.6120346
С	3.6957714	2.0695012	-0.3745106
С	2.7409987	3.1351193	-0.1907745
С	2.2141440	3.3148294	1.1137269
С	1.9192370	3.4946433	-1.2981597
С	0.3738066	3.1262771	2.5089263
С	-0.9986374	2.7581959	2.6209109
С	-1.8716780	3.1227555	1.5549540
С	-1.3105969	1.5799483	3.3595553
С	1.4063256	2.2834071	3.0338548
С	-0.7218057	-0.6084096	3.8432490
С	1.0987100	1.0652075	3.6980641
С	-0.2755195	0.7499932	3.9036674
С	3.6881855	1.3225724	-1.6025747
С	2.3894448	0.5715678	-3.5169921
С	2.8246503	1.6445961	-2.7012547
С	1.9660211	2.7632338	-2.5317233
С	3.3139975	-2.3402976	-1.4307539
С	2.7503371	-0.7876862	-3.2247388
С	3.5582495	-1.1146615	-2.1032017
С	-3.9252500	0.0770300	-0.3225307
С	-0.0311178	-3.1797283	-2.7590616
С	1.6560573	-1.6336147	-3.6083165
С	1.3405657	-2.8079269	-2.8653664
С	2.2148086	-3.1781069	-1.8027518
Sc	-1.0685179	-2.3364308	-3.2815379
Sc	1.0675951	0.5671618	-4.0841091
Sc	-0.7484115	-1.1175925	-3.9368607
Ν	0.6201275	-0.8012561	-4.1403934

General description of calibration curves construction for charge assessment on encapsulated fragment for X@YY endohedral system.

- 1. At the initial stage, 1s orbital energies for encapsulated fragment X taken in various charge states has been obtained.
- 2. At the next stage calibration curve of 1s orbital energy on charge state for specie of interest has been constructed.
- 3. Charge prediction is performed on the basis of the calibration curve obtained above and the 1s orbital energy value for encapsulated fragment X in X@YY system.

In the case when encapsulated fragment represented by a group of atoms calibration curve as well as charge prediction can be performed for any of the atoms constituting the fragment X.

Cl+B39 (VdV	V) [0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.1732	0.0198	-0.0696	-0.0696	-0.1962	6.93E-02
2	В	0.0095	0.0017	0.0185	0.0185	0.0339	1.23E-01
3	В	-0.0488	-0.0309	0.0229	0.0229	0.0455	-5.73E-02
4	В	0.1000	0.0544	0.0062	0.0061	0.0318	4.76E-03
5	В	-0.1612	0.0044	0.0537	0.0537	0.1528	2.27E-02
6	В	0.2034	0.0187	-0.0707	-0.0707	-0.2103	4.55E-02
7	В	0.2119	0.0198	-0.0647	-0.0647	-0.2076	3.31E-02
8	В	0.2114	0.0434	0.0015	0.0010	-0.0506	5.69E-02
9	В	-0.2075	-0.0062	0.0465	0.0465	0.1178	-1.64E-02
10	В	0.0958	0.0150	-0.0642	-0.0642	-0.2009	2.18E-01
11	В	-0.1235	-0.0058	0.0427	0.0427	0.0863	-1.73E-01
12	В	-0.1158	-0.0415	0.0639	0.0617	0.1323	3.95E-02
13	В	0.0690	-0.0135	0.0074	0.0074	-0.0241	5.66E-02
14	В	-0.0317	-0.0014	0.0380	0.0380	0.1070	-4.51E-02
15	В	0.2076	0.0256	-0.0630	-0.0630	-0.2011	2.01E-02
16	В	0.2185	0.0359	-0.0047	-0.0052	-0.0855	-6.48E-02
17	В	-0.0918	-0.0113	0.0379	0.0379	0.1044	4.77E-02
18	В	0.1784	0.0214	-0.0669	-0.0669	-0.2240	-8.79E-02
19	В	-0.1421	-0.0046	0.0471	0.0471	0.1285	3.77E-02
20	В	-0.0280	-0.0043	0.0372	0.0372	0.1097	-7.76E-02
21	В	-0.0481	-0.0247	0.0276	0.0276	0.0684	-3.17E-02
22	В	-0.0271	-0.0069	0.0764	0.0742	0.1845	8.52E-02
23	В	0.0551	0.0599	0.0053	0.0052	0.0345	5.87E-02
24	В	-0.2079	-0.0147	0.0442	0.0442	0.1290	-1.57E-02
25	В	-0.0684	-0.0036	0.0404	0.0404	0.1230	3.87E-02
26	В	-0.0909	-0.0052	0.0372	0.0372	0.1016	1.17E-02
27	В	-0.0217	0.0276	0.0503	0.0503	0.1184	-1.44E-01
28	В	-0.1593	0.0019	0.0490	0.0490	0.1477	1.24E-03
29	В	-0.0489	-0.0031	0.0371	0.0371	0.1051	-4.42E-02
30	В	0.1305	0.0155	-0.0616	-0.0616	-0.1862	2.07E-01
31	В	0.1451	0.0156	-0.0678	-0.0678	-0.2367	1.86E-01
32	В	0.2000	0.0206	-0.0678	-0.0678	-0.1985	3.18E-02
33	В	-0.0073	-0.0195	0.0297	0.0297	0.0704	-2.06E-02
34	В	-0.1594	-0.0394	0.0637	0.0615	0.1390	9.79E-03
35	В	0.1026	0.0413	-0.0014	-0.0014	-0.0065	-2.78E-02
36	В	0.0317	-0.0113	0.0081	0.0081	-0.0022	7.22E-02
37	В	0.2404	0.0417	-0.0033	-0.0040	-0.0677	6.65E-02
38	В	-0.2416	-0.0090	0.0528	0.0528	0.1665	-2.02E-02
39	В	-0.1435	0.0117	0.0543	0.0543	0.1401	-1.38E-01
40	Cl	-0.4098	-0.2392	-0.3935	-0.3851	-0.4803	-5.47E-01
	F1(B39)	0.4098	0.2392	0.3935	0.3851	0.4803	0.580
	F2(CI)	-0.4098	-0.2392	-0.3935	-0.3851	-0.4803	-0.547
	Total	0.0000	0.0000	0.0000	0.0000	0.0000	0.033

F@B39 [0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.1870	0.0150	-0.0751	-0.0755	-0.2092	0.0497
2	В	-0.0539	-0.0140	0.0017	0.0009	-0.0373	0.1462
3	В	-0.0060	-0.0289	0.0250	0.0240	0.0734	-0.0011
4	В	0.2197	0.0461	0.0007	0.0003	0.0777	-0.0122
5	В	-0.1540	-0.0016	0.0542	0.0529	0.1732	0.0646
6	В	0.1870	0.0150	-0.0750	-0.0754	-0.2105	0.0467
7	В	0.2249	0.0305	-0.0550	-0.0555	-0.2012	-0.0481
8	В	0.2080	0.0278	-0.0285	-0.0288	-0.1146	-0.0338
9	В	-0.1540	-0.0016	0.0541	0.0529	0.1832	0.0646
10	В	0.1522	0.0112	-0.0721	-0.0728	-0.2501	0.2267
11	В	-0.1558	0.0171	0.0638	0.0629	0.1990	-0.1515
12	В	-0.1301	0.0052	0.0553	0.0548	0.0882	0.0146
13	В	-0.0539	-0.0140	0.0018	0.0010	-0.0379	0.1462
14	В	-0.0405	-0.0029	0.0375	0.0370	0.1189	-0.0416
15	В	0.2249	0.0305	-0.0550	-0.0555	-0.1930	-0.0509
16	В	0.2080	0.0278	-0.0286	-0.0289	-0.1151	-0.0357
17	В	-0.0832	0.0009	0.0467	0.0458	0.1375	0.0597
18	В	0.2249	0.0305	-0.0550	-0.0555	-0.1937	-0.0501
19	В	-0.1540	-0.0016	0.0542	0.0529	0.1815	0.0648
20	В	-0.0405	-0.0029	0.0376	0.0371	0.1179	-0.0414
21	В	-0.0060	-0.0289	0.0252	0.0241	0.0713	-0.0010
22	В	-0.1301	0.0052	0.0553	0.0548	0.0914	0.0145
23	В	0.2197	0.0461	0.0007	0.0002	0.0729	-0.0126
24	В	-0.1674	-0.0063	0.0568	0.0555	0.2126	0.0252
25	В	-0.0832	0.0009	0.0468	0.0459	0.1412	0.0596
26	В	-0.0832	0.0009	0.0467	0.0458	0.1394	0.0595
27	В	-0.1558	0.0171	0.0639	0.0630	0.1984	-0.1515
28	В	-0.1674	-0.0063	0.0568	0.0554	0.2063	0.0250
29	В	-0.0405	-0.0029	0.0376	0.0371	0.1183	-0.0416
30	В	0.1522	0.0112	-0.0721	-0.0727	-0.2377	0.2260
31	В	0.1522	0.0112	-0.0720	-0.0727	-0.2357	0.2256
32	В	0.1870	0.0150	-0.0751	-0.0755	-0.2144	0.0468
33	В	-0.0060	-0.0289	0.0251	0.0240	0.0752	-0.0010
34	В	-0.1301	0.0052	0.0553	0.0548	0.0889	0.0146
35	В	0.2197	0.0461	0.0007	0.0003	0.0728	-0.0131
36	В	-0.0539	-0.0140	0.0018	0.0010	-0.0412	0.1463
3/	В	0.2080	0.0278	-0.0285	-0.0289	-0.1094	-0.0370
38	В	-0.1674	-0.0063	0.0569	0.0555	0.2117	0.0251
39	В	-0.1558	0.0171	0.0640	0.0631	0.1926	-0.1515
40	F	-0.6031	-0.3004	-0.3336	-0.3051	-0.8424	-0.8221
	LJ(R2A) LT(R2A)	0.6031	0.3004	0.3339	0.3055	0.8424	0.8765
	r∠(r) Total	-0.6031	-0.3004	-0.3336	-0.3051	-0.8424	-0.8221
<u> </u>	ruldi	0.0000	0.0000	0.0003	0.0003	0.0000	0.0544

F calibration curve constraction:

Charges on F	F 1s orbital energies
-2	-24.21387
-1	-24.42497
0	-24.86812
1	-25.46937
2	-26.23521



 $Q_{predicted} = -0.585$

S21

Orbital energies in F@B39 complex F 1s -24.59440

F 1s

Cl@B39 [I	0,1]	Mulliken Schem	Lowdin Scheme	Hirshfeld Schem	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.3405	0.0122	-0.0639	-0.0653	-0.1689	-1.63E-02
2	В	-0.0502	-0.0319	0.0009	-0.0022	-0.0146	1.08E-01
3	В	-0.0605	-0.0627	0.0153	0.0112	0.0603	-1.70E-03
4	В	0.2794	0.0354	-0.0018	-0.0034	0.0835	-1.38E-02
5	В	-0.3442	-0.0528	0.0422	0.0373	0.1659	1.99E-02
6	В	0.3268	0.0092	-0.0672	-0.0686	-0.1735	1.40E-02
7	В	0.3759	0.0105	-0.0634	-0.0655	-0.2058	-5.22E-02
8	В	0.2918	0.0153	-0.0287	-0.0299	-0.0698	-5.58E-02
9	В	-0.3331	-0.0538	0.0372	0.0323	0.1499	6.82E-02
10	В	0.2735	-0.0087	-0.0720	-0.0747	-0.2142	2.01E-01
11	В	-0.2486	-0.0283	0.0330	0.0295	0.1032	-1.48E-01
12	В	-0.2195	-0.0200	0.0354	0.0335	0.0276	2.69E-02
13	В	-0.0230	-0.0375	-0.0003	-0.0035	0.0023	1.15E-01
14	В	-0.1047	-0.0152	0.0239	0.0219	0.0572	-5.86E-03
15	В	0.3285	-0.0014	-0.0768	-0.0789	-0.2152	-2.65E-02
16	В	0.3185	0.0237	-0.0162	-0.0174	-0.0462	-6.70E-02
17	В	-0.1650	-0.0400	0.0258	0.0225	0.1065	1.00E-01
18	В	0.3342	0.0048	-0.0719	-0.0740	-0.2172	-4.61E-02
19	В	-0.3295	-0.0552	0.0499	0.0450	0.1933	3.61E-02
20	В	-0.0853	-0.0115	0.0396	0.0377	0.1644	-2.76E-02
21	В	-0.0631	-0.0608	0.0113	0.0073	0.0373	-1.45E-02
22	В	-0.2105	-0.0217	0.0366	0.0348	0.0410	2.08E-02
23	в	0.2602	0.0384	0.0013	-0.0003	0.0892	1.19E-04
24	В	-0.3431	-0.0736	0.0320	0.0266	0.1656	5.1/E-02
25	В	-0.1633	-0.0539	0.0182	0.0149	0.1119	9.24E-02
26	В	-0.1431	-0.0305	0.0295	0.0262	0.1080	7.97E-02
27	В	-0.2633	-0.0351	0.0244	0.0210	0.0965	-1.11E-01
28	В	-0.3467	-0.0673	0.0368	0.0314	0.1583	3.83E-03
29	В	-0.1204	-0.0306	0.0103	0.0083	0.0139	3.42E-02
50 21	D	0.3003	-0.0042	-0.0625	-0.0650	-0.1828	1.62E-01
31 22	D	0.2605	0.0066	-0.0492	-0.0319	-0.1550	1.002-01
32	D	0.3033	0.0430	-0.0233	-0.0274	-0.0380	1 24E 02
33	B	-0.0370	-0.0313	0.0147	0.0107	0.0033	-1.24L-02 2 37E-02
35	B	0.2127	0.0240	-0.0136	-0.0152	0.0440	1 70E-02
35	R	-0.04/9	-0.0231	0.0130	-0.0132	-0 0042	1.70L-02 1.74F-01
37	B	0.0448	0.0392	-0 0206	-0.0022	-0.0042	-6 25F-02
38	B	-0 3531	-0.0627	0.0200	0.0219	0.1880	2 94F-02
39	B	-0 2686	-0.0319	0.0475	0.0423	0.1000	-9 43F-02
40	ci	-0.1105	0.7580	0.0023	0.1141	-0.5598	-6.18E-01
	F1(B39)	0.1105	-0.7580	-0.0023	-0.1141	0.5597	0.6579
	F2(CI)	-0.1105	0.7580	0.0023	0.1141	-0.5598	-0.6181
	Total	0.0000	0.0000	0.0000	0.0000	0.0000	0.0398

Cl calibration curve constraction:

Charges on Cl	Cl 1s orbital energies
-2	-101.37098
-1	-101.51657
0	-101.75375
1	-102.07354
2	-102.47303



 $Q_{predicted} = -0.475$

Orbital energies in Cl@B39 complex Cl 1s -101.62826

Cl 1s

Atom Number Element Charge density Charge density <thcharge density<="" th=""> Charge density<th>Br@B39</th><th>[0,1]</th><th>Mulliken Scheme</th><th>Lowdin Scheme</th><th>Hirshfeld Scheme</th><th>CM5 Scheme</th><th>NPA Scheme</th><th>Bader Scheme</th></thcharge>	Br@B39	[0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
1 B 0.2947 0.0018 -0.0738 -0.0765 -0.1927 1.286-02 2 B -0.0728 -0.0751 0.0064 -0.0012 0.0485 1.956-02 4 B 0.09956 -0.0162 0.0136 0.0224 0.120 6.016-02 5 B -0.2685 -0.0662 0.0136 0.0224 0.0485 -6.826-02 6 B 0.3000 0.0211 -0.0434 -0.0495 -6.386-02 7 B 0.4004 0.0098 -0.0524 -0.0333 0.1694 2.346-02 9 B -0.3002 -0.0708 0.0425 0.0333 0.1694 2.346-02 10 B -0.3071 -0.0427 0.0214 0.0150 0.0578 -1.056-01 11 B -0.1701 -0.0427 0.0214 0.0133 0.01327 -0.0688 0.01007 1.0164 0.0272 -2.496-02 13 B -0.0367 -0.0298 -0.0688	Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
2 8 -0.0235 -0.0473 -0.0067 -0.0121 -0.0485 -1.055-02 3 8 -0.0758 -0.0751 0.0064 -0.0123 0.0485 -1.955-02 4 8 0.0956 0.0116 -0.0203 0.0610 9.435-03 5 8 0.2685 -0.0662 0.0316 0.0224 0.0336 6.746-02 7 8 0.4004 0.0098 -0.0655 -0.0694 -0.2058 -6.826-02 9 8 0.1643 0.0175 -0.0219 -0.022 -0.0485 -6.386-02 9 8 0.3392 0.0079 -0.0444 -0.0444 -0.449 -1.429 1.246-01 11 8 -0.0477 -0.0431 -0.0252 0.0333 0.1654 1.246-02 12 B -0.0477 -0.0443 -0.0282 0.0224 0.0137 -1.0557 13 8 0.1607 -0.0083 -0.0649 -0.0688 -0.1900 -6.96	1	В	0.2947	0.0018	-0.0738	-0.0765	-0.1927	1.28E-02
3 8 0.0728 0.0751 0.0064 0.0203 0.0610 9.43E-03 4 8 0.0956 0.0160 -0.0173 -0.0203 0.0610 9.43E-03 5 8 0.22685 -0.0662 0.0316 -0.0224 -0.0358 6-7.4E-02 7 8 0.4004 0.0098 -0.0655 -0.0644 -0.0242 -0.0242 -0.0242 -0.0242 -0.0242 -0.0425 6-3.3E-02 9 8 -0.3002 -0.0708 0.0425 0.0333 0.1664 2.34E-02 10 8 0.3002 -0.0708 0.0424 0.0142 0.1429 1.24E-01 11 8 -0.1701 -0.0427 0.0214 0.0150 0.0578 -1.05E-01 12 8 -0.0677 -0.0244 0.0282 0.0244 0.1327 -2.49E-02 13 8 -0.0367 -0.0443 -0.0255 -0.0507 -6.09E-02 14 8 0.1609 <	2	В	-0.0235	-0.0473	-0.0067	-0.0127	-0.0101	1.02E-01
4 8 0.0956 0.0196 -0.0173 -0.023 0.0610 9.43E-03 5 8 -0.2685 -0.0662 0.0316 0.0224 0.1320 6.01E-02 6 8 0.3300 0.0281 -0.0434 -0.0441 -0.0886 -6.74E-02 7 8 0.4004 0.0098 -0.0219 -0.0242 -0.0495 -6.38E-02 9 8 -0.3002 -0.0708 0.0425 0.0333 0.1694 2.34E-02 10 8 0.3392 0.0079 -0.0444 -0.0424 -0.1429 1.24E-01 11 8 -0.0377 -0.0314 0.0316 0.0222 0.0333 1.95E-02 12 8 -0.0477 -0.0483 -0.0037 -0.0007 1.11E-01 14 8 0.0467 -0.0244 -0.0222 -0.0331 1.0120 6.0560 15 8 0.1609 -0.0177 -0.0231 -0.0255 -0.0507 -6.39E-02 <	3	В	-0.0728	-0.0751	0.0064	-0.0012	0.0485	-1.95E-02
5 B -0.2685 -0.0662 0.0316 0.0224 0.1320 6.01E-02 6 B 0.3300 0.0281 -0.0434 -0.0461 -0.0836 -6.74E-02 7 B 0.40404 0.0098 -0.0655 -0.0694 -0.2058 -6.82E-02 8 B 0.1643 0.0175 -0.0219 -0.0242 -0.0495 -6.38E-02 9 B 0.3302 0.0079 -0.0444 -0.1499 1.24E-01 11 B -0.1701 -0.0427 0.0214 0.0150 0.0578 +1.05E-01 12 B -0.0677 -0.0314 0.0322 0.0244 0.1327 -2.49E-02 13 B -0.0677 -0.0231 -0.055 -0.0007 1.11E-01 14 B 0.0667 0.089 -0.0648 0.1900 6.69E-02 15 B 0.0407 -0.0656 0.0112 0.0050 0.0944 9.11E-02 16 B	4	В	0.0956	0.0196	-0.0173	-0.0203	0.0610	9.43E-03
6 8 0.3300 0.0281 -0.0434 -0.0613 -0.0694 -0.2086 -6.82E.02 7 B 0.4004 0.0098 -0.0655 -0.0694 -0.2088 -6.82E.02 9 B 0.0302 -0.0708 0.0445 0.0333 0.1694 2.34E.02 10 B 0.3392 0.0079 -0.0444 -0.0194 -0.1429 1.24E.01 11 B -0.1701 -0.0427 0.0214 0.0150 0.0578 1.05E.01 12 B -0.0367 -0.0343 -0.037 -0.0007 1.11E.01 14 B -0.0367 -0.0244 0.0225 -0.0507 -6.39E.02 15 B 0.0467 0.0089 -0.0649 -0.0688 -0.1900 -6.99E.02 16 B 0.1609 0.0177 -0.0231 -0.0255 -0.0507 -6.39E.02 17 B -0.2218 -0.0655 -0.0143 0.0321 -0.166 5.38E.03 <td>5</td> <td>В</td> <td>-0.2685</td> <td>-0.0662</td> <td>0.0316</td> <td>0.0224</td> <td>0.1320</td> <td>6.01E-02</td>	5	В	-0.2685	-0.0662	0.0316	0.0224	0.1320	6.01E-02
7 B 0.4004 0.0098 -0.655 -0.0694 -0.2058 -6.382-02 8 B 0.1643 0.0175 -0.0219 -0.0242 -0.0495 -6.386-02 9 B -0.3002 -0.0708 0.0425 0.0333 0.1694 2.34E-01 10 B 0.0302 -0.0708 0.0214 0.0150 0.0578 -1.05E-01 11 B -0.1071 -0.0427 0.0214 0.0150 0.0578 -1.05E-01 12 B -0.0677 -0.0433 -0.037 -0.007 -1.11E-01 14 B -0.0467 -0.0244 0.0282 0.0244 0.1327 -2.49E-02 15 B -0.0467 -0.0385 -0.012 0.0050 0.0944 -9.11E-02 16 B -0.2218 -0.0665 0.0112 0.0050 0.0944 -9.11E-02 18 B -0.2318 -0.0657 -0.074 0.0822 -2.2144 -2.34E-02	6	В	0.3300	0.0281	-0.0434	-0.0461	-0.0836	-6.74E-02
8 8 0.1643 0.0175 -0.0219 -0.0422 -0.0425 -6.38E.02 9 8 -0.3002 -0.0708 0.0425 0.0333 0.1694 2.34E.02 10 8 -0.3392 0.0079 -0.0444 -0.0494 -0.1429 1.24E.01 11 8 -0.0873 -0.0314 0.0316 0.0282 0.0383 1.93E.02 13 8 -0.0477 -0.0483 -0.0377 -0.0097 -0.0007 1.11E.01 14 8 -0.0367 -0.0244 0.0282 0.0244 0.1327 -2.49E.02 15 8 0.4067 0.089 -0.0648 -0.1900 -6.09E.02 16 8 0.1609 0.0177 -0.0215 -0.055 -0.055 -0.055 -0.050 -0.69E.02 -2.2144 -2.94E.02 19 8 -0.231 -0.0657 -0.022 -0.166 -2.42E.02 20 8 -0.0411 -0.057 -0.0224 <t< td=""><td>7</td><td>В</td><td>0.4004</td><td>0.0098</td><td>-0.0655</td><td>-0.0694</td><td>-0.2058</td><td>-6.82E-02</td></t<>	7	В	0.4004	0.0098	-0.0655	-0.0694	-0.2058	-6.82E-02
9 8 -0.3002 -0.0708 0.0425 0.0333 0.1694 2.34E-02 10 8 0.3392 0.0079 -0.0444 -0.0494 -0.1429 1.24E-01 11 8 -0.0873 -0.0314 0.0316 0.0282 0.0383 1.93E-02 13 8 -0.0477 -0.0483 -0.0037 -0.0097 -0.0007 1.11E-01 14 8 -0.0477 -0.0843 -0.037 -0.0225 -0.0507 -6.09E-02 15 8 0.1609 0.0177 -0.0211 -0.0525 -0.0507 -6.39E-02 16 8 0.3649 -0.0035 -0.012 -0.0022 -0.2144 -2.94E-02 18 8 0.3649 -0.0655 -0.012 -0.0186 -2.42E-02 20 8 -0.0647 -0.0555 -0.0022 -0.0186 -2.42E-02 21 8 -0.1025 -0.0024 -0.0186 -2.42E-02 22 8 -0.1	8	В	0.1643	0.0175	-0.0219	-0.0242	-0.0495	-6.38E-02
10 B 0.3392 0.0079 -0.0444 -0.0494 -0.1429 1.24E-01 11 B -0.1701 -0.0427 0.0214 0.0150 0.0578 -1.05E-01 12 B -0.0873 -0.0314 0.0316 0.0282 0.0383 1.39E-02 13 B -0.0367 -0.0244 0.0282 0.0244 0.1327 -2.49E-02 15 B 0.0667 -0.0244 0.0282 -0.0244 0.1327 -2.49E-02 16 B 0.1669 0.0177 -0.0231 -0.0255 -0.0507 -6.39E-02 17 B -0.2218 -0.0665 0.0112 0.0050 0.0944 9.11E-02 18 B 0.3649 -0.0355 -0.0574 -0.022 -0.146 1.63E-02 20 B -0.0441 -0.0575 0.0564 -0.0022 -0.0186 -2.42E-02 21 B -0.0411 -0.657 0.054 -0.0224 0.0186	9	В	-0.3002	-0.0708	0.0425	0.0333	0.1694	2.34E-02
11 B -0.1701 -0.0427 0.0214 0.0150 0.0578 -1.05E01 12 B -0.0873 -0.0314 0.0316 0.0282 0.0383 1.93E02 13 B -0.0477 -0.0483 -0.0077 -0.007 1.11E01 14 B -0.0367 -0.0244 0.0282 0.0244 0.1327 -2.49E02 15 B 0.4067 0.0089 -0.0649 -0.0658 -0.190 -6.09E02 16 B 0.1609 0.0177 -0.0231 -0.0225 -0.0507 -6.39E02 17 B -0.2218 -0.0665 0.0112 0.0050 0.0944 9.11E02 18 B -0.3203 -0.0681 0.0413 0.0321 0.1766 5.03E03 20 B -0.0647 -0.0365 0.014 0.0077 0.0463 1.63E-02 21 B -0.0105 -0.0283 0.0320 -0.0266 0.0272 2.03E-02	10	В	0.3392	0.0079	-0.0444	-0.0494	-0.1429	1.24E-01
12 B -0.0873 -0.0314 0.0316 0.0282 0.0383 1.93F-02 13 B -0.0477 -0.0483 -0.0037 -0.0044 0.1327 7.2.49F-02 15 B 0.4067 0.0089 -0.0649 -0.0688 -0.1900 -6.09F-02 16 B 0.1609 0.0177 -0.0231 -0.0255 -0.0507 -5.39F-02 17 B -0.2218 -0.0665 0.0112 0.0080 0.0944 -9.11E-02 18 B 0.3649 -0.0035 -0.0784 -0.0822 -0.2144 -2.94F-02 19 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03F-03 20 B -0.0647 -0.0365 0.0114 0.0077 0.0463 1.63F-02 21 B -0.0141 -0.0657 0.0054 -0.022 -0.0186 -1.27F-02 23 B -0.299 -0.0854 0.0374 0.0788 8.94F-02	11	В	-0.1701	-0.0427	0.0214	0.0150	0.0578	-1.05E-01
13 B -0.0477 -0.0483 -0.0037 -0.0097 -0.0007 1.11:e11 14 B -0.0367 -0.0244 0.0282 0.0244 0.1327 -2.49E-02 15 B 0.04067 0.0089 -0.0688 -0.1900 -6.09E-02 16 B 0.1609 0.0177 -0.0231 -0.0255 -0.0507 -6.39E-02 17 B -0.2218 -0.0665 0.0112 0.0050 0.0444 9.11E-02 18 B -0.3649 -0.0355 -0.0784 -0.0822 -0.2144 -2.94E-02 19 B -0.3203 -0.0681 0.0413 0.0321 0.1766 5.03E-03 20 B -0.0057 0.0054 -0.0022 -0.0166 -2.42E-02 21 B -0.1028 0.0292 -0.0061 -0.0092 0.0816 -1.27E-02 23 B -0.1284 0.0533 0.0155 0.0093 0.0836 9.84E-02	12	В	-0.0873	-0.0314	0.0316	0.0282	0.0383	1.93E-02
14 B -0.0367 -0.0244 0.0282 0.0244 0.1327 -2.49Fe02 15 B 0.4067 0.0089 -0.0649 -0.0688 -0.1900 -6.09Fe02 16 B 0.1609 0.0177 -0.0231 -0.0255 -0.0507 -6.39Fe02 17 B -0.2218 -0.0665 0.0112 0.0050 0.0944 9.11Fe02 18 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03Fe03 20 B -0.0647 -0.0355 0.0114 0.0077 0.0463 1.63Fe02 21 B -0.0411 -0.0657 0.0054 -0.0022 -0.0186 -2.42Fe02 23 B 0.1298 0.0292 -0.061 -0.0092 0.0816 -1.27Fe02 24 B -0.2333 0.0155 0.0093 0.0836 9.84Fe02 25 B -0.1527 -0.043 0.0212 0.0148 0.0809 -1.48Fe01	13	В	-0.0477	-0.0483	-0.0037	-0.0097	-0.0007	1.11E-01
15 B 0.4067 0.0089 -0.0649 -0.0688 -0.1900 -6.09E-02 16 B 0.1609 0.0177 -0.0231 -0.0255 -0.0507 -6.39E-02 17 B -0.218 -0.0665 0.0112 0.0050 0.0944 9.11E-02 18 B 0.3649 -0.0355 -0.0784 -0.0822 -0.2144 -2.94E-02 19 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03E-03 20 B -0.0411 -0.0657 0.0054 -0.0022 -0.0186 -2.42E-02 21 B -0.1005 -0.0283 0.0320 0.0226 0.0272 2.03E-02 23 B 0.1298 0.0292 -0.0661 -0.0092 0.0816 -1.27E-02 24 B -0.2184 -0.0532 0.0136 0.0074 0.0788 8.94E-02 25 B -0.1527 -0.0443 0.0127 0.1382 3.24E-02 <td>14</td> <td>В</td> <td>-0.0367</td> <td>-0.0244</td> <td>0.0282</td> <td>0.0244</td> <td>0.1327</td> <td>-2.49E-02</td>	14	В	-0.0367	-0.0244	0.0282	0.0244	0.1327	-2.49E-02
16 B 0.1609 0.0177 -0.0231 -0.0255 -0.0507 -6.39F-02 17 B -0.2218 -0.0665 0.0112 0.0050 0.0944 9.11E-02 18 B 0.3649 -0.0035 -0.0784 -0.0822 -0.2144 -2.94F-02 19 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03E-03 20 B -0.0647 -0.0365 0.0114 0.0077 0.0463 1.63E-02 21 B -0.0411 -0.0657 0.0054 -0.0022 -0.0186 -2.42E-02 22 B -0.1005 -0.0283 0.0320 0.0286 0.0274 0.1572 3.12E-02 23 B -0.1299 -0.0854 0.0374 0.0274 0.1572 3.12E-02 24 B -0.2909 -0.0853 0.0155 0.0993 0.0836 9.84E-02 26 B -0.1527 -0.0443 0.0217 0.1582	15	В	0.4067	0.0089	-0.0649	-0.0688	-0.1900	-6.09E-02
17 B -0.2218 -0.0665 0.0112 0.0050 0.0944 9.11F-02 18 B 0.3649 -0.0035 -0.0784 -0.0822 -0.2144 -2.94E-02 19 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03E-03 20 B -0.0647 -0.0365 0.0114 0.0077 0.0463 1.63E-02 21 B -0.0411 -0.0657 0.0054 -0.0022 -0.0186 -2.42E-02 22 B -0.1005 -0.0283 0.0320 0.0286 0.0272 2.03E-02 23 B 0.1298 0.0292 -0.0061 -0.0992 0.0816 -1.27E-02 24 B -0.2184 -0.0532 0.0136 0.0074 0.0788 8.94E-02 25 B -0.1848 -0.0532 0.0136 0.0074 0.0778 8.94E-02 26 B -0.2184 -0.0533 0.0157 0.0127 0.1382 3	16	В	0.1609	0.0177	-0.0231	-0.0255	-0.0507	-6.39E-02
18 B 0.3649 -0.0035 -0.0784 -0.0822 -0.2144 -2.94F-02 19 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03F-03 20 B -0.0647 -0.0365 0.0114 0.0077 0.0463 1.63F-02 21 B -0.0105 -0.0283 0.0320 0.0286 0.0272 2.03F-02 23 B 0.1298 0.0292 -0.0661 -0.0092 0.0816 -1.27F-02 24 B -0.2909 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0532 0.0136 0.0074 0.0788 8.94E-02 26 B -0.2184 -0.0533 0.0155 0.0093 0.0836 9.84E-02 27 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.7	17	В	-0.2218	-0.0665	0.0112	0.0050	0.0944	9.11E-02
19 B -0.3203 -0.0681 0.0413 0.0321 0.1706 5.03E-03 20 B -0.0647 -0.0365 0.0114 0.0077 0.0463 1.63E-02 21 B -0.0411 -0.0657 0.0024 -0.0022 -0.0186 -2.42E-02 22 B -0.1005 -0.0283 0.0320 0.0286 0.0272 2.03E-02 23 B 0.1298 0.0292 -0.0061 -0.0092 0.0816 -1.27F-02 24 B -0.2909 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0532 0.0136 0.0074 0.0788 8.94E-02 26 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.2589 -0.0913 0.0228 0.0127 0.1382 3.24E-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.7	18	В	0.3649	-0.0035	-0.0784	-0.0822	-0.2144	-2.94E-02
20 B -0.0647 -0.0365 0.0114 0.0077 0.0463 1.63E-02 21 B -0.0411 -0.0657 0.0054 -0.0022 -0.0186 -2.42E-02 22 B -0.1005 -0.0283 0.0320 0.0286 0.0272 2.03E-02 23 B 0.1298 0.0292 -0.0061 -0.0092 0.0816 -1.27E-02 24 B -0.2909 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0533 0.0155 0.0093 0.0836 9.84E-02 26 B -0.2184 -0.0533 0.0122 0.0148 0.0809 -1.48E-01 28 B -0.554 -0.0295 0.0164 0.0127 0.1382 3.24E-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.526 2.70E-04 30 B 0.3239 -0.0151 -0.0574 -0.0624 -0.1592 1.5	19	В	-0.3203	-0.0681	0.0413	0.0321	0.1706	5.03E-03
21 B -0.0411 -0.0657 0.0054 -0.0022 -0.0186 -2.42E-02 22 B -0.1005 -0.0283 0.0320 0.0286 0.0272 2.03E-02 23 B 0.1298 0.0292 -0.061 -0.0092 0.0816 -1.27E-02 24 B -0.2099 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0532 0.0136 0.0074 0.0788 8.94E-02 26 B -0.2184 -0.0533 0.0155 0.0093 0.0836 9.84E-02 27 B -0.1527 -0.0443 0.0212 0.0148 0.809 -1.48E-01 28 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0624 -0.1592 1.54E-01 31 B 0.3069 0.0104 -0.0636 -0.0662 -0.1553 -2	20	В	-0.0647	-0.0365	0.0114	0.0077	0.0463	1.63E-02
22 B -0.1005 -0.0283 0.0320 0.0286 0.0272 2.03E-02 23 B 0.1298 0.0292 -0.061 -0.092 0.0816 -1.27F-02 24 B -0.2909 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0533 0.0155 0.0093 0.0836 9.84E-02 26 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.5589 -0.0913 0.0228 0.0127 0.1382 3.24E-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0578 -0.0808 -0.2028 1.88E-01 31 B 0.311 -0.0036 -0.0624 -0.1553 -2.55E-02 33 B -0.0508 -0.0740 0.0071 -0.0662 -0.1553 -2.55E-02	21	В	-0.0411	-0.0657	0.0054	-0.0022	-0.0186	-2.42E-02
23 B 0.1298 0.0292 -0.0061 -0.0092 0.0816 -1.27E-02 24 B -0.2909 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0532 0.0136 0.0074 0.0788 8.94E-02 26 B -0.2184 -0.0533 0.0155 0.0093 0.0836 9.84E-02 27 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.2589 -0.0913 0.0228 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0808 -0.2028 1.88E-01 31 B 0.3311 -0.0054 -0.0624 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0636 -0.0624 -0.1592 1.54E-01 33 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02	22	В	-0.1005	-0.0283	0.0320	0.0286	0.0272	2.03E-02
24 B -0.2909 -0.0854 0.0374 0.0274 0.1572 3.12E-02 25 B -0.1848 -0.0532 0.0136 0.0074 0.0788 8.94E-02 26 B -0.1527 -0.0443 0.0212 0.0148 0.0836 9.84E-02 27 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.2589 -0.0913 0.0228 0.0127 0.0526 2.70E-04 30 B -0.3239 -0.0151 -0.0758 -0.0808 -0.2028 1.88E-01 31 B 0.3311 -0.0036 -0.0574 -0.0624 -0.1553 -2.55E-02 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0522 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.014 -0.0145 0.0648	23	В	0.1298	0.0292	-0.0061	-0.0092	0.0816	-1.27E-02
25 B -0.1848 -0.0532 0.0136 0.0074 0.0788 8.94E-02 26 B -0.2184 -0.0533 0.0155 0.0093 0.0836 9.84E-02 27 B -0.1527 -0.0443 0.0212 0.0148 0.0896 9.448E-01 28 B -0.2589 -0.0913 0.0228 0.0127 0.1382 3.24E-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0808 -0.2028 1.88E-01 31 B 0.3069 0.0104 -0.0654 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0666 -0.0562 -0.1553 -2.55E-02 33 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02	24	В	-0.2909	-0.0854	0.0374	0.0274	0.1572	3.12E-02
26 B -0.2184 -0.0533 0.0155 0.0093 0.0836 9.844-02 27 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.2589 -0.0913 0.0228 0.0127 0.1382 3.24E-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0808 -0.2028 1.88E-01 31 B 0.3069 0.0104 -0.0624 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0666 -0.0624 -0.1592 1.54E-01 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.014 -0.0415 0.0648 1.18E-02	25	В	-0.1848	-0.0532	0.0136	0.0074	0.0788	8.94E-02
27 B -0.1527 -0.0443 0.0212 0.0148 0.0809 -1.48E-01 28 B -0.2589 -0.0913 0.0228 0.0127 0.1382 3.24E-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0808 -0.2028 1.88E-01 31 B 0.3311 -0.0036 -0.0574 -0.0624 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0636 -0.0662 -0.1553 -2.55E-02 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0922 -0.0298 0.0334 0.3000 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.014 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0552 -0.0084 <t< td=""><td>26</td><td>В</td><td>-0.2184</td><td>-0.0533</td><td>0.0155</td><td>0.0093</td><td>0.0836</td><td>9.84E-02</td></t<>	26	В	-0.2184	-0.0533	0.0155	0.0093	0.0836	9.84E-02
28 B -0.2589 -0.0913 0.0228 0.0127 0.1382 3.24t-02 29 B -0.0504 -0.0295 0.0164 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0608 -0.2028 1.88E-01 31 B 0.3311 -0.0036 -0.0574 -0.0624 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0636 -0.0662 -0.1553 -2.55E-02 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0522 -0.0084 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 <	27	В	-0.1527	-0.0443	0.0212	0.0148	0.0809	-1.48E-01
29 B -0.0504 -0.0295 0.0144 0.0127 0.0526 2.70E-04 30 B 0.3239 -0.0151 -0.0758 -0.0808 -0.2028 1.88E-01 31 B 0.3311 -0.0036 -0.0574 -0.0624 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.6636 -0.0662 -0.1553 -2.55E-02 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0552 -0.0144 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-03 38 B -0.2939 -0.0477 0.0193 0.1355 -5.64E-03 <	28	В	-0.2589	-0.0913	0.0228	0.0127	0.1382	3.24E-02
30 B 0.3239 -0.0131 -0.0805 -0.0805 -0.0228 1.88E-01 31 B 0.3311 -0.0036 -0.0574 -0.0624 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0636 -0.0662 -0.1553 -2.55E-02 33 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0455 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0552 -0.084 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-03 38 B -0.2939 -0.0872 0.0293 0.0193 0.1355 -5.64E-03 39 B -0.1939 -0.0467 0.0193 0.0129 0.0821 <t< td=""><td>29</td><td>В</td><td>-0.0504</td><td>-0.0295</td><td>0.0164</td><td>0.0127</td><td>0.0526</td><td>2.70E-04</td></t<>	29	В	-0.0504	-0.0295	0.0164	0.0127	0.0526	2.70E-04
51 b 0.3311 -0.0030 -0.0574 -0.0024 -0.1024 -0.1592 1.54E-01 32 B 0.3069 0.0104 -0.0636 -0.0624 -0.1553 -2.55E-02 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0922 -0.0298 0.034 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0522 -0.0984 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-02 38 B -0.2939 -0.0872 0.0293 0.0133 0.1355 -5.64E-03 39 B -0.1939 -0.0467 0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172	30	В	0.3239	-0.0151	-0.0758	-0.0808	-0.2028	1.88E-01
32 B 0.3069 0.0104 -0.068 -0.0662 -0.1533 -2.35E-02 33 B -0.0508 -0.0740 0.0071 -0.0005 0.0368 -1.32E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0052 -0.0084 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-02 38 B -0.2939 -0.0872 0.0293 0.0193 0.1355 5.64E-03 39 B -0.1399 -0.0467 0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 0.2090 0.4172 -0.2576 0.4047	31	В	0.3311	-0.0036	-0.0574	-0.0624	-0.1592	1.54E-01
3.3 B -0.0508 -0.0740 0.001 -0.0005 0.0388 -1.32E-02 34 B -0.0922 -0.0298 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0052 -0.0084 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-02 38 B -0.2939 -0.0872 0.0293 0.0193 0.1355 -5.64E-03 39 B -0.13261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 40 Br -0.3261 -1.1415 -0.2091 -0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 0.2090 0.4172 -0.2576 -0.3566	32	В	0.3069	0.0104	-0.0036	-0.0662	-0.1553	-2.55E-02
3-4 B -0.0222 -0.0233 0.0334 0.0300 0.0434 1.55E-02 35 B 0.1013 0.0263 -0.0114 -0.0145 0.0648 1.18E-02 36 B -0.0338 -0.0421 0.0007 -0.0052 -0.0084 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-02 38 B -0.2939 -0.0872 0.0293 0.0193 0.1355 -5.64E-03 39 B -0.1939 -0.0467 0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 0.2090 0.4172 -0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	24	D	-0.0508	-0.0740	0.0071	-0.0005	0.0308	-1.52E-UZ
33 B 0.0113 0.0223 0.0114 0.0143 0.0048 1.161-02 36 B -0.0338 -0.0421 0.0007 -0.0052 -0.0084 9.00E-02 37 B 0.1525 0.0118 -0.0312 -0.0335 -0.0714 -5.45E-02 38 B -0.2939 -0.0872 0.0293 0.0193 0.1355 -5.64E-03 39 B -0.1320 -0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 -0.2091 -0.4172 0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	25	D	-0.0322	-0.0258	0.0334	0.0300	0.0434	1.332-02
37 B 0.1525 0.0118 -0.0312 -0.0325 -0.0714 -5.45E-02 38 B -0.2939 -0.0872 0.0212 0.0135 -5.64E-03 39 B -0.1939 -0.0467 0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 -0.2091 -0.4172 0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	35	R	-U U330 0.1012	-0.0205	0.0114	-0.0145	-0.0048	1.10E-02
38 B -0.2939 -0.0872 0.0293 0.0133 -0.1355 -5.64E-03 39 B -0.1939 -0.0467 0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 -0.2091 -0.4172 0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	30	B	-0.0556	-0.0421	-0.0007	-0.0052	-0.0084	-5 455 02
39 B -0.193 -0.0457 0.0193 0.0193 0.0193 0.0129 0.0821 -1.15E-01 40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 -0.2091 -0.4172 0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	37	B	-0 2020	-0.0110	-0.0312	-0.0355	-0.0714	-5.451-02
40 Br -0.3261 1.1415 0.2090 0.4172 -0.2576 -3.57E-01 F1(B39) 0.3261 -1.1415 -0.2091 -0.4172 0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	39	B	-0.2939	-0.0872	0.0293	0.0193	0.1333	-1.15F-01
F1(B39) 0.3261 -1.1415 -0.2091 -0.4172 0.2576 0.4047 F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	40	Br	-0.1939	1 1415	0.0193	0.0129 0 4172	-0 2576	-3 57F-01
F2(Br) -0.3261 1.1415 0.2090 0.4172 -0.2576 -0.3566	40	F1(B39)	0 3261	-1 1415	-0 2090	-0 4172	0.2576	0 4047
		F2(Br)	-0 3261	1 1415	0 2091	0.4172	-0 2576	-0 3566
Total 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0481		Total	0.0000	0.0000	0.0000	0.0000	0.0000	0.0481

Br calibration curve constraction:

Charges on Br	Br 1s orbital energies
-2	-483.02043
-1	-483.11004
0	-483.29595
1	-483.55083
2	-483.85900



 $Q_{predicted} = -0.251$

Orbital energies in Br@B39 complex Br 1s -483.23916

Br 1s

NO@B39	[0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.3144	0.0278	-0.0474	-0.0474	-0.0936	-6.65E-02
2	В	-0.0637	-0.0368	-0.0115	-0.0120	-0.0352	1.02E-01
3	В	-0.1195	-0.0633	0.0021	0.0020	0.0202	-1.62E-02
4	В	0.2371	0.0271	-0.0151	-0.0158	0.0665	-1.38E-02
5	В	-0.3697	-0.0423	0.0241	0.0237	0.1332	5.53E-03
6	В	0.3144	0.0278	-0.0475	-0.0474	-0.0929	-6.77E-02
7	В	0.3760	0.0049	-0.0774	-0.0775	-0.2009	-4.55E-02
8	В	0.2782	0.0166	-0.0286	-0.0292	-0.0471	-7.25E-02
9	В	-0.3697	-0.0423	0.0240	0.0236	0.1147	5.55E-03
10	В	0.3997	-0.0064	-0.0785	-0.0789	-0.1939	1.77E-01
11	В	-0.3405	-0.0346	0.0127	0.0118	0.0429	-1.43E-01
12	В	-0.2120	-0.0345	0.0265	0.0255	0.0295	1.02E-02
13	В	-0.0637	-0.0368	-0.0115	-0.0120	-0.0317	1.01E-01
14	В	-0.0525	-0.0315	0.0122	0.0124	0.0611	1.38E-02
15	В	0.3760	0.0049	-0.0774	-0.0775	-0.2036	-4.65E-02
16	В	0.2782	0.0166	-0.0286	-0.0293	-0.0521	-7.12E-02
17	В	-0.1452	-0.0522	0.0146	0.0146	0.0853	6.66E-02
18	В	0.3760	0.0049	-0.0773	-0.0775	-0.2100	-4.72E-02
19	В	-0.3697	-0.0423	0.0241	0.0237	0.1290	5.67E-03
20	В	-0.0525	-0.0315	0.0122	0.0123	0.0624	1.38E-02
21	В	-0.1195	-0.0633	0.0021	0.0020	0.0202	-1.64E-02
22	В	-0.2120	-0.0345	0.0266	0.0255	0.0271	1.02E-02
23	В	0.2371	0.0271	-0.0151	-0.0157	0.0666	-1.45E-02
24	В	-0.4504	-0.0557	0.0137	0.0132	0.1038	-1.24E-02
25	В	-0.1452	-0.0522	0.0146	0.0146	0.0839	6.66E-02
26	В	-0.1452	-0.0522	0.0146	0.0146	0.0878	6.67E-02
27	В	-0.3405	-0.0346	0.0127	0.0118	0.0383	-1.43E-01
28	В	-0.4504	-0.0557	0.0138	0.0133	0.1100	-1.26E-02
29	В	-0.0525	-0.0315	0.0122	0.0124	0.0621	1.37E-02
30	В	0.3997	-0.0064	-0.0786	-0.0789	-0.1923	1.77E-01
31	В	0.3997	-0.0064	-0.0785	-0.0789	-0.2103	1.77E-01
32	В	0.3144	0.0278	-0.0474	-0.0473	-0.0938	-6.80E-02
33	В	-0.1195	-0.0633	0.0021	0.0021	0.0170	-1.59E-02
34	В	-0.2120	-0.0345	0.0266	0.0255	0.0265	1.01E-02
35	В	0.2371	0.0271	-0.0151	-0.0157	0.0715	-1.33E-02
36	В	-0.0637	-0.0368	-0.0115	-0.0120	-0.0308	1.01E-01
37	В	0.2782	0.0166	-0.0286	-0.0292	-0.0527	-7.18E-02
38	В	-0.4504	-0.0557	0.0138	0.0133	0.1110	-1.25E-02
39	В	-0.3405	-0.0346	0.0127	0.0118	0.0432	-1.43E-01
40	0	0.2170	0.4615	0.1731	0.2507	-0.2357	-4.47E-01
41	N	0.2274	0.3810	0.2853	0.2223	0.3625	4.77E-01
	F1(B39)	-0.4444	-0.8425	-0.4577	-0.4722	-0.1268	0.0095
	F2(NO)	0.4444	0.8425	0.4585	0.4730	0.1268	0.0297
	iotal	0.0000	0.0000	0.0008	0.0008	0.0000	0.0392

N+O calibration curve constraction:

Charg	ges on NO	O 1s orbital energies	N 1s orbital energies
	-2	-18.92336	-14.07920
	-1	-19.10629	-14.26065
	0	-19.34540	-14.51986
	1	-19.66771	-14.86562
	2	-20.02529	-15.28306



 $Q_{predicted}^{0} = 0.212$

 Orbital energies in NO@B39 complex

 O 1s
 -19.41203

 N 1s
 -14.60064





CN@B39	[0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.1781	0.0118	-0.0759	-0.0759	-0.2013	5.43E-02
2	В	-0.0573	-0.0242	-0.0040	-0.0060	-0.0488	1.36E-01
3	В	-0.1132	-0.0454	0.0179	0.0171	0.0651	1.35E-03
4	В	0.1468	0.0352	-0.0042	-0.0064	0.0868	-1.09E-02
5	В	-0.1237	-0.0107	0.0500	0.0481	0.1745	5.01E-02
6	В	0.1781	0.0118	-0.0758	-0.0758	-0.2024	5.43E-02
7	В	0.3409	0.0312	-0.0530	-0.0536	-0.1959	-5.40E-02
8	В	0.0740	0.0178	-0.0346	-0.0368	-0.1080	-1.50E-02
9	В	-0.1237	-0.0107	0.0500	0.0482	0.1692	5.00E-02
10	В	0.2959	0.0118	-0.0697	-0.0710	-0.2394	2.20E-01
11	В	-0.1545	-0.0012	0.0596	0.0565	0.2121	-1.61E-01
12	В	-0.0125	-0.0242	0.0461	0.0423	0.1219	3.21E-02
13	В	-0.0573	-0.0242	-0.0039	-0.0060	-0.0491	1.36E-01
14	В	-0.0316	-0.0195	0.0354	0.0354	0.1411	-2.23E-02
15	В	0.3409	0.0312	-0.0531	-0.0536	-0.1897	-5.44E-02
16	В	0.0740	0.0178	-0.0346	-0.0368	-0.1133	-1.85E-02
17	В	-0.1433	-0.0178	0.0410	0.0406	0.1421	7.12E-02
18	В	0.3409	0.0312	-0.0530	-0.0536	-0.1887	-5.22E-02
19	В	-0.1237	-0.0107	0.0500	0.0482	0.1711	5.00E-02
20	В	-0.0316	-0.0195	0.0355	0.0355	0.1411	-2.21E-02
21	В	-0.1132	-0.0454	0.0179	0.0171	0.0594	1.38E-03
22	В	-0.0125	-0.0242	0.0461	0.0423	0.1216	3.19E-02
23	В	0.1468	0.0352	-0.0043	-0.0064	0.0865	-1.10E-02
24	В	-0.1354	-0.0188	0.0508	0.0488	0.2100	1.44E-02
25	В	-0.1433	-0.0178	0.0410	0.0406	0.1455	7.11E-02
26	В	-0.1433	-0.0178	0.0409	0.0406	0.1432	7.10E-02
27	В	-0.1545	-0.0012	0.0596	0.0565	0.2123	-1.61E-01
28	В	-0.1354	-0.0188	0.0508	0.0488	0.2030	1.43E-02
29	В	-0.0316	-0.0195	0.0354	0.0354	0.1399	-2.24E-02
30	В	0.2959	0.0118	-0.0697	-0.0710	-0.2319	2.19E-01
31	В	0.2959	0.0118	-0.0697	-0.0710	-0.2315	2.20E-01
32	В	0.1781	0.0118	-0.0759	-0.0759	-0.2018	5.35E-02
33	В	-0.1132	-0.0454	0.0178	0.0170	0.0609	1.24E-03
34	В	-0.0125	-0.0242	0.0461	0.0423	0.1188	3.21E-02
35	В	0.1468	0.0352	-0.0043	-0.0065	0.0895	-8.44E-03
36	В	-0.0573	-0.0242	-0.0040	-0.0060	-0.0547	1.36E-01
3/	В	0.0740	0.0178	-0.0346	-0.0367	-0.1058	-1.93E-02
38	В	-0.1354	-0.0188	0.0508	0.0488	0.2112	1.44E-U2
39	B C	-0.1545	-0.0012	0.0597	0.0566	0.2058	-1.01E-01
40		-0.8426	-0.0595	-0.0455	0.1361	0.10/2	0.89E-UI
41	IN E1(D20)	0.0500	0.2210	-0.1319	-0.2529	-1.2375	-1.392+00
	- T(D22)	0.7926	-0.1021	0.1774	0.1174	1.0703	0.9427
	Total	-0.7920	0.1021	0.1774	-0.1108	-1.0703	-0.8992
	iotai	0.0000	0.0000	0.0006	0.0008	0.0000	0.0450

N+C calibration curve constraction:

Charges on CN	N 1s orbital energies	C 1s orbital energies
-2	-14.14861	-10.02157
-1	-14.26022	-10.11569
0	-14.44832	-10.34491
1	-14.72820	-10.63958
2	-15.05867	-10.99190



 $Q_{predicted}^{N} = -0.763$

 Orbital energies in CN@B39 complex

 N 1s
 -14.30035

 C 1s
 -10.16208





FO@B39 [0,1]		Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.2678	0.0281	-0.0473	-0.0488	-0.1054	-2.06E-02
2	В	-0.0174	-0.0191	0.0042	0.0031	0.0089	1.14E-01
3	В	-0.0884	-0.0413	0.0108	0.0087	0.0198	-2.14E-02
4	В	0.1817	0.0293	-0.0120	-0.0128	0.0719	1.79E-02
5	В	-0.2005	-0.0192	0.0398	0.0381	0.1448	5.47E-02
6	В	0.2951	0.0559	-0.0158	-0.0172	-0.0155	-1.44E-01
7	В	0.2288	0.0089	-0.0763	-0.0771	-0.2363	-3.56E-02
8	В	0.1909	0.0155	-0.0303	-0.0311	-0.0722	-3.17E-02
9	В	-0.2087	-0.0188	0.0416	0.0399	0.1588	2.42E-02
10	В	0.2101	0.0182	-0.0509	-0.0518	-0.1651	1.74E-01
11	В	-0.1984	-0.0199	0.0301	0.0287	0.1038	-9.59E-02
12	В	-0.0984	-0.0289	0.0355	0.0340	0.0581	1.73E-02
13	В	-0.0349	-0.0182	0.0040	0.0029	-0.0021	1.11E-01
14	В	-0.0221	-0.0208	0.0339	0.0314	0.1534	-1.63E-02
15	В	0.2471	0.0132	-0.0709	-0.0718	-0.2269	-3.14E-02
16	В	0.1917	0.0119	-0.0345	-0.0354	-0.0749	-3.25E-02
17	В	-0.1304	-0.0364	0.0211	0.0187	0.1083	8.06E-02
18	В	0.2349	0.0124	-0.0682	-0.0691	-0.2176	-4.51E-02
19	В	-0.1972	-0.0140	0.0366	0.0348	0.1343	1.96E-02
20	В	-0.0539	-0.0321	0.0010	-0.0014	-0.0289	4.49E-02
21	В	-0.0930	-0.0356	0.0169	0.0148	0.0058	7.76E-03
22	В	-0.0995	-0.0287	0.0356	0.0341	0.0560	2.06E-02
23	В	0.1949	0.0306	-0.0123	-0.0132	0.0673	1.87E-02
24	В	-0.2336	-0.0203	0.0438	0.0419	0.1828	8.03E-03
25	В	-0.1315	-0.0147	0.0398	0.0375	0.1233	6.31E-02
26	В	-0.1426	-0.0382	0.0246	0.0223	0.1154	8.36E-02
27	В	-0.1771	-0.0134	0.0397	0.0384	0.1362	-1.58E-01
28	В	-0.2189	-0.0257	0.0401	0.0382	0.1804	4.35E-02
29	В	-0.0307	-0.0099	0.0301	0.0277	0.0972	-2.43E-02
30	В	0.1688	0.0069	-0.0689	-0.0698	-0.2134	2.15E-01
31	В	0.1872	0.0096	-0.0636	-0.0645	-0.1955	1.82E-01
32	В	0.2566	-0.0019	-0.0845	-0.0859	-0.2234	3.77E-02
33	В	-0.0684	-0.0455	0.0131	0.0110	0.0566	-5.21E-03
34	В	-0.0912	-0.0272	0.0357	0.0342	0.0529	1.58E-02
35	В	0.1949	0.0370	-0.0037	-0.0046	0.0826	7.10E-03
36	В	-0.0470	-0.0148	0.0033	0.0022	-0.0058	9.67E-02
37	В	0.1918	0.0131	-0.0327	-0.0335	-0.0734	-3.46E-02
38	В	-0.2169	-0.0264	0.0340	0.0320	0.1583	1.71E-02
39	В	-0.1746	-0.0165	0.0298	0.0285	0.1118	-1.16E-01
40	F	-0.0284	0.2473	0.0715	0.1227	-0.1761	-3.01E-01
41	0	-0.2388	0.0496	-0.0444	-0.0372	-0.3561	-3.18E-01
	F1(B39)	0.2672	-0.2969	-0.0263	-0.0848	0.5322	0.6618
	F2(FO)	-0.2672	0.2969	0.0270	0.0855	-0.5322	-0.6192
	Total	0.0000	0.0000	0.0007	0.0007	0.0000	0.0426

F+O calibration curve constraction:

Charges on FO	F 1s orbital energies	O 1s orbital energies
-2	-24.42790	-18.82396
-1	-24.63991	-19.03829
0	-24.87414	-19.37617
1	-25.21402	-19.75222
2	-25.60464	-20.20892



 $Q_{predicted}^F = -0.253$

 Orbital energies in FO@B39 complex

 F 1s
 -24.81417

 O 1s
 -19.24582





CF@B39	[0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.1922	0.0246	-0.0526	-0.0554	-0.1061	-5.84E-02
2	В	-0.0395	-0.0336	-0.0109	-0.0129	-0.0239	9.94E-02
3	В	-0.0168	-0.0666	0.0044	0.0002	0.0375	-3.00E-02
4	В	0.1659	0.0272	-0.0167	-0.0181	0.0561	-9.02E-03
5	В	-0.1957	-0.0418	0.0254	0.0219	0.1366	1.89E-03
6	В	0.1922	0.0246	-0.0526	-0.0554	-0.1061	-5.68E-02
7	В	0.2673	0.0078	-0.0748	-0.0766	-0.1986	-5.26E-02
8	В	0.2112	0.0157	-0.0299	-0.0312	-0.0572	-6.80E-02
9	В	-0.1957	-0.0418	0.0253	0.0218	0.1366	1.90E-03
10	В	0.2938	-0.0044	-0.0782	-0.0800	-0.2001	1.71E-01
11	В	-0.2829	-0.0306	0.0124	0.0100	0.0448	-1.38E-01
12	В	-0.1985	-0.0345	0.0257	0.0235	0.0265	5.16E-03
13	В	-0.0395	-0.0336	-0.0109	-0.0129	-0.0239	9.92E-02
14	В	-0.0226	-0.0393	0.0097	0.0050	0.0760	1.79E-02
15	В	0.2673	0.0078	-0.0747	-0.0765	-0.1986	-5.20E-02
16	В	0.2112	0.0157	-0.0300	-0.0313	-0.0572	-6.82E-02
17	В	-0.0600	-0.0589	0.0147	0.0101	0.0901	6.52E-02
18	В	0.2673	0.0078	-0.0748	-0.0765	-0.1986	-5.31E-02
19	В	-0.1957	-0.0418	0.0255	0.0220	0.1366	1.85E-03
20	В	-0.0226	-0.0393	0.0097	0.0049	0.0760	1.78E-02
21	В	-0.0168	-0.0666	0.0045	0.0002	0.0375	-2.99E-02
22	В	-0.1985	-0.0345	0.0258	0.0235	0.0265	5.10E-03
23	В	0.1659	0.0272	-0.0167	-0.0181	0.0561	-9.48E-03
24	В	-0.3191	-0.0540	0.0135	0.0096	0.1183	-1.80E-02
25	В	-0.0600	-0.0589	0.0147	0.0101	0.0901	6.52E-02
26	В	-0.0600	-0.0589	0.0147	0.0101	0.0901	6.53E-02
27	В	-0.2829	-0.0306	0.0124	0.0100	0.0448	-1.38E-01
28	В	-0.3191	-0.0540	0.0135	0.0097	0.1183	-1.82E-02
29	В	-0.0226	-0.0393	0.0098	0.0050	0.0760	1.77E-02
30	В	0.2938	-0.0044	-0.0783	-0.0801	-0.2001	1.71E-01
31	В	0.2938	-0.0044	-0.0783	-0.0801	-0.2001	1./1E-01
32	В	0.1922	0.0246	-0.0526	-0.0554	-0.1061	-5.81E-02
33	В	-0.0168	-0.0666	0.0045	0.0002	0.0375	-2.98E-02
34	В	-0.1985	-0.0345	0.0258	0.0236	0.0265	4.96E-03
35	В	0.1659	0.0272	-0.0166	-0.0180	0.0561	-9.24E-03
36	В	-0.0395	-0.0336	-0.0108	-0.0129	-0.0239	9.93E-02
3/	В	0.2112	0.0157	-0.0299	-0.0312	-0.05/2	-6.79E-02
38	В	-0.3191	-0.0540	0.0135	0.0097	0.1183	-1.80E-02
39	B C	-0.2829	-0.0306	0.0123	0.0099	0.0448	-1.38E-01
40		-0.1074	0.3372	0.3282	0.4286	0.5243	8.29E-U1
41	F E1(P20)	0.1210	0.5281	0.1439	0.1534	-0.3235	-7.45E-UI
	E3(CE)	-0.0135	-0.0053	-0.4717	-0.3610	-0.0008	-0.0411
	Total	0.0133	0.8055	0.4721	0.3820	0.0008	0.0802
	iotai	0.0000	0.0000	0.0005	0.0005	0.0000	0.0451

F+C calibration curve constraction:

Charges on CF	F 1s orbital energies	C 1s orbital energies
-2	-24.60253	-10.03886
-1	-24.72069	-10.16461
0	-24.87854	-10.37149
1	-25.12975	-10.71409
2	-25.41892	-11.12917



 $Q_{predicted}^F = 0.176$

 Orbital energies in CF@B39 complex

 F 1s
 -24.92486

 C 1s
 -10.45571



 $Q_{predicted}^{c} = 0.257$

Cu@B39	[0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.2796	0.0151	-0.0758	-0.0802	-0.1689	-1.41E-02
2	В	-0.0214	-0.0243	-0.0119	-0.0215	-0.0456	7.33E-02
3	В	-0.0726	-0.0381	0.0071	-0.0052	0.0223	-6.73E-02
4	В	0.1881	0.0382	-0.0154	-0.0203	0.0685	-2.24E-02
5	В	-0.3339	-0.0233	0.0302	0.0153	0.0875	-2.13E-02
6	В	0.2811	0.0151	-0.0758	-0.0802	-0.1699	-1.19E-02
7	В	0.3700	0.0250	-0.0700	-0.0763	-0.1806	-5.61E-02
8	В	0.2836	0.0263	-0.0292	-0.0330	-0.0550	-7.41E-02
9	В	-0.3298	-0.0232	0.0302	0.0153	0.0890	-2.12E-02
10	В	0.2451	0.0132	-0.0710	-0.0791	-0.1887	1.48E-01
11	В	-0.2477	-0.0190	0.0123	0.0019	0.0180	-1.68E-01
12	В	-0.1839	-0.0183	0.0267	0.0211	0.0127	-7.99E-03
13	В	-0.0184	-0.0243	-0.0118	-0.0215	-0.0462	7.32E-02
14	В	-0.0647	-0.0229	0.0097	0.0037	0.0640	-2.53E-02
15	В	0.3714	0.0250	-0.0700	-0.0763	-0.1740	-5.75E-02
16	В	0.2834	0.0264	-0.0292	-0.0330	-0.0504	-7.41E-02
17	В	-0.1700	-0.0358	0.0085	-0.0016	0.0462	5.49E-02
18	В	0.3688	0.0250	-0.0699	-0.0762	-0.1742	-5.83E-02
19	В	-0.3299	-0.0232	0.0303	0.0154	0.0910	-2.13E-02
20	В	-0.0658	-0.0229	0.0098	0.0037	0.0638	-2.51E-02
21	В	-0.0724	-0.0381	0.0071	-0.0052	0.0178	-6.72E-02
22	В	-0.1875	-0.0183	0.0266	0.0211	0.0142	-8.13E-03
23	В	0.1907	0.0382	-0.0154	-0.0204	0.0665	-2.08E-02
24	В	-0.3355	-0.0385	0.0166	0.0002	0.0588	-4.53E-02
25	В	-0.1766	-0.0358	0.0084	-0.0017	0.0496	5.48E-02
26	В	-0.1731	-0.0358	0.0084	-0.0016	0.0474	5.49E-02
27	В	-0.2490	-0.0190	0.0123	0.0019	0.0219	-1.68E-01
28	В	-0.3347	-0.0385	0.0166	0.0003	0.0530	-4.51E-02
29	В	-0.0658	-0.0229	0.0096	0.0036	0.0627	-2.54E-02
30	В	0.2425	0.0132	-0.0710	-0.0791	-0.1811	1.49E-01
31	В	0.2480	0.0132	-0.0710	-0.0791	-0.1724	1.49E-01
32	В	0.2816	0.0152	-0.0759	-0.0802	-0.1695	-1.58E-02
33	В	-0.0734	-0.0381	0.0070	-0.0052	0.0183	-6.72E-02
34	В	-0.1874	-0.0183	0.0267	0.0211	0.0146	-8.00E-03
35	В	0.1909	0.0383	-0.0154	-0.0204	0.0668	-2.12E-02
36	В	-0.0206	-0.0243	-0.0119	-0.0215	-0.0494	7.34E-02
37	В	0.2853	0.0263	-0.0292	-0.0330	-0.0534	-7.35E-02
38	В	-0.3362	-0.0385	0.0166	0.0002	0.0573	-4.55E-02
39	В	-0.2469	-0.0190	0.0124	0.0019	0.0136	-1.68E-01
40	Cu	0.1872	0.3064	0.4871	0.8255	0.7541	7.19E-01
	F1(B39)	-0.1872	-0.3064	-0.4869	-0.8253	-0.7541	-0.6760
	F2(Cu)	0.1872	0.3064	0.4871	0.8255	0.7541	0.7191
1	Total	0.0000	0.0000	0.0001	0.0001	0.0000	0.0431

Cu calibration curve constraction:

 Charges on Cu
 Cu 1s orbital energies
 Cu 2s orb

 -2
 -323.17838
 -38

 -1
 -323.2079
 -38

 0
 -323.30118
 -39

 1
 -323.4751
 -39

 2
 -323.40751
 -39





nergies in Cu@B39 comple:
-323.36111
-38.94670
-4.37551



 $Q_{predicted} = 0.416$



 $Q_{predicted} = 0.398$





Atom Number Element Charge density Charge density <thcharge density<="" th=""> Charge density<th>Ag@B39</th><th>[0,1]</th><th>Mulliken Scheme</th><th>Lowdin Scheme</th><th>Hirshfeld Scheme</th><th>CM5 Scheme</th><th>NPA Scheme</th><th>Bader Scheme</th></thcharge>	Ag@B39	[0,1]	Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
1 8 0.3475 0.0105 -0.0769 -0.0831 -0.1713 8.116-03 2 8 -0.0589 -0.0366 -0.0124 -0.0260 -0.0442 7.586-02 3 8 -0.1483 -0.0487 0.0066 -0.0123 0.0644 -2.10F-02 5 8 -0.3339 -0.0358 0.0298 0.0087 0.0833 -1.372-0.0644 6 8 0.4576 0.0193 -0.0796 -0.132 -6.04600 7 8 0.4576 0.0193 -0.0796 -0.0235 -0.0184 -0.0003 7.00F02 9 8 -0.2351 0.0224 -0.0295 -0.0484 -0.0036 -1.87F02 10 8 -0.1437 -0.0245 0.0263 0.0184 0.0147 -7.58F03 11 8 -0.1539 -0.0246 0.00261 -0.0433 -7.0F02 13 8 -0.0756 -0.0224 0.0294 -0.0348 -0.0556 -7.06F02	Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
2 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0442 7.58F-02 3 B -0.1438 -0.0447 -0.0666 -0.0108 0.0210 -6.51F-02 4 B -0.1339 -0.0336 -0.0152 -0.0223 0.0644 -2.10F-02 5 B -0.3339 -0.0388 0.0298 0.0087 0.0633 -1.87F-02 6 B 0.4375 0.0103 -0.0769 -0.0380 -0.1522 -6.64F-03 7 B 0.4576 0.0025 -0.0348 -0.0503 -7.06F-02 9 B -0.3345 0.0027 -0.0797 -0.687-1 -0.120 -0.0227 0.0197 -1.68E-01 11 B -0.2345 -0.0224 -0.0207 -0.0147 -7.58E-03 13 B -0.0759 -0.0244 -0.0206 -0.0435 -7.57E-03 14 B -0.2766 -0.0244 -0.0797 -0.1748 -4.79E-02	1	В	0.3475	0.0105	-0.0769	-0.0831	-0.1713	-8.11E-03
3 8 -0.1483 -0.0487 0.0066 -0.0123 0.0644 -2.10E-02 5 B -0.3339 -0.0358 0.0228 0.0087 0.0833 -1.87E-02 6 B 0.3475 0.0105 -0.0796 -0.0833 -0.1732 -6.04E-03 7 B 0.4576 0.0193 -0.0796 -0.0323 -0.0122 -6.04E-03 7 B 0.4576 0.0193 -0.0796 -0.0323 -7.00E-02 9 B -0.3339 -0.0358 0.0295 -0.0348 -0.0503 -7.00E-02 10 B 0.3345 -0.027 -0.0171 -0.0833 -0.1331 1.59E-01 11 B -0.2365 -0.0274 0.0206 -0.0435 7.57E-02 14 B -0.0756 -0.0294 0.0091 0.0005 -0.651 -2.51E-02 15 B 0.4576 0.0193 -0.0707 -0.1748 -4.79E-02 16 B	2	В	-0.0539	-0.0336	-0.0124	-0.0260	-0.0442	7.58E-02
4 8 0.1399 0.0336 -0.0152 -0.023 0.0644 -2.10F-02 5 B -0.3339 -0.0358 0.0298 0.0083 -1.87F-02 6 B 0.3475 0.0105 -0.0769 -0.0830 -0.1732 -6.64E-03 7 B 0.4576 0.0193 -0.0769 -0.0348 -0.0503 -7.00F-02 9 B -0.3339 -0.0358 0.0299 0.0087 0.0968 -1.87F-02 10 B 0.3345 0.0057 -0.0120 -0.0027 0.0197 -1.68E-01 11 B -0.2356 -0.0247 0.0120 -0.0027 -0.1437 -5.58E-03 13 B -0.0599 -0.0345 -0.0124 -0.0207 -0.1748 -4.79E-02 14 B 0.0576 -0.0244 -0.0348 -0.0556 -7.00E-02 15 B 0.4576 0.0193 -0.0707 -0.0796 -0.1756 -4.86E-02 <t< td=""><td>3</td><td>В</td><td>-0.1483</td><td>-0.0487</td><td>0.0066</td><td>-0.0108</td><td>0.0210</td><td>-6.51E-02</td></t<>	3	В	-0.1483	-0.0487	0.0066	-0.0108	0.0210	-6.51E-02
5 8 -0.3339 -0.0358 0.0298 0.0079 -0.0830 -0.1732 -6.04-03 6 8 0.4576 0.0193 -0.0769 -0.0830 -0.1732 -6.04-03 7 8 0.4576 0.0193 -0.0796 -0.0796 -0.1823 -4.61E-02 8 8 0.2331 -0.0224 -0.0295 -0.0383 -0.1831 1.59F-01 10 8 0.3345 0.0057 -0.0719 -0.0833 -0.1831 1.59F-01 11 8 -0.2365 -0.0287 0.0120 -0.0027 0.0147 -7.58F-03 13 8 -0.0559 -0.0294 0.0091 0.0005 0.0661 -2.51E-02 15 8 0.4576 0.0193 -0.0776 -0.0748 -0.7278 -0.0749 -0.0748 -0.0749 -0.0748 -0.056 -7.00E-02 17 8 0.2376 -0.0449 0.0006 0.0661 -2.51E-02 15 8 0.4576	4	В	0.1399	0.0336	-0.0152	-0.0223	0.0644	-2.10E-02
6 8 0.3475 0.0105 -0.0796 -0.0300 -0.1732 -6.04E-33 7 8 0.4375 0.0193 -0.0706 -0.0348 -0.0503 -7.06E-02 9 8 -0.3339 -0.0358 0.0229 0.0087 -0.0668 -1.877-02 10 8 0.3339 -0.0287 -0.0120 -0.0027 0.0197 -1.68E-01 11 8 -0.2365 -0.0287 0.0120 -0.027 0.0197 -1.68E-01 12 8 -0.1437 -0.0245 0.0124 -0.0260 -0.0435 7.57E-02 14 8 -0.0756 -0.0294 0.0091 0.0005 0.0651 -2.51E-02 15 8 0.4576 0.0124 -0.0246 -0.0448 -7.06E-02 16 8 0.2376 -0.0449 0.0080 -0.0663 0.0481 5.58E-02 17 B -0.1756 -0.0294 0.0091 0.0006 0.648 -2.50E-02 <td>5</td> <td>В</td> <td>-0.3339</td> <td>-0.0358</td> <td>0.0298</td> <td>0.0087</td> <td>0.0833</td> <td>-1.87E-02</td>	5	В	-0.3339	-0.0358	0.0298	0.0087	0.0833	-1.87E-02
7 8 0.4576 0.0193 -0.0708 -0.0346 -0.0506 -1.823 -4.616-02 8 8 0.2331 -0.0358 0.0299 -0.0348 -0.0508 -1.876-02 10 8 0.3345 0.0057 -0.0719 -0.0833 -0.1881 1.596-01 11 8 -0.2365 -0.0287 0.0120 -0.0027 0.0197 -1.68E-01 12 8 -0.0137 -0.0245 0.0260 -0.0435 7.57E-02 14 8 -0.0756 -0.0294 0.0091 0.0005 0.6651 -2.51E-02 15 8 0.4576 0.0193 -0.0708 -0.0063 0.0481 5.58E-02 16 8 0.4576 0.0193 -0.0707 -0.0448 -0.0563 -0.0481 -0.88 -0.856 -7.00E-02 17 8 -0.2376 -0.0449 0.0080 -0.0663 0.0481 5.58E-02 19 8 -0.1375 -0.0294 <t< td=""><td>6</td><td>В</td><td>0.3475</td><td>0.0105</td><td>-0.0769</td><td>-0.0830</td><td>-0.1732</td><td>-6.04E-03</td></t<>	6	В	0.3475	0.0105	-0.0769	-0.0830	-0.1732	-6.04E-03
8 6 0.2531 0.0224 -0.0225 -0.0348 -0.0503 -7.00E.02 9 8 -0.3345 0.0057 -0.0719 -0.0833 -0.1831 1.187E.02 10 8 -0.3345 0.0057 -0.0719 -0.0833 -0.1831 1.187E.02 11 8 -0.0236 -0.0263 0.0104 -0.0477 -7.58E.03 13 8 -0.0539 -0.0336 -0.0124 -0.0260 -0.0435 7.57E.02 14 8 -0.0756 -0.0294 0.0091 -0.0005 0.0651 -2.51E.02 15 8 0.4576 0.0193 -0.0708 -0.0797 -0.1748 -4.79E.02 16 8 0.2531 0.0224 -0.0290 0.0063 0.0481 5.58E.02 19 8 -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E.02 20 8 -0.1483 -0.0487 0.0262 0.0183 0.0151 -7.74E.03	7	В	0.4576	0.0193	-0.0708	-0.0796	-0.1823	-4.61E-02
9 8 -0.3339 -0.0358 0.0229 0.0087 0.0968 -1.87E-02 10 8 0.3345 0.0057 -0.0171 -0.0083 -0.1831 1.59E-01 11 8 -0.2365 -0.0287 0.0126 -0.0027 0.0197 -1.68E-01 12 8 -0.0756 -0.0294 0.0263 -0.0134 -0.0447 -7.58E-03 14 8 -0.0756 -0.0294 -0.0977 -0.1748 -4.79E-02 16 8 0.2531 0.0224 -0.0294 -0.0348 -0.0556 -7.00E-02 17 8 -0.2376 -0.0494 -0.0080 -0.0088 0.0481 5.58E-02 18 8 -0.4576 0.0193 -0.0707 -0.0796 -1.756 -4.86E-02 20 8 -0.1483 -0.0294 0.0088 0.0896 -1.85E-02 21 8 -0.1483 -0.0245 0.0262 0.0183 0.0151 -7.74E-03	8	В	0.2531	0.0224	-0.0295	-0.0348	-0.0503	-7.00E-02
10 B 0.3345 0.0057 -0.0719 -0.0833 -0.1831 1.59E-10 11 B -0.2365 -0.0285 0.0120 -0.0027 0.0197 -1.68E-01 12 B -0.1437 -0.0245 0.0265 -0.0435 -7.57E-02 14 B -0.0756 -0.0294 -0.0091 -0.0005 0.0651 -2.51E-02 15 B 0.4576 -0.0193 -0.0797 -0.1748 -4.79E-02 16 B 0.2531 0.0224 -0.0294 -0.0348 -0.0556 -7.00E-02 17 B -0.2376 -0.0449 0.0080 -0.0663 0.0481 5.58E-02 18 B -0.4576 0.0193 -0.0796 -0.1756 -4.86E-02 19 B -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E-02 20 B -0.1437 -0.0244 0.0066 -0.0108 0.0257 -5.0E-02 21 <t< td=""><td>9</td><td>В</td><td>-0.3339</td><td>-0.0358</td><td>0.0299</td><td>0.0087</td><td>0.0968</td><td>-1.87E-02</td></t<>	9	В	-0.3339	-0.0358	0.0299	0.0087	0.0968	-1.87E-02
11 B -0.2365 -0.0287 0.0120 -0.0027 0.0137 -1.68E-01 12 B -0.1437 -0.0245 0.0263 0.0184 0.0147 -7.58E-03 13 B -0.0539 -0.0326 -0.0124 -0.0260 -0.0435 7.57E-02 14 B -0.0756 -0.0294 -0.0348 -0.0756 -7.00E-02 15 B 0.4576 0.0193 -0.0708 -0.0797 -0.1748 -4.79E-02 16 B 0.23376 -0.0449 0.0080 -0.0348 -0.0556 -7.00E-02 17 B -0.3339 -0.0797 -0.1756 -4.86E-02 18 B -0.4576 -0.0994 0.0091 0.0066 0.0648 -2.50E-02 19 B -0.3339 -0.0244 0.0075 -0.0108 0.0257 -6.50E-02 21 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 22	10	В	0.3345	0.0057	-0.0719	-0.0833	-0.1831	1.59E-01
12 B -0.1437 -0.0245 0.0263 0.0184 0.0147 -7.58E-33 13 B -0.0539 -0.0336 -0.0260 -0.0435 7.57E-02 14 B -0.0756 -0.0294 0.0091 0.0005 0.0651 -2.51E-02 15 B 0.4576 0.0193 -0.0708 -0.0797 -0.1748 -4.79E-02 16 B 0.2376 -0.0449 0.0080 -0.063 0.0481 5.58E-02 18 B 0.4576 0.0193 -0.0707 -0.0796 -0.1756 +4.86E-02 19 B -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E-02 20 B -0.0756 -0.0294 0.0091 0.0006 0.0648 -2.50E-02 21 B -0.1483 -0.0449 0.0079 -0.0223 0.0641 -1.98E-02 23 B -0.2376 -0.0449 0.0079 -0.0064 0.0594 -5.59E-02 <	11	В	-0.2365	-0.0287	0.0120	-0.0027	0.0197	-1.68E-01
13 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0435 7.57-02 14 B -0.0756 -0.0294 0.0091 0.0005 0.0651 -2.51E-02 15 B 0.4576 0.0193 -0.0797 -0.1748 -4.79E-02 16 B 0.2376 -0.0449 0.0080 -0.0633 0.0481 5.58E-02 17 B -0.3339 -0.0358 0.0299 0.0088 0.0481 5.58E-02 19 B -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E-02 20 B -0.0756 -0.0294 0.0091 0.0006 0.0648 -2.50E-02 21 B -0.1437 -0.0244 0.0062 0.0183 0.0151 -7.74E-03 23 B -0.1379 -0.0449 0.0079 -0.0664 4.27E-02 24 B -0.3504 -0.0523 0.0163 -0.0427 0.0164 -5.5E-02 26	12	В	-0.1437	-0.0245	0.0263	0.0184	0.0147	-7.58E-03
14 B -0.0756 -0.0294 0.0091 0.0005 0.0651 -2.51F-02 15 B 0.4576 0.0193 -0.0708 -0.0797 -0.1748 -4.79E-02 16 B 0.23376 -0.0449 0.0080 -0.0348 -0.0556 -7.00E-02 17 B -0.3339 -0.0358 0.0299 -0.0796 -1.756 -4.86E-02 19 B -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E-02 20 B -0.0756 -0.0294 0.0091 0.0006 0.0648 -2.50E-02 21 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.2376 -0.0449 0.0079 -0.0664 0.554 -5.5Fe-02 25 B -0.2376 -0.0244 0.00057 0.0067 0.0521	13	В	-0.0539	-0.0336	-0.0124	-0.0260	-0.0435	7.57E-02
15 B 0.4376 0.0193 -0.0708 -0.0797 -0.1748 -4.79E-02 16 B 0.2331 0.0224 -0.0294 -0.0348 -0.0556 -7.00E-02 17 B 0.2376 -0.0449 0.0080 -0.0763 0.0481 5.58E-02 18 B 0.4576 0.0193 -0.0707 -0.0796 -0.1756 -4.86E-02 19 B -0.3339 -0.0358 0.0299 0.0086 0.0896 -1.85E-02 20 B -0.1433 -0.0487 0.0066 -0.0108 0.0257 -6.50E-02 21 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.2376 -0.0449 0.0079 -0.0064 0.554 -4.27E-02 25 B -0.2365 -0.027 0.0188 -1.68E-01 -6.8E-01	14	В	-0.0756	-0.0294	0.0091	0.0005	0.0651	-2.51E-02
16 B 0.0231 0.0224 -0.0244 -0.0348 -0.0556 -7.00-10 17 B -0.2376 -0.0449 0.0080 -0.0663 0.0481 5.58-02 18 B -0.4576 0.0193 -0.0707 -0.0796 -0.1756 -4.86E-02 19 B -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E-02 20 B -0.1483 -0.0244 0.0066 -0.0108 0.0257 -6.50E-02 21 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 23 B 0.1399 0.036 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.2376 -0.0449 0.0079 -0.0663 0.0490 5.57E-02 25 B -0.2365 -0.0287 0.0120 -0.027 0.0188 -1.68E-01 28 B -0.3504 -0.0523 0.0164 -0.0667 0.0521 <	15	В	0.4576	0.0193	-0.0708	-0.0797	-0.1748	-4.79E-02
17 B -0.2376 -0.0449 0.0083 -0.0063 0.0481 5.58F-02 18 B 0.4576 0.0193 -0.0707 -0.0796 -0.1756 -4.86E-02 19 B -0.3339 -0.0358 0.0299 0.0088 0.0896 -1.85E-02 20 B -0.0756 -0.0294 0.0091 0.0006 0.0648 -2.50E-02 21 B -0.1483 -0.0487 0.0066 -0.0108 0.0257 -6.50E-02 21 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.2376 -0.0449 0.0079 -0.0663 0.0490 5.57E-02 25 B -0.2376 -0.0247 0.01027 0.0188 -1.68E-01 28 B -0.3504 -0.0523 0.0164 -0.0667 0.0524 -0.0294 </td <td>16</td> <td>В</td> <td>0.2531</td> <td>0.0224</td> <td>-0.0294</td> <td>-0.0348</td> <td>-0.0556</td> <td>-7.00E-02</td>	16	В	0.2531	0.0224	-0.0294	-0.0348	-0.0556	-7.00E-02
18 B 0.4376 0.0193 -0.0707 -0.0796 -0.1756 -4.86t-02 19 B -0.03339 -0.0358 0.0299 0.0088 0.0896 -1.85t-02 20 B -0.0756 -0.0294 0.0091 0.0006 0.6648 -2.50t-02 21 B -0.1483 -0.0487 0.0262 0.0183 0.0151 -7.74t-03 23 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74t-03 23 B -0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98t-02 24 B -0.3504 -0.0523 0.0163 -0.0067 0.0564 4.27t-02 25 B -0.2376 -0.0449 0.0079 -0.0064 0.0594 5.57t-02 26 B -0.2365 -0.0294 0.0090 0.0005 0.0640 -2.52t-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640	17	В	-0.2376	-0.0449	0.0080	-0.0063	0.0481	5.58E-02
19 B -0.333 -0.0358 0.0299 0.0088 0.0896 -1.85t-02 20 B -0.0756 -0.0294 0.0091 0.0006 0.0648 -2.50t-02 21 B -0.1483 -0.0487 0.0026 0.0183 0.0151 -7.74t-03 22 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74t-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98t-02 24 B -0.3504 -0.0523 0.0163 -0.0067 0.0564 -4.27t-02 25 B -0.2376 -0.0449 0.0079 -0.064 0.0504 5.59t-02 26 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 1.68t-01 28 B -0.3345 -0.0523 0.0164 -0.0067 0.521 -4.29t-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640	18	В	0.4576	0.0193	-0.0707	-0.0796	-0.1756	-4.86E-02
20 B -0.0756 -0.024 0.0091 0.0006 0.0488 -2.50E-02 21 B -0.1483 -0.0487 0.0066 -0.0108 0.0257 -6.50E-02 22 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.3504 -0.0523 0.0163 -0.0067 0.0564 -4.27E-02 25 B -0.2376 -0.0449 0.0079 -0.0063 0.0490 5.57E-02 26 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.0556 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.6400 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739	19	В	-0.3339	-0.0358	0.0299	0.0088	0.0896	-1.85E-02
21 B -0.1483 -0.0487 0.0066 -0.0108 0.0257 -6.50E-02 22 B -0.1437 -0.0245 0.0262 0.0183 0.0151 -7.74E-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.3504 -0.0523 0.0163 -0.0067 0.0564 -4.27E-02 25 B -0.2376 -0.0449 0.0079 -0.0063 0.0490 5.57E-02 26 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.3504 -0.0523 0.0164 -0.0067 0.0521 -4.29E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60E-01 31 B 0.34345 0.0057 -0.0719 -0.0833 -0.1739	20	В	-0.0756	-0.0294	0.0091	0.0006	0.0648	-2.50E-02
22 B -0.1437 -0.0243 0.0183 0.0131 -7.74E-03 23 B 0.1399 0.0336 -0.0153 -0.0223 0.0641 -1.98E-02 24 B -0.3504 -0.0523 0.0163 -0.0067 0.0564 -4.27E-02 25 B -0.2376 -0.0449 0.0079 -0.0064 0.0504 5.59E-02 26 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.3504 -0.0523 0.0164 -0.0667 0.0521 -4.29E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02	21	В	-0.1483	-0.0487	0.0066	-0.0108	0.0257	-6.50E-02
23 B 0.1339 0.0336 -0.0223 0.0041 -1.98E-02 24 B -0.3504 -0.0523 0.0163 -0.0067 0.0564 -4.27E-02 25 B -0.2376 -0.0449 0.0079 -0.0064 0.0504 5.59E-02 26 B -0.2376 -0.0449 0.0079 -0.0063 0.0490 5.57E-02 27 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.0556 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60E-01 31 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 <	22	В	-0.1437	-0.0245	0.0262	0.0183	0.0151	-7.74E-03
24 B -0.3504 -0.0523 0.0165 -0.0067 0.0544 -4.77-02 25 B -0.2376 -0.0449 0.0079 -0.0063 0.0490 5.57E-02 26 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.3504 -0.0523 0.0164 -0.0067 0.0521 -4.29E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0245 0.0223 0.0629 -1.95E-02 35 B 0.1399 0.0336 -0.0153 -0.0223 0.6629 -1.95E-02	23	В	0.1399	0.0336	-0.0153	-0.0223	0.0641	-1.98E-02
25 B -0.2376 -0.0449 0.0079 -0.0064 0.0504 5.59E-02 26 B -0.2376 -0.0449 0.0079 -0.0063 0.0490 5.57E-02 27 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.3504 -0.0224 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60E-01 32 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.047 0.0065 -0.108 0.0216 6.50E-02 34 B -0.1437 -0.0245 0.0262 0.0183 0.0133 -7.71E-02 35 B 0.1399 0.0336 -0.0124 -0.0260 -0.0487 <t< td=""><td>24</td><td>В</td><td>-0.3504</td><td>-0.0523</td><td>0.0163</td><td>-0.0067</td><td>0.0564</td><td>-4.27E-02</td></t<>	24	В	-0.3504	-0.0523	0.0163	-0.0067	0.0564	-4.27E-02
26 B -0.2376 -0.0439 0.0079 -0.0063 0.0490 5.57E-02 27 B -0.2365 -0.0287 0.0120 -0.0027 0.0188 -1.68E-01 28 B -0.3504 -0.0523 0.0164 -0.0067 0.0521 -4.29E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0247 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 36 B -0.0539 -0.0287 0.0121 -0.0260 -0.0487	25	В	-0.2376	-0.0449	0.0079	-0.0064	0.0504	5.59E-02
27 B -0.2365 -0.027 0.0120 -0.0027 0.0188 -1.168-01 28 B -0.3504 -0.0523 0.0164 -0.0067 0.0521 -4.29E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60E-01 32 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0245 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 36 B -0.2531 0.0224 -0.0294 -0.0348 -0.0490	20	В	-0.2376	-0.0449	0.0079	-0.0063	0.0490	5.57E-02
28 B -0.3504 -0.0523 0.0164 -0.0067 0.0221 -4.29E-02 29 B -0.0756 -0.0294 0.0090 0.0005 0.0640 -2.52E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60E-01 32 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0245 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0153 -0.0223 0.0629 -1.95E-02 36 B -0.0539 -0.0346 -0.0487 7.57E-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 <	27	В	-0.2365	-0.0287	0.0120	-0.0027	0.0188	-1.08E-01
25 B -0.0756 -0.0234 0.0005 0.0005 0.0040 -2.32E-02 30 B 0.3345 0.0057 -0.0719 -0.0833 -0.1762 1.60E-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60E-01 32 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0245 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0153 -0.0223 0.0629 -1.95E-02 36 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 38 B -0.3504 -0.0523 0.0164 -0.0607 0.0586	20	D	-0.5504	-0.0323	0.0104	-0.0007	0.0521	-4.29E-02
30 B 0.3343 0.0037 -0.0719 -0.0833 -0.1702 1.00c-01 31 B 0.3345 0.0057 -0.0719 -0.0833 -0.1739 1.60c-01 32 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0245 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0124 -0.0223 0.0629 -1.95E-02 36 B -0.0539 -0.0346 -0.0244 -0.0244 -0.0240 -0.0487 7.57E-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 38 B -0.3504 -0.0523 0.0164 -0.0667 0.0586 -4.27E-02 39 B -0.2365 -0.0287 0.0121 -0.0027	29	D	-0.0736	-0.0294	0.0090	0.0003	0.0040	-2.52E-02
31 B 0.3343 0.0007 -0.0833 -0.1735 -1.001-31 32 B 0.3475 0.0105 -0.0769 -0.0831 -0.1719 -9.58E-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1437 -0.0245 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 36 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 38 B -0.3504 -0.0523 0.0164 -0.0667 0.0586 -4.27E-02 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 -0.7376 -0.5444	21	D	0.3345	0.0057	-0.0719	-0.0855	-0.1782	1.60E-01
32 B 0.3473 0.0103 -0.0831 -0.1175 -9.361-03 33 B -0.1483 -0.0487 0.0065 -0.0108 0.0216 -6.50E-02 34 B -0.1483 -0.0245 0.0262 0.0183 0.0133 -7.71E-03 35 B 0.1399 0.0336 -0.0153 -0.0223 0.0629 -1.95E-02 36 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 38 B -0.3504 -0.0523 0.0164 -0.0067 0.0586 -4.27E-02 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861	22	D	0.3345	0.0037	-0.0719	-0.0833	-0.1739	0.595.02
33 B 0.1403 0.0403 0.0003 0.0103 0.0103 0.0103 0.0103 0.0103 0.0103 0.0103 0.0110 0.0004 0.0103 0.0113 0.0103 0.771E03 35 B 0.1339 0.0336 -0.0123 0.0223 0.0629 -1.95E02 36 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0487 7.57E02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E02 38 B -0.3504 -0.0523 0.0164 -0.0067 0.0586 -4.27E02 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E01 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861 Total 0.0000 0.0001 0.0001 0.0000 0.0418	32	B	-0 1/83	-0.0103	-0.0703	-0.0831	-0.1719	-5.582-03
34 B 0.1437 0.0243 0.0252 0.0233 0.0213 0.0133 0.0223 0.0629 -1.95E-02 36 B -0.0539 -0.0336 -0.0153 -0.0223 0.0629 -1.95E-02 36 B -0.0539 -0.0336 -0.0124 -0.0260 -0.0487 7.57E-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 38 B -0.3504 -0.0523 0.0164 -0.0067 0.0586 -4.27E-02 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 F1(B39) -0.1418 -0.6196 -0.5058 -0.9843 -0.7376 0.5861 Total 0.0000 0.0001 0.0001 0.0001 0.0001 0.0001	34	B	-0.1485	-0.0487	0.0005	0.0103	0.0210	-0.30E-02
35 B 0.0539 0.0336 0.0124 0.0260 0.0425 7.576-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0497 7.576-02 37 B 0.2531 0.0224 -0.0294 -0.0348 -0.0490 -6.95E-02 38 B -0.3504 -0.0523 0.0164 -0.0067 0.0586 -4.27E-02 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5844 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5844 Total 0.0000 0.0001 0.0001 0.0000 0.0418	35	B	0.1457	0.0245	-0.0202	-0.0223	0.0133	-1.95E-02
37 B 0.0535 0.0224 0.0294 0.02348 -0.0490 -6.956-02 38 B -0.3504 -0.0523 0.0164 -0.0667 0.0586 -4.27E-02 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 40 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5444 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5844 Total 0.0000 0.0001 0.0001 0.0001 0.0001 0.0001	36	B	-0.0539	-0.0336	-0.0124	-0.0260	-0.0487	7 57E-02
38 B -0.3504 -0.0217 0.0217 -0.0067 0.0506 -0.30160 39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 F1(B39) -0.1418 -0.6196 -0.5058 -0.9843 -0.7376 -0.5444 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861 Total 0.0000 0.0001 0.0001 0.0000 0.0418	37	B	0.0535	0.0330	-0.0124	-0.0200	-0.0490	-6 95F-02
39 B -0.2365 -0.0287 0.0121 -0.0027 0.0164 -1.68E-01 40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 F1(B39) -0.1418 -0.6196 -0.5058 -0.9843 -0.7376 -0.5444 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861 Total 0.0000 0.0001 0.0001 0.0001 0.0001 0.0001	38	B	-0 3504	-0.0523	0.0164	-0.0067	0.0586	-4 27F-02
40 Ag 0.1418 0.6196 0.5059 0.9843 0.7376 5.86E-01 F1(B39) -0.1418 -0.6196 -0.5058 -0.9843 -0.7376 -0.5444 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861 Total 0.0000 0.0001 0.0001 0.0001 0.0001 0.0001	39	В	-0.2365	-0.0287	0.0121	-0.0027	0.0164	-1.68F-01
F1(B39) -0.1418 -0.6196 -0.5058 -0.9843 -0.7376 -0.5444 F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861 Total 0.0000 0.0001 0.0001 0.0001 0.0001 0.0001	40	Ag	0.1418	0.6196	0.5059	0.9843	0.7376	5.86F-01
F2(Ag) 0.1418 0.6196 0.5059 0.9843 0.7376 0.5861 Total 0.0000 0.0000 0.0001 0.0001 0.0000 0.0418		F1(B39)	-0 1418	-0 6196	-0 5055	-0 9843	-0 7376	-0 5444
Total 0.000 0.0000 0.0001 0.0001 0.0000 0.048		F2(Ag)	0.1418	0.6196	0.5059	0.9843	0.7376	0.5861
		Total	0.0000	0.0000	0.0001	0,0001	0.0000	0.0418

Ag calibration curve constraction:

Charges on Ag	Ag 4s orbital energies
-2	-3.67322
-1	-3.67644
0	-3.75852
1	-3.89155
2	-4.27212



 $Q_{predicted} = 0.443$

Orbital energies in Ag@B39 complex Ag 4s -3.81311

Au@B39 [0,1]		Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
1	В	0.3406	0.0089	-0.0811	-0.0865	-0.1838	5.42E-04
2	В	-0.0424	-0.0365	-0.0142	-0.0259	-0.0472	7.73E-02
3	В	-0.1203	-0.0514	0.0068	-0.0082	0.0212	-6.52E-02
4	В	0.1307	0.0332	-0.0168	-0.0229	0.0641	-1.81E-02
5	В	-0.3016	-0.0412	0.0301	0.0119	0.0921	-1.39E-02
6	В	0.3385	0.0089	-0.0811	-0.0864	-0.1911	2.72E-03
7	В	0.4507	0.0180	-0.0739	-0.0816	-0.1915	-3.97E-02
8	В	0.2016	0.0220	-0.0321	-0.0367	-0.0613	-6.09E-02
9	В	-0.3001	-0.0412	0.0302	0.0120	0.0987	-1.36E-02
10	В	0.3613	0.0065	-0.0718	-0.0817	-0.1843	1.57E-01
11	В	-0.1681	-0.0319	0.0115	-0.0012	0.0186	-1.63E-01
12	В	-0.0955	-0.0249	0.0250	0.0182	0.0199	-3.17E-03
13	В	-0.0391	-0.0365	-0.0141	-0.0259	-0.0465	7.72E-02
14	В	-0.0763	-0.0306	0.0074	0.0000	0.0709	-2.07E-02
15	В	0.4485	0.0180	-0.0740	-0.0816	-0.1844	-4.16E-02
16	В	0.2028	0.0220	-0.0320	-0.0366	-0.0625	-6.00E-02
17	В	-0.2170	-0.0484	0.0064	-0.0059	0.0498	5.89E-02
18	В	0.4482	0.0180	-0.0739	-0.0815	-0.1842	-4.25E-02
19	В	-0.3003	-0.0412	0.0302	0.0120	0.0878	-1.38E-02
20	В	-0.0746	-0.0306	0.0074	0.0000	0.0721	-2.04E-02
21	В	-0.1178	-0.0514	0.0068	-0.0082	0.0299	-0.52E-02
22	D	-0.0987	-0.0249	0.0250	0.0181	0.0211	-5.29E-05
25	D	0.1310	0.0332	-0.0105	-0.0223	0.0081	-1.821-02
24	D	-0.2044	-0.0587	0.0163	-0.0034	0.0521	-5.45E-02
25	D	-0.2235	-0.0485	0.0003	-0.0000	0.0531	5.881-02
20	B	-0.2155	-0.0405	0.0005	-0.0000	0.0508	-1 63E-02
27	B	-0.1055	-0.0515	0.0115	-0.0012	0.0130	-3.44F-02
20	B	-0.2043	-0.0306	0.0103	-0.0034	0.0475	-3.44E-02
30	B	0.3583	0.0065	-0.0718	-0.0817	-0 1770	1 58F-01
31	В	0.3615	0.0065	-0.0718	-0.0817	-0.1755	1.58E-01
32	В	0.3396	0.0089	-0.0812	-0.0865	-0.1843	-6.84E-04
33	В	-0.1204	-0.0514	0.0067	-0.0082	0.0202	-6.53E-02
34	В	-0.0992	-0.0249	0.0250	0.0182	0.0195	-3.16E-03
35	В	0.1331	0.0333	-0.0169	-0.0229	0.0635	-1.66E-02
36	В	-0.0420	-0.0365	-0.0142	-0.0259	-0.0511	7.73E-02
37	В	0.2028	0.0220	-0.0320	-0.0366	-0.0548	-6.08E-02
38	В	-0.2648	-0.0587	0.0165	-0.0034	0.0547	-3.44E-02
39	В	-0.1667	-0.0319	0.0116	-0.0011	0.0135	-1.63E-01
40	Au	-0.5885	0.7055	0.5596	0.9720	0.7995	4.17E-01
	F1(B39)	0.5885	-0.7055	-0.5592	-0.9717	-0.7995	-0.3758
	F2(Au)	-0.5885	0.7055	0.5596	0.9720	0.7995	0.4170
L	Total	0.0000	0.0000	0.0004	0.0004	0.0000	0.0412

Au calibration curve constraction:

Charges on Au	Au 5s orbital energies
-2	-4.05093
-1	-4.06707
0	-4.16613
1	-4.30664
2	-4.6373



Orbital energies in Au@B39 complex Au 5s -4.22134

 $Q_{predicted} = 0.441$

Atom Number Former Oblige density Charge density Charge density Charge density Charge density Charge density 1 C 0.0178 0.0188 0.0009 0.0138 0.0009 3 C 0.0786 0.0128 0.0028 0.0134 0.0148 4 C 0.0488 0.0022 0.0134 0.0124 0.0228 0.0134 5 C 0.0137 0.0144 0.0172 0.0228 0.0131 7 C 0.0004 0.0115 0.0012 0.0127 0.0228 0.0177 10 C 0.0563 0.0153 0.0012 0.0107 0.0107 11 C 0.0563 0.0151 0.0012 0.0028 0.0107 13 C 0.0564 0.0103 0.0028 0.0107 0.0039 0.0444 14 C 0.0567 0.0077 0.0060 0.0171 0.0069 0.0171 15 C 0.0561 0.0	Sc3N@B39 [0,1]		Mulliken Scheme	Lowdin Scheme	Hirshfeld Scheme	CM5 Scheme	NPA Scheme	Bader Scheme
1 C 0.0179 -0.0166 -0.0179 -0.0138 2 C 0.0778 -0.0131 0.0099 -0.0001 3 C 0.0976 -0.0331 -0.0147 -0.1062 4 C 0.0448 -0.0219 -0.0445 -0.0279 -0.0445 6 C 0.0992 -0.0144 -0.0127 -0.0224 -0.0445 7 C 0.0004 -0.0121 -0.0115 -0.0171 -0.0226 -0.0147 9 C -0.1785 -0.0121 -0.0127 -0.0226 -0.0147 111 C -0.0213 -0.0127 -0.0266 -0.0131 -0.0177 -0.0464 -0.086 -0.0227 -0.0147 112 C -0.0565 -0.0131 -0.0177 -0.0167 -0.0167 -0.0167 -0.0167 -0.0167 -0.0264 -0.089 -0.0271 -0.0169 -0.0171 -0.0169 -0.0171 -0.0164 -0.0181 -0.0172 -0.0197 -0.0171 </th <th>Atom Number</th> <th>Element</th> <th>Charge density</th> <th>Charge density</th> <th>Charge density</th> <th>Charge density</th> <th>Charge density</th> <th>Charge density</th>	Atom Number	Element	Charge density	Charge density	Charge density	Charge density	Charge density	Charge density
2 C 0.0788 0.0118 0.0099 0.0001 0.0004 3 C 0.0483 0.0021 0.0933 0.0334 0.0767 5 C 0.0117 0.0144 0.0128 0.0334 0.0767 5 C 0.0137 0.0144 0.0128 0.0131 0.0128 0.0131 6 C 0.0982 0.0134 0.0127 0.0225 0.0317 10 C 0.0463 0.0137 0.0122 0.0177 11 C 0.0254 0.0373 0.0172 0.0147 12 C 0.0564 0.0169 0.0172 0.0167 13 C 0.0574 0.0061 0.0172 0.0275 0.0377 14 C 0.0577 0.0077 0.0171 0.0448 0.0022 0.0334 0.0271 0.0449 0.0281 0.0273 0.0374 0.0444 0.0281 0.0274 0.0374 0.0444 0.0281 0.0444 0.0	1	С	0.0179	-0.0106	-0.0109	-0.0175	-0.0188	
3 C 0.0976 -0.0038 0.0159 0.0472 -0.1062 5 C 0.0137 0.0149 0.0245 0.0259 0.0435 6 C 0.0062 0.0116 0.0074 0.0135 7 C 0.0006 -0.0123 0.0178 0.0225 0.0276 9 C -0.1785 0.0014 0.0178 0.0225 0.0177 10 C -0.0603 -0.0154 0.0178 0.0127 -0.0177 11 C -0.0213 -0.0178 -0.0179 -0.0177 -0.0175 -0.0175 14 C 0.0554 -0.0175 -0.0225 -0.0397 -0.0211 -0.0616 -0.0175 -0.0225 -0.0297 -0.0171 -0.0406 -0.0171 -0.0407 -0.0171 -0.0406 -0.0171 -0.0407 -0.0171 -0.0408 -0.0271 -0.0408 -0.0171 -0.0408 -0.0171 -0.0408 -0.0171 -0.0408 -0.0171 -0.0408 -0.017	2	С	-0.0788	-0.0118	0.0099	-0.0001	-0.0004	
4 C 0.0483 -0.0221 -0.0934 -0.0345 5 C -0.0344 -0.0144 -0.0196 -0.0226 -0.0443 6 C -0.0982 -0.0144 -0.0175 -0.0171 -0.0225 -0.0343 7 C -0.0064 -0.0125 -0.0171 -0.0225 -0.0171 10 C -0.0463 -0.0154 -0.0058 -0.0027 -0.0471 11 C -0.0456 -0.0154 -0.0174 -0.0184 -0.0174 13 C -0.0554 -0.0164 -0.0172 -0.0224 -0.0187 14 C -0.0554 -0.0164 -0.0173 -0.0894 -0.0171 15 C -0.0567 -0.0771 -0.0498 -0.0221 -0.0331 16 C -0.0571 -0.0771 -0.0498 -0.0221 -0.0331 17 C 0.0571 -0.0771 -0.0498 -0.0224 -0.0498 12	3	С	0.0976	-0.0038	-0.0159	-0.0472	-0.1062	
S C 0.0137 0.0140 0.0245 0.0253 0.0435 7 C 0.0092 0.0116 0.0224 0.0311 9 C 0.0765 0.0115 0.0171 0.0224 0.0311 10 C 0.0603 0.0154 0.0088 0.0012 0.0167 11 C 0.0213 0.0070 0.0082 0.0267 0.0667 12 C 0.0254 0.0070 0.0142 0.0264 0.0168 13 C 0.0254 0.0070 0.0142 0.0264 0.0533 14 C 0.0244 0.0084 0.0132 0.0264 0.0233 0.0581 15 C 0.0364 0.0171 0.0409 0.0221 0.0371 16 C 0.0364 0.0171 0.0409 0.0221 0.0331 17 C 0.0254 0.0022 0.0233 0.0543 18 C 0.0364 0.0171 0.026	4	C	0.0483	-0.0021	-0.0093	-0.0334	-0.0767	
b C 0.0385 0.0138 0.022 0.0138 0.0248 0.0384 8 C 0.1356 0.0115 0.0117 0.0225 0.0311 9 C 0.1565 0.0114 0.0124 0.0117 0.0224 0.0417 10 C 0.0665 0.0134 0.0238 0.0012 0.0167 11 C 0.0655 0.0039 0.0056 0.0339 0.0064 0.0169 12 C 0.0654 0.0039 0.0059 0.0446 0.0085 13 C 0.0057 0.0077 0.0039 0.0446 0.0085 14 C 0.0557 0.0074 0.0137 -0.008 0.0231 0.0541 15 C 0.0562 0.0072 0.0141 0.0446 0.0815 16 C 0.0562 0.0068 0.0171 0.0464 0.0815 16 C 0.0562 0.0068 0.0171 0.0463 0.0733	5	C	-0.0137	-0.0149	-0.0245	-0.0259	-0.0435	
j C 0.0182 0.0183 0.0183 0.0183 9 C 0.0175 0.0117 0.0023 0.0117 10 C 0.0213 0.0034 0.0034 0.0034 0.0017 11 C 0.0210 0.0037 0.0034 0.0037 0.0167 12 C 0.0544 0.0039 0.0034 0.0168 0.017 13 C 0.0564 0.0159 0.0225 0.037 14 C 0.0575 0.0039 0.0464 0.0351 15 C 0.0575 0.0037 0.0132 0.0464 0.0851 16 C 0.0575 0.0037 0.0132 0.0464 0.0851 17 C 0.0575 0.0037 0.0137 0.0406 0.0951 18 C 0.0556 0.0072 0.0137 0.0406 0.057 14 C 0.0556 0.0224 0.0203 0.0171 0.0464 0.0481<	6		-0.0982	-0.0140	-0.0196	-0.0226	-0.0343	
9 C 0.075 0.0178 0.0228 0.0276 10 C 0.0603 0.0177 0.0068 0.0171 0.0267 0.0667 11 C 0.0255 0.0313 0.0070 0.0142 0.0466 13 C 0.0555 0.0313 0.0029 0.0269 0.0253 14 C 0.0544 0.0080 0.0329 0.0263 0.0337 15 C 0.0376 0.0081 0.0122 0.0263 0.0387 15 C 0.0376 0.0081 0.0122 0.0263 0.0383 16 C 0.0376 0.0084 0.0171 0.0469 0.0383 17 C 0.0667 0.0022 0.0334 0.0773 20 C 0.0455 0.0084 0.0171 0.0463 0.0172 21 C 0.0554 0.0084 0.0170 0.0234 0.058 22 C 0.0554 0.0084 0.017	8	C C	-0.1586	-0.0102	-0.0118	-0.0225	-0.0439	
10 C 0.0637 0.0082 0.012 0.017 11 C 0.0233 0.0077 0.0004 0.0177 13 C 0.029 0.0770 0.012 0.0044 0.0177 14 C 0.0546 0.0139 0.0025 0.0337 15 C 0.0656 0.0151 0.0225 0.0337 16 C 0.0551 0.0081 -0.0125 0.0337 17 C 0.0557 0.0277 -0.0253 0.0683 19 C 0.1155 0.0074 -0.0171 -0.0496 -0.0181 21 C 0.0662 -0.0084 -0.0170 -0.0631 -0.0723 22 C 0.0562 -0.0084 -0.0170 -0.0611 -0.0843 23 C 0.0562 -0.0084 -0.0170 -0.063 -0.0858 24 C 0.0562 -0.0084 -0.0170 -0.063 -0.0588 25	9	c	-0.1380	-0.0113	-0.0171	-0.0223	-0.0276	
11 C -0.0213 -0.037 -0.0627 -0.0647 12 C -0.0565 -0.0132 -0.0177 -0.0246 -0.0766 13 C 0.0565 -0.0132 -0.0269 -0.0766 14 C 0.0564 -0.0080 -0.0250 -0.0397 15 C 0.0376 -0.0081 -0.0250 -0.0397 16 C 0.0376 -0.0079 -0.0464 -0.0581 18 C 0.0577 -0.0130 -0.0244 -0.0891 19 C 0.0155 -0.0072 -0.0141 -0.0344 -0.0819 21 C 0.0562 -0.0072 -0.0130 -0.0235 -0.0563 22 C 0.0562 -0.0072 -0.0130 -0.0133 -0.073 23 C 0.0562 -0.0073 -0.0130 -0.0137 -0.0814 24 C 0.0552 -0.0080 -0.0137 -0.0263 -0.0558	10	c	-0.0603	-0.0154	0.0058	0.0012	0.0147	
12 C -0.0565 -0.0129 -0.0142 -0.0234 -0.0176 14 C 0.0544 -0.0036 -0.0142 -0.0346 -0.0786 15 C 0.0036 -0.0159 -0.0220 -0.0533 16 C -0.0376 -0.00130 -0.0221 -0.0598 18 C 0.0397 -0.0040 -0.0121 -0.0400 -0.0212 20 C 0.1155 -0.0074 -0.0331 -0.0334 -0.0131 21 C 0.0365 -0.0072 -0.0133 -0.0334 -0.0171 22 C 0.0367 -0.0334 -0.0133 -0.0334 -0.0171 23 C 0.0364 -0.0134 -0.0138 -0.0173 -0.0384 -0.0561 24 C 0.0364 -0.0138 -0.0178 -0.0138 -0.0171 25 C 0.0166 -0.0284 -0.0284 -0.0284 -0.0284 26 0.0173 <td< td=""><td>11</td><td>С</td><td>-0.0213</td><td>-0.0037</td><td>-0.0082</td><td>-0.0267</td><td>-0.0647</td><td></td></td<>	11	С	-0.0213	-0.0037	-0.0082	-0.0267	-0.0647	
13 C 0.0024 -0.0076 -0.0132 -0.0864 -0.01459 14 C 0.0636 -0.0159 -0.0225 -0.0337 15 C 0.0357 -0.00152 -0.0225 -0.0337 17 C 0.0257 -0.0015 -0.0225 -0.0325 18 C 0.0357 -0.0015 -0.0464 -0.0325 20 C 0.0115 -0.0044 -0.0131 -0.0338 -0.0323 21 C 0.0634 -0.0127 -0.0331 -0.0333 -0.0531 223 C 0.0634 -0.0027 -0.0141 -0.0344 -0.0632 234 C 0.0524 -0.0026 -0.0130 -0.0140 -0.0443 24 C 0.0354 -0.0027 -0.0131 -0.0140 -0.0224 -0.0224 -0.0224 -0.0224 -0.0224 -0.0224 -0.0224 -0.0323 -0.2244 -0.0333 -0.2244 -0.0333 -0.2244 -0.0331	12	С	-0.0565	-0.0131	-0.0177	-0.0204	-0.0167	
14 C 0.0544 -0.0080 -0.0329 -0.0806 -0.1459 15 C -0.0375 -0.0013 -0.0251 -0.0375 17 C 0.0251 -0.00130 -0.0251 -0.0398 18 C 0.0397 -0.0217 -0.0409 -0.0221 20 C 0.1155 -0.0074 -0.0374 -0.0434 -0.0181 21 C 0.0656 -0.0072 -0.0133 -0.0773 -0.0384 -0.0173 22 C 0.0456 -0.0024 -0.0338 -0.0773 23 C 0.0456 -0.0084 -0.0130 -0.0261 -0.0434 24 C 0.0566 -0.0130 -0.0274 -0.0130 -0.0274 26 C 0.0134 -0.0064 -0.0137 -0.0284 -0.0484 27 C 0.0267 -0.0135 -0.0274 -0.0383 -0.0429 36 C 0.0141 -0.0171 -0.027	13	С	0.1029	-0.0070	-0.0142	-0.0346	-0.0786	
15 C 0.088 0.0152 0.0225 0.0397 17 C 0.0251 0.0061 0.0152 0.0225 1.0397 18 C 0.0557 0.0071 0.0069 0.0466 0.0825 19 C 0.1155 0.0074 0.0377 0.0496 0.0423 20 C 0.0157 0.0032 0.0233 0.0543 21 C 0.0664 0.0170 0.0434 0.0532 24 C 0.0652 0.0032 0.0268 0.0226 25 C 0.0562 0.0032 0.0268 0.0428 26 C 0.0524 0.0060 0.0130 0.0268 0.0288 27 C 0.0596 0.02058 0.0206 0.0248 0.0224 0.0224 30 C -0.139 0.0115 0.0174 0.0224 0.0224 31 C 0.1616 0.0115 0.0174 0.0226 0.0333	14	C	0.0544	-0.0080	-0.0329	-0.0804	-0.1459	
Ib C -0.0351 -0.0051 -0.0130 -0.0221 -0.0398 138 C 0.0551 -0.0054 -0.0130 -0.0221 -0.0398 139 C 0.1155 -0.0074 -0.0171 -0.0409 -0.0221 20 C 0.1155 -0.0074 -0.0337 -0.0409 -0.0319 21 C 0.0648 -0.0022 -0.0033 -0.0773 22 C 0.0648 -0.0022 -0.0033 -0.0773 24 C 0.0656 -0.0030 -0.0233 -0.0411 25 C 0.0156 -0.01010 -0.0243 -0.0693 26 C 0.0226 -0.0101 -0.0243 -0.0243 28 C -0.1139 -0.0171 -0.0226 -0.0343 30 C -0.0127 -0.0138 -0.0124 -0.0323 31 C -0.0161 -0.0115 -0.0171 -0.0226 -0.0343 33	15	C	0.0636	-0.0169	0.0029	-0.0260	-0.0533	
1/2 C 0.0257 0.0058 0.0243 0.0058 199 C 0.0105 0.0024 0.0117 0.0404 0.0823 199 C 0.0115 0.0074 0.0137 0.0404 0.0823 200 C 0.0543 0.0072 0.0141 0.0324 0.00543 221 C 0.0654 0.0002 0.0094 0.0338 0.0773 244 C 0.0552 0.0084 0.0170 0.0441 0.0083 25 C 0.0134 0.0028 0.0032 0.0040 0.0433 26 C 0.0134 0.0074 0.0328 0.0081 0.0449 29 C 0.0147 0.0126 0.0232 0.0449 0.0421 30 C 0.0147 0.0126 0.0232 0.0433 31 C 0.0158 0.0126 0.0333 32 C 0.0161 0.0179 0.0024 0.0033	16		-0.0376	-0.0081	-0.0152	-0.0225	-0.0397	
10 C 0.0106 0.0084 0.0111 0.0409 0.0921 20 C 0.1155 0.0074 0.0377 0.0966 0.1444 21 C 0.0654 0.0171 0.0032 0.0253 0.0543 23 C 0.0652 0.0004 0.0333 0.0773 24 C 0.0556 0.0002 0.0263 0.0645 25 C 0.0334 0.0074 0.0378 0.0044 26 C 0.0327 0.0108 0.0117 0.0045 0.0423 30 C 0.0115 0.0117 0.0044 0.0333 0.0421 31 C 0.0115 0.0117 0.0094 0.0421 0.0333 32 C 0.0103 0.0117 0.0094 0.0421 0.0333 33 C 0.0115 0.0117 0.0094 0.0421 0.0333 33 C 0.0105 0.0015 0.0224 0.0034	17		0.0251	-0.0061	-0.0130	-0.0261	-0.0598	
20 C 0.1155 0.0072 0.0141 0.0344 0.0149 21 C 0.0654 0.0022 0.0032 0.0233 0.0773 24 C 0.0564 0.0002 0.0094 0.0338 0.0773 24 C 0.0562 0.0084 0.0170 0.4410 0.0663 25 C 0.0324 0.0070 0.4410 0.0663 26 C 0.0324 0.0074 0.0136 0.0084 0.0170 0.0410 0.0663 27 C 0.0566 0.0208 0.0061 0.0441 0.0133 0.0133 0.0144 29 C 0.0117 0.0104 0.0124 0.0226 0.0333 31 C 0.0150 0.0124 0.0123 0.0226 0.0333 32 C 0.0101 0.0114 0.0195 0.0226 0.0343 33 C 0.0162 0.0119 0.0029 0.0026 0.0333	19	c	0.1016	-0.0084	-0.0035	-0.0409	-0.0823	
21 CC 0.0657 0.0072 0.0141 0.0254 0.0054 22 C 0.0634 0.0127 0.0333 0.0373 24 C 0.0562 0.0080 0.0127 0.0798 0.1445 25 C 0.0354 0.0080 0.0170 0.0410 0.0663 26 C 0.0356 0.0208 0.0061 0.0451 0.0814 28 C 0.0139 0.0074 0.0378 0.0083 0.0421 31 C 0.0101 0.0117 0.0084 0.0421 31 C 0.0101 0.0117 0.0224 0.0333 33 C 0.0101 0.0115 0.0127 0.0331 34 C 0.0636 0.0152 0.0224 0.0333 35 C 0.0587 0.0133 0.0251 0.0973 36 C 0.1170 0.0043 0.0171 0.0412 0.0873 36 C	20	c	0.1155	-0.0074	-0.0377	-0.0906	-0.1448	
22 C 0.0634 -0.0167 0.0032 -0.0253 -0.0733 24 C 0.0562 -0.0800 -0.0327 -0.0798 -0.1445 25 C 0.1054 -0.0804 -0.0130 -0.0451 -0.0884 26 C 0.0396 -0.0208 -0.0661 -0.0814 28 C 0.0113 -0.0275 -0.0260 -0.0449 29 C -0.0147 -0.0130 -0.0245 -0.0260 -0.0449 30 C -0.0207 -0.0130 -0.0170 -0.0224 -0.0333 31 C -0.1618 -0.0115 -0.0170 -0.0224 -0.0333 33 C -0.0181 -0.0119 -0.0271 -0.0125 -0.0287 34 C -0.0366 -0.0162 -0.0213 -0.0271 -0.0125 35 C 0.1170 -0.0774 -0.0379 -0.0909 -0.1485 36 C 0.1170 -0.0	21	c	0.0967	-0.0072	-0.0141	-0.0344	-0.0819	
23 C 0.0458 -0.0022 -0.0994 -0.0338 -0.0773 24 C 0.0552 -0.0034 -0.0170 -0.0440 -0.0956 25 C 0.0324 -0.0066 -0.0253 -0.0588 27 C 0.0324 -0.0074 -0.0275 -0.0998 -0.1449 28 C 0.1139 -0.0074 -0.0276 -0.0421 30 C -0.0107 -0.013 -0.017 -0.0224 -0.0333 31 C -0.1568 -0.0111 -0.0195 -0.0226 -0.0333 33 C -0.1618 -0.0119 0.0099 -0.0000 0.0002 35 C 0.0666 -0.0127 -0.0464 -0.0338 -0.0171 -0.0412 -0.0973 36 C 0.0587 -0.0209 -0.0663 -0.0126 -0.0226 37 C 0.0587 -0.0213 -0.0456 -0.0231 38 C 0.0587 </td <td>22</td> <td>С</td> <td>0.0634</td> <td>-0.0167</td> <td>0.0032</td> <td>-0.0253</td> <td>-0.0543</td> <td></td>	22	С	0.0634	-0.0167	0.0032	-0.0253	-0.0543	
24 C 0.0562 -0.0806 -0.0327 -0.0798 -0.1445 25 C 0.0334 -0.0061 -0.0133 -0.0588 277 C 0.0596 -0.0208 -0.0245 -0.0884 28 C 0.01147 -0.0150 -0.0245 -0.0260 -0.0429 300 C -0.0147 -0.0150 -0.0224 -0.0333 31 C -0.1588 -0.0115 -0.0170 -0.0224 -0.0333 331 C -0.1618 -0.0115 -0.0170 -0.0224 -0.0333 34 C -0.0636 -0.0157 -0.0648 -0.0027 355 C 0.0646 -0.0037 -0.0468 -0.0267 37 C 0.0657 -0.0207 -0.0468 -0.0973 38 C 0.1170 -0.0074 -0.0373 -0.0296 -0.1488 399 C 0.0587 -0.0209 -0.0148 -0.0661 411<	23	С	0.0458	-0.0022	-0.0094	-0.0338	-0.0773	
25 C 0.0154 -0.0084 -0.0170 -0.0410 -0.0963 26 C 0.0324 -0.0061 -0.0451 -0.0588 27 C 0.0596 -0.0228 -0.0661 -0.0451 -0.0584 28 C -0.0147 -0.0130 -0.0245 -0.0260 -0.0429 30 C -0.027 -0.0131 -0.0170 -0.0224 -0.0333 31 C -0.1618 -0.0119 -0.0099 -0.0000 -0.0002 35 C -0.0612 -0.0119 -0.0099 -0.0000 -0.0027 36 C 0.0612 -0.013 -0.017 -0.0226 -0.0103 37 C 0.1995 -0.0038 -0.017 -0.0468 -0.1096 38 C 0.1170 -0.0071 -0.0456 -0.0849 40 C 0.0392 -0.0063 -0.0456 -0.0484 41 C 0.0606 -0.0072 -0.0141<	24	С	0.0562	-0.0080	-0.0327	-0.0798	-0.1445	
26 C 0.0324 -0.0060 -0.0130 -0.0253 -0.0588 27 C 0.0596 -0.0274 -0.0378 -0.0908 -0.0449 28 C 0.1139 -0.0147 -0.0150 -0.0245 -0.0226 -0.0323 30 C -0.0027 -0.0103 0.0117 0.0094 -0.0421 31 C -0.1568 -0.0170 -0.0224 -0.0333 32 C -0.1618 -0.0115 -0.0170 -0.0224 -0.0333 33 C -0.0612 -0.0119 0.0099 0.0000 0.0002 35 C 0.0636 -0.0171 -0.0412 -0.0973 36 C 0.1070 -0.0246 -0.0468 -0.0468 40 C 0.0353 -0.0171 -0.0412 -0.0973 41 C 0.0607 -0.033 -02246 -0.0464 42 C 0.0606 -0.0172 -0.0141 -0.0875 <td>25</td> <td>С</td> <td>0.1054</td> <td>-0.0084</td> <td>-0.0170</td> <td>-0.0410</td> <td>-0.0963</td> <td></td>	25	С	0.1054	-0.0084	-0.0170	-0.0410	-0.0963	
27 C 0.0396 -0.0208 -0.0061 -0.0451 -0.0841 28 C 0.0147 -0.0150 -0.0245 -0.0260 -0.0429 30 C -0.0156 -0.0170 -0.0224 -0.0333 31 C -0.0161 -0.0170 -0.0224 -0.0333 32 C -0.0101 -0.0170 -0.0224 -0.0333 34 C -0.0612 -0.0119 -0.0770 -0.0224 -0.0333 34 C -0.0812 -0.0119 -0.0170 -0.0224 -0.0303 35 C 0.0812 -0.0177 -0.0468 -0.1096 37 C 0.1095 -0.0209 -0.0468 -0.1096 38 C 0.0157 -0.0468 -0.0493 -0.0849 40 C 0.0351 -0.0255 -0.0616 41 C 0.0352 -0.0245 -0.0444 42 C 0.0602 -0.0154	26	С	0.0324	-0.0060	-0.0130	-0.0263	-0.0588	
28 C 0.0143 0.0074 0.0036 0.0429 30 C 0.0017 0.01245 0.02266 0.0421 31 C 0.1568 0.0115 0.0170 0.0224 0.0333 32 C 0.1018 0.0115 0.0170 0.0224 0.0333 33 C 0.1618 0.0115 0.0170 0.0224 0.0333 34 C 0.0636 0.0157 0.0468 0.0196 35 C 0.0636 0.0171 0.0411 0.0297 36 C 0.1170 0.0245 0.0265 0.0649 40 C 0.0392 0.0129 0.0265 0.0644 41 C 0.0392 0.0129 0.0265 0.0644 42 C 0.0696 0.0129 0.0226 0.0444 42 C 0.0690 0.0129 0.0226 0.0229 43 C 0.0590 0.0174 0.0141	27	C	0.0596	-0.0208	-0.0061	-0.0451	-0.0814	
2.5 C -0.0125 -0.0126 -0.0127 -0.0103 0.0117 0.0094 0.0421 31 C -0.0568 -0.0115 -0.0170 -0.0226 -0.0343 33 C -0.06112 -0.0115 -0.0170 -0.0226 -0.0343 33 C -0.0612 -0.0113 -0.0213 -0.0297 36 C -0.0636 -0.0112 -0.0412 -0.0973 36 C 0.0196 -0.0063 -0.0117 -0.0412 -0.0973 38 C 0.1170 -0.0074 -0.0379 -0.0495 -0.0616 40 C -0.0353 -0.0059 -0.0129 -0.0256 -0.0616 41 C -0.0332 -0.0084 -0.0156 -0.0249 -0.0551 43 C 0.0548 -0.0081 -0.0256 -0.0616 44 C 0.0548 -0.0081 -0.0267 -0.0656 45 C -0.0590 -	28		-0.0147	-0.0074	-0.0378	-0.0908	-0.1449	
3.5 C 0.0121 0.0121 0.0124 0.0023 32 C -0.1001 -0.0141 -0.0195 -0.0224 -0.0303 33 C -0.6618 -0.0115 -0.0170 -0.0224 -0.0303 34 C -0.0636 -0.0119 0.0099 0.0000 0.0002 35 C 0.0636 -0.0157 -0.0468 -0.1996 37 C 0.0195 -0.0638 -0.0171 -0.0416 -0.0373 38 C 0.0195 -0.0603 -0.0456 -0.0849 40 C 0.0333 -0.0226 -0.0404 41 C 0.0362 -0.0156 -0.0226 -0.0404 42 C 0.0660 -0.0235 -0.0794 -0.1463 43 C 0.0266 -0.0249 -0.0166 44 C 0.058 -0.0012 -0.0266 -0.0342 45 C -0.0258 -0.0121 -0.	30	C C	-0.0147	-0.0100	0.0243	0.0200	0.0423	
32 C -0.1001 -0.0141 -0.0195 -0.0226 -0.0343 33 C -0.6618 -0.0119 -0.0099 -0.0000 0.0002 35 C 0.0636 -0.0152 -0.0213 -0.0251 -0.0297 36 C 0.0946 -0.0038 -0.0157 -0.0468 -0.0973 38 C 0.0170 -0.0074 -0.0399 -0.0042 -0.0973 38 C 0.0587 -0.029 -0.063 -0.04456 -0.0849 40 C 0.0383 -0.0079 -0.0129 -0.0265 -0.0616 41 C -0.0392 -0.0084 -0.0156 -0.0249 -0.0551 43 C 0.0588 -0.0021 -0.0141 -0.0267 -0.0656 44 C 0.0588 -0.0012 -0.0137 -0.0231 -0.0137 45 C -0.0508 -0.0123 -0.0175 -0.021 -0.0137 46	31	c	-0.1568	-0.0115	-0.0170	-0.0224	-0.0323	
33 C -0.1518 -0.0170 -0.0224 -0.0303 34 C -0.0812 -0.0199 0.0000 0.0002 35 C 0.0946 -0.0182 -0.0251 -0.0297 36 C 0.1095 -0.0038 -0.0157 -0.0468 -0.1096 37 C 0.1197 -0.0074 -0.0379 -0.0499 -0.1458 39 C 0.0587 -0.029 -0.0663 -0.0441 -0.0343 40 C -0.0392 -0.0084 -0.0156 -0.0246 -0.0044 41 C -0.0548 -0.0080 -0.0333 -0.0343 -0.0804 43 C -0.0548 -0.0081 -0.0247 -0.0141 -0.0343 -0.0804 44 C -0.0747 -0.0141 -0.0343 -0.0804 -0.0121 -0.0137 45 C -0.0588 -0.0021 -0.0137 -0.0221 -0.0137 46 C -0.	32	С	-0.1001	-0.0141	-0.0195	-0.0226	-0.0343	
34 C -0.0812 -0.0119 0.0099 0.0000 0.0002 35 C 0.0636 -0.0152 -0.0251 -0.0297 36 C 0.1095 -0.0683 -0.0157 -0.0468 -0.0099 37 C 0.1170 -0.0074 -0.0379 -0.0099 -0.1458 39 C 0.0587 -0.029 -0.0255 -0.0616 40 C 0.0353 -0.079 -0.0226 -0.0404 42 C 0.0660 -0.0157 0.0026 -0.0444 43 C 0.0264 -0.0167 0.0333 -0.0294 -0.0163 44 C 0.0584 -0.0080 -0.0325 -0.0794 -0.1463 45 C -0.0231 -0.038 -0.0175 -0.0220 -0.0231 47 C -0.0174 -0.0144 -0.0175 -0.0221 -0.0137 48 C -0.0508 -0.0172 -0.0147 -0.0141	33	С	-0.1618	-0.0115	-0.0170	-0.0224	-0.0303	
35 C 0.0636 -0.0162 -0.0213 -0.0237 36 C 0.0946 -0.0038 -0.0157 -0.0468 -0.1096 37 C 0.1095 -0.0083 -0.0171 -0.0412 -0.0973 38 C 0.1170 -0.0074 -0.0379 -0.0999 -0.1458 40 C 0.0353 -0.0059 -0.0129 -0.0265 -0.0616 41 C -0.0392 -0.0147 -0.0333 -0.0294 -0.0551 43 C 0.0660 -0.0072 -0.0141 -0.0343 -0.0804 44 C 0.0548 -0.0081 -0.0227 -0.0656 45 C -0.0590 -0.0154 0.0088 0.0012 0.0137 45 C -0.0508 -0.0179 -0.0175 -0.0221 -0.0137 46 C -0.0508 -0.0129 -0.0175 -0.0210 -0.0137 47 C 0.0174 -0.0176	34	С	-0.0812	-0.0119	0.0099	0.0000	0.0002	
36 C 0.0946 -0.038 -0.017 -0.0412 -0.0973 38 C 0.1170 -0.0074 -0.0379 -0.0999 -0.0412 -0.0973 39 C 0.0587 -0.0209 -0.0063 -0.0455 -0.0644 40 C 0.0352 -0.0054 -0.0156 -0.0226 -0.0404 41 C -0.0392 -0.0084 -0.0156 -0.0226 -0.0404 42 C 0.0602 -0.0172 -0.0141 -0.0343 -0.0804 43 C 0.058 -0.0023 -0.0172 -0.0144 -0.0178 -0.0229 -0.0231 44 C -0.0508 -0.0178 -0.0229 -0.0231 -0.0176 -0.0180 47 C -0.1747 -0.0144 -0.0178 -0.0229 -0.0231 48 C -0.0508 -0.0123 -0.0176 -0.0342 -0.0131 50 C 0.0209 -0.0123 -0.0176	35	С	0.0636	-0.0162	-0.0213	-0.0251	-0.0297	
37 C 0.1095 -0.0083 -0.0171 -0.0492 -0.0993 38 C 0.0587 -0.0299 -0.0663 -0.0456 -0.0849 40 C 0.0353 -0.059 -0.0129 -0.0265 -0.0616 41 C -0.0392 -0.0084 -0.0156 -0.0246 -0.0444 42 C 0.0602 -0.0167 0.0033 -0.0249 -0.0551 43 C 0.0568 -0.0080 -0.0325 -0.0794 -0.1463 45 C -0.0590 -0.0144 -0.0177 -0.0180 -0.0129 46 C -0.0508 -0.0129 -0.021 -0.0181 -0.0181 47 C -0.0747 -0.0144 -0.0178 -0.021 -0.0181 48 C -0.0508 -0.0123 -0.0147 -0.0181 -0.0160 51 C 0.0029 -0.0123 -0.0177 -0.0118 -0.0231 52	36	С	0.0946	-0.0038	-0.0157	-0.0468	-0.1096	
38 C 0.1170 -0.0074 -0.0399 -0.0456 -0.0456 40 C 0.0353 -0.0059 -0.0129 -0.0265 -0.0616 41 C -0.0392 -0.0084 -0.0156 -0.0249 -0.0541 42 C 0.00602 -0.0167 -0.0141 -0.0343 -0.0804 43 C 0.0548 -0.0038 -0.027 -0.0141 -0.0343 -0.0804 44 C -0.0548 -0.0038 -0.0217 -0.0414 -0.0361 -0.0267 -0.0656 46 C -0.0590 -0.0124 -0.0178 -0.0229 -0.0211 47 C -0.0129 -0.0129 -0.0121 -0.0141 -0.0181 -0.0181 48 C -0.0508 -0.0123 -0.0147 -0.0181 -0.0160 50 C 0.0209 -0.0123 -0.0177 -0.0213 -0.0230 51 C 0.00736 -0.0083 -0.0176 </td <td>37</td> <td>С</td> <td>0.1095</td> <td>-0.0083</td> <td>-0.0171</td> <td>-0.0412</td> <td>-0.0973</td> <td></td>	37	С	0.1095	-0.0083	-0.0171	-0.0412	-0.0973	
55 C 0.0337 0.0209 -0.0435 -0.04435 -0.04435 40 C 0.0332 -0.0084 -0.0156 -0.0226 -0.0404 41 C 0.0602 -0.0167 0.0033 -0.0249 -0.0551 43 C 0.0548 -0.0080 -0.0325 -0.0794 -0.1463 44 C 0.0559 -0.0154 0.0081 -0.02267 -0.0656 46 C -0.0590 -0.0144 -0.0178 -0.0229 -0.0231 477 C -0.1747 -0.0144 -0.0178 -0.0229 -0.0317 48 C -0.0508 -0.022 -0.096 -0.0342 -0.0812 50 C 0.0209 -0.0178 -0.0181 -0.0160 51 C -0.0702 -0.0118 0.0002 0.0021 52 C 0.0024 -0.0157 -0.0158 -0.0158 54 C -0.0785 -0.0119 -0.017	38	C	0.1170	-0.0074	-0.0379	-0.0909	-0.1458	
40 C 0.0332 0.0034 0.0112 0.0112 0.0013 41 C 0.0602 0.0084 0.0155 0.0226 0.0094 42 C 0.0602 0.0167 0.0033 -0.0249 -0.0551 43 C 0.0960 -0.0072 -0.0141 -0.0343 -0.084 44 C 0.0258 -0.0088 -0.0027 -0.0143 -0.0656 46 C -0.0590 -0.0154 0.0058 0.0012 -0.0137 48 C -0.0508 -0.0178 -0.0266 -0.0137 49 C 0.0020 -0.0141 -0.0185 -0.026 -0.0129 50 C 0.0024 -0.0123 -0.0197 -0.0213 -0.0230 51 C 0.0024 -0.0123 -0.0197 -0.0231 -0.0230 52 C 0.0024 -0.0125 -0.0253 -0.0328 54 C -0.0736 -0.0083	39		0.0587	-0.0209	-0.0083	-0.0436	-0.0849	
42 C 0.0602 0.0167 0.0163 0.0224 0.0551 43 C 0.0660 0.0072 -0.0141 -0.0343 -0.0804 44 C 0.0548 -0.0080 -0.0325 -0.0794 -0.1463 45 C -0.0231 -0.0038 -0.0227 -0.0656 46 C -0.0590 -0.0154 0.0058 0.0012 0.0137 48 C -0.0508 -0.0229 -0.0231 -0.0137 49 C 0.0508 -0.0022 -0.0096 -0.0342 -0.0812 50 C 0.0024 -0.017 -0.0213 -0.0129 51 C -0.0702 -0.018 0.0085 0.0026 0.0129 52 C 0.0073 -0.0197 -0.0213 -0.0230 -0.0123 53 C -0.0785 -0.0118 0.0001 -0.0074 -0.018 54 C -0.0786 -0.00173 -0.0174	40	C	-0.0392	-0.0039	-0.0129	-0.0203	-0.0010	
43 C 0.0960 -0.0072 -0.0141 -0.0343 -0.0804 44 C 0.0548 -0.0080 -0.0325 -0.0794 -0.163 45 C -0.0231 -0.0038 -0.00267 -0.0656 46 C -0.0590 -0.0144 -0.0178 -0.0229 -0.0231 47 C -0.1747 -0.0144 -0.0178 -0.0229 -0.0317 48 C -0.0508 -0.022 -0.0342 -0.0812 50 C 0.0209 -0.0123 -0.0147 -0.0181 -0.0160 51 C -0.0702 -0.018 0.0085 0.0026 0.0123 52 C 0.0024 -0.0123 -0.0176 -0.0174 54 C -0.0785 -0.018 0.0002 0.0021 55 C 0.0156 -0.017 -0.0033 -0.0174 56 C 0.0678 -0.0157 -0.0167 -0.018	42	c	0.0602	-0.0167	0.0033	-0.0249	-0.0551	
44 C 0.0548 -0.0080 -0.0325 -0.0794 -0.1463 45 C -0.0231 -0.0038 -0.0081 -0.0267 -0.0656 46 C -0.0590 -0.0154 0.0058 0.0022 -0.0231 47 C -0.1747 -0.0144 -0.0178 -0.0229 -0.0231 48 C -0.0508 -0.022 -0.0017 -0.0342 -0.0812 50 C 0.0209 -0.0123 -0.0147 -0.0141 -0.0160 51 C -0.0702 -0.0118 0.0085 0.0026 0.0129 52 C 0.0024 -0.0137 -0.0231 -0.0230 53 C 0.0073 -0.0160 -0.0174 -0.0188 54 C -0.0785 -0.018 0.0107 -0.0174 56 C 0.0624 -0.0157 -0.0253 -0.0328 57 C 0.0678 -0.0087 -0.0176 -0.0108 <td>43</td> <td>С</td> <td>0.0960</td> <td>-0.0072</td> <td>-0.0141</td> <td>-0.0343</td> <td>-0.0804</td> <td></td>	43	С	0.0960	-0.0072	-0.0141	-0.0343	-0.0804	
45 C -0.0231 -0.0038 -0.0811 -0.0267 -0.0656 46 C -0.0590 -0.0154 0.0058 0.0122 0.0231 47 C -0.1747 -0.0144 -0.0175 -0.0201 -0.0137 48 C -0.0508 -0.022 -0.0096 -0.0342 -0.0812 50 C 0.0209 -0.0123 -0.0147 -0.0181 -0.0160 51 C -0.0702 -0.018 0.0026 0.0129 52 C 0.0024 -0.0123 -0.0171 -0.0213 -0.0230 53 C 0.0073 -0.0039 -0.0160 -0.0473 -0.0230 54 C -0.0785 -0.018 0.0100 -0.0021 0.0213 55 C 0.0156 -0.017 -0.0157 -0.0163 -0.0323 57 C 0.0736 -0.083 -0.0157 -0.0163 -0.0121 60 C 0.0678	44	С	0.0548	-0.0080	-0.0325	-0.0794	-0.1463	
46 C -0.0590 -0.0154 0.0058 0.0012 0.0180 47 C -0.1747 -0.0144 -0.0175 -0.0229 -0.0231 48 C -0.0508 -0.0022 -0.0096 -0.0342 -0.0812 50 C 0.0209 -0.0123 -0.0147 -0.0181 -0.0160 51 C -0.0702 -0.0118 0.0085 0.0026 0.0129 52 C 0.0073 -0.0133 -0.0137 -0.058 54 C -0.0785 -0.0118 0.0100 -0.0017 -0.0158 54 C -0.0785 -0.0118 0.0100 -0.0017 -0.0123 -0.0253 -0.0328 55 C 0.0156 -0.017 -0.019 -0.0176 -0.0174 56 C 0.0678 -0.0083 -0.0157 -0.0163 -0.0163 59 C 0.0678 -0.0073 0.0069 -0.0163 59 C	45	С	-0.0231	-0.0038	-0.0081	-0.0267	-0.0656	
47 C -0.1747 -0.0144 -0.0175 -0.0229 -0.0231 48 C -0.0508 -0.0129 -0.0175 -0.0201 -0.0137 49 C 0.0508 -0.0022 -0.0096 -0.0342 -0.0812 50 C 0.0209 -0.0123 -0.0147 -0.0181 -0.0230 51 C -0.0702 -0.0118 0.0085 0.0026 0.0129 52 C 0.0024 -0.0123 -0.0107 -0.0137 -0.0230 53 C 0.0973 -0.039 -0.0160 -0.0473 -0.1058 54 C -0.0785 -0.0118 0.0100 -0.0021 -0.0578 55 C 0.0156 -0.0177 -0.0167 -0.0108 58 C -0.1218 -0.0083 -0.0157 -0.0163 59 C 0.0678 -0.0083 -0.0157 -0.0166 -0.0104 61 C -0.0008 -0.017<	46	С	-0.0590	-0.0154	0.0058	0.0012	0.0180	
48 C -0.0508 -0.0129 -0.0175 -0.0201 -0.0137 49 C 0.0508 -0.0022 -0.096 -0.0342 -0.0812 50 C 0.0209 -0.0123 -0.0147 -0.0181 -0.0209 51 C -0.0702 -0.0118 0.0085 0.0021 -0.0230 53 C 0.0973 -0.039 -0.0160 -0.0473 -0.1058 54 C -0.0785 -0.017 -0.0199 -0.0176 -0.0174 56 C 0.0156 -0.0107 -0.0199 -0.0167 -0.0128 57 C 0.0624 -0.0152 -0.0253 -0.0328 57 C 0.0678 -0.0081 -0.0167 -0.0108 58 C -0.1218 -0.0087 -0.0157 -0.0166 -0.0104 61 C 0.0695 -0.0824 -0.0157 -0.0166 -0.0104 61 C -0.0206 -0.0107<	47	С	-0.1747	-0.0144	-0.0178	-0.0229	-0.0231	
49 C 0.0338 -0.0342 -0.0342 -0.01342 50 C 0.0209 -0.0123 -0.0147 -0.0181 -0.0160 51 C -0.0702 -0.0118 0.0085 0.0024 -0.0230 53 C 0.0973 -0.0039 -0.0160 -0.0473 -0.1058 54 C -0.0785 -0.0118 0.0100 -0.0002 0.0021 55 C 0.0156 -0.0107 -0.0109 -0.0176 -0.0174 56 C 0.0624 -0.0157 -0.0167 -0.0108 58 C -0.1218 -0.0083 -0.0157 -0.0167 -0.0112 60 C 0.06695 -0.082 -0.0157 -0.0166 -0.0104 61 C -0.0038 -0.0107 -0.0110 -0.0174 -0.188 63 C -0.0038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 </td <td>48</td> <td>C</td> <td>-0.0508</td> <td>-0.0129</td> <td>-0.0175</td> <td>-0.0201</td> <td>-0.0137</td> <td></td>	48	C	-0.0508	-0.0129	-0.0175	-0.0201	-0.0137	
30 C 0.0123 0.0112 0.0111 0.0111 0.0110 51 C 0.0702 -0.0118 0.0085 0.0026 0.0129 52 C 0.0024 -0.0123 -0.0197 -0.0213 -0.0230 53 C 0.0973 -0.0039 -0.0160 -0.0473 -0.1058 54 C -0.0785 -0.0118 0.0100 -0.0002 0.0021 55 C 0.0156 -0.017 -0.019 -0.0176 -0.0174 56 C 0.0624 -0.0162 -0.0253 -0.0328 57 C 0.0736 -0.0083 -0.0157 -0.0167 58 C -0.1218 -0.0082 -0.0157 -0.0166 -0.0104 61 C 0.0678 -0.0082 -0.0157 -0.0166 -0.0104 61 C 0.0206 -0.0107 -0.0110 -0.0174 -0.188 63 C -0.0302 -0.0381	49		0.0508	-0.0022	-0.0096	-0.0342	-0.0812	
52 C 0.0024 -0.0123 -0.023 -0.023 53 C 0.0073 -0.0039 -0.0160 -0.0473 -0.0230 54 C -0.0785 -0.0118 0.0100 -0.0002 0.0021 55 C 0.0156 -0.017 -0.019 -0.0176 -0.0174 56 C 0.0624 -0.0162 -0.0253 -0.0328 57 C 0.0736 -0.0083 -0.0157 -0.0167 -0.0108 58 C -0.1218 -0.0087 0.0073 0.0069 0.0163 59 C 0.0678 -0.0083 -0.0157 -0.0166 -0.0112 60 C 0.06095 -0.0082 -0.0157 -0.0166 -0.0112 61 C -0.1008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0117 -0.0144 -0.018 63 C -0.0302 -0.0245 -0.0259	51	C	-0.0203	-0.0123	0.0147	0.0181	0.0100	
53 C 0.0973 -0.039 -0.0160 -0.0473 -0.1058 54 C -0.0785 -0.0118 0.0100 -0.0002 0.0021 55 C 0.0156 -0.0107 -0.019 -0.0176 -0.0174 56 C 0.0624 -0.0162 -0.0253 -0.0328 57 C 0.0736 -0.0083 -0.0157 -0.0163 58 C -0.1218 -0.0087 0.0073 0.0069 0.0163 59 C 0.0678 -0.0083 -0.0158 -0.0121 -0.0124 60 C 0.0695 -0.0022 -0.0157 -0.0166 -0.0104 61 C -0.0038 -0.017 -0.0166 -0.0104 63 C -0.0038 -0.017 -0.0174 -0.0188 63 C -0.0108 -0.017 -0.0259 -0.0435 65 C -0.0302 -0.0388 -0.084 -0.0267 -0.0617	52	c	0.0024	-0.0123	-0.0197	-0.0213	-0.0230	
54 C -0.0785 -0.0118 0.0100 -0.0002 0.0021 55 C 0.0156 -0.0107 -0.0109 -0.0176 -0.0174 56 C 0.0624 -0.0162 -0.0215 -0.0253 -0.0328 57 C 0.0736 -0.0083 -0.0177 -0.0108 58 C -0.1218 -0.0087 -0.0158 -0.0167 -0.0112 60 C 0.0678 -0.0083 -0.0157 -0.0166 -0.0104 61 C -0.1008 -0.0141 -0.0195 -0.0256 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0308 -0.0103 0.017 -0.0184 -0.0259 -0.0435 65 C -0.0302 -0.0038 -0.0204 -0.0257 -0.0617 66 C -0.0557 -0.0174 -0.0177 -0.0203 -0.0154 67 <td< td=""><td>53</td><td>С</td><td>0.0973</td><td>-0.0039</td><td>-0.0160</td><td>-0.0473</td><td>-0.1058</td><td></td></td<>	53	С	0.0973	-0.0039	-0.0160	-0.0473	-0.1058	
55 C 0.0156 -0.0107 -0.0109 -0.0176 -0.0174 56 C 0.0624 -0.0162 -0.0215 -0.0253 -0.0328 57 C 0.0736 -0.0083 -0.0177 -0.0167 -0.0108 58 C -0.1218 -0.0087 0.0073 0.0069 0.0163 59 C 0.0678 -0.0082 -0.0157 -0.0166 -0.104 60 C -0.0206 -0.0121 -0.0166 -0.104 61 C -0.1008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0308 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0129 -0.0177 -0.0203 -0.0154 65 C -0.0557 -0.014 -0.0177 -0.0203 -0.0154 66 C -0.0557 <td>54</td> <td>С</td> <td>-0.0785</td> <td>-0.0118</td> <td>0.0100</td> <td>-0.0002</td> <td>0.0021</td> <td></td>	54	С	-0.0785	-0.0118	0.0100	-0.0002	0.0021	
56 C 0.0624 -0.0162 -0.0215 -0.0253 -0.0328 57 C 0.0736 -0.0083 -0.0157 -0.0167 -0.0108 58 C -0.1218 -0.0087 0.0073 0.0069 0.0163 59 C 0.0678 -0.0083 -0.0157 -0.0166 -0.012 60 C 0.0695 -0.0082 -0.0157 -0.0166 -0.0104 61 C -0.1008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0308 -0.0125 -0.0259 -0.0435 64 C -0.0108 -0.0149 -0.0245 -0.0203 -0.0154 65 C -0.0302 -0.038 -0.0177 -0.0203 -0.0154 66 C -0.0557 -0.014 -0.0177 -0.0203 -0.0154 67 C -0.0557	55	С	0.0156	-0.0107	-0.0109	-0.0176	-0.0174	
57 C 0.0736 -0.0083 -0.0157 -0.0167 -0.0108 58 C -0.1218 -0.0087 0.0073 0.0069 0.0163 59 C 0.0678 -0.0083 -0.0157 -0.0166 -0.0104 60 C 0.0695 -0.0082 -0.0157 -0.0166 -0.0104 61 C -0.0008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 -0.0255 -0.0435 65 C -0.0302 -0.038 -0.0203 -0.0154 66 C -0.0557 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0144 -0.0177 -0.0203 -0.0270 68 C -0.1759 -0.0144 -0.0148	56	С	0.0624	-0.0162	-0.0215	-0.0253	-0.0328	
58 C -0.1218 -0.0087 0.0073 0.0069 0.0163 59 C 0.0678 -0.0083 -0.0158 -0.0167 -0.0112 60 C 0.0695 -0.0082 -0.0157 -0.0166 -0.0104 61 C -0.1008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 -0.0245 -0.0259 -0.0435 65 C -0.0302 -0.038 -0.0177 -0.0203 -0.0157 66 C -0.0535 -0.0129 -0.0177 -0.0203 -0.0152 67 C -0.0557 -0.0144 -0.0179 -0.0230 -0.0270 68 C -0.1759 -0.0144 -0.0148 -0.0181 -0.0165 70 C	57	С	0.0736	-0.0083	-0.0157	-0.0167	-0.0108	
59 C 0.0087s -0.008s -0.0167 -0.0112 60 C 0.0695 -0.0082 -0.0157 -0.0166 -0.0104 61 C -0.1008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 -0.0245 -0.0259 -0.0435 65 C -0.0302 -0.0038 -0.0017 -0.0203 -0.0154 66 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0123 -0.0181 -0.0165 70 C 0.0204 -0.0124 -0.0148 -0.0181 -0.0129 71 C -0.0702 -0.018	58	C	-0.1218	-0.0087	0.0073	0.0069	0.0163	
60 C 0.0055 -0.0022 -0.0106 -0.0106 -0.0104 61 C -0.1008 -0.0141 -0.0195 -0.0226 -0.0352 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 -0.0245 -0.0259 -0.0435 65 C -0.0302 -0.0038 -0.0017 -0.0203 -0.0154 66 C -0.0555 -0.0129 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0123 -0.0181 -0.0165 70 C 0.0204 -0.0123 -0.0213 -0.0229 71 C -0.0702 -0.018	59		0.0678	-0.0083	-0.0158	-0.0167	-0.0112	
61 C 0.1010 0.0111 0.0111 0.01212 0.0212 62 C 0.0206 -0.0107 -0.0110 -0.0174 -0.0188 63 C -0.0038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 -0.0245 -0.0259 -0.0435 65 C -0.0302 -0.0038 -0.0084 -0.0267 -0.0617 66 C -0.0535 -0.0129 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0123 -0.0148 -0.0181 -0.0165 70 C 0.0204 -0.0123 -0.0197 -0.0213 -0.0229 71 C -0.0702 -0.018 0.0083 0.0026 0.0146 72 C	61	C C	-0.10095	-0.0082	-0.0137	-0.0166	-0.0104	
63 C -1.011 0.0111 0.0117 0.0094 0.0444 64 C -0.0038 -0.0103 0.0117 0.0094 0.0444 64 C -0.0108 -0.0149 -0.0245 -0.0259 -0.0435 65 C -0.0302 -0.0038 -0.0084 -0.0267 -0.0617 66 C -0.0535 -0.0129 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0144 -0.0179 -0.0230 -0.0270 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0042 -0.0123 -0.0197 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0253 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	62	c	0.0206	-0.0141	-0.0195	-0.0220	-0.0332	
64 C -0.0108 -0.0149 -0.0245 -0.0259 -0.0435 65 C -0.0302 -0.0038 -0.0084 -0.0267 -0.0617 66 C -0.0535 -0.0129 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0123 -0.0148 -0.0181 -0.0165 70 C 0.0042 -0.0123 -0.0197 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0253 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	63	č	-0.0038	-0.0103	0.0110	0.0094	0.0444	
65 C -0.0302 -0.0038 -0.0084 -0.0267 -0.0617 66 C -0.0535 -0.0129 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0124 -0.0148 -0.0181 -0.0165 70 C 0.0042 -0.0123 -0.0197 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0243 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	64	C	-0.0108	-0.0149	-0.0245	-0.0259	-0.0435	
66 C -0.0535 -0.0129 -0.0177 -0.0203 -0.0154 67 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0124 -0.0148 -0.0181 -0.0165 70 C 0.0042 -0.0123 -0.0177 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0243 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	65	С	-0.0302	-0.0038	-0.0084	-0.0267	-0.0617	
67 C -0.0557 -0.0154 0.0056 0.0010 0.0162 68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0124 -0.0148 -0.0181 -0.0165 70 C 0.0042 -0.0123 -0.0177 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0233 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	66	С	-0.0535	-0.0129	-0.0177	-0.0203	-0.0154	
68 C -0.1759 -0.0144 -0.0179 -0.0230 -0.0270 69 C 0.0204 -0.0124 -0.0148 -0.0181 -0.0165 70 C 0.0042 -0.0123 -0.017 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0253 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	67	С	-0.0557	-0.0154	0.0056	0.0010	0.0162	
69 C 0.0204 -0.0124 -0.0148 -0.0181 -0.0165 70 C 0.0042 -0.0123 -0.0197 -0.0213 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0253 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	68	С	-0.1759	-0.0144	-0.0179	-0.0230	-0.0270	
70 C 0.0042 -0.0123 -0.0123 -0.0229 71 C -0.0702 -0.0118 0.0083 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0253 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	69	C	0.0204	-0.0124	-0.0148	-0.0181	-0.0165	
71 C -0.0102 -0.0116 0.0005 0.0026 0.0146 72 C 0.0612 -0.0163 -0.0215 -0.0253 -0.0345 73 C 0.0391 -0.0098 -0.0195 -0.0204 -0.0291	/U 71		0.0042	-0.0123	-0.0197	-0.0213	-0.0229	
73 C 0.0391 -0.098 -0.0195 -0.0204 -0.0291	71		-0.0702	-0.0118	-0.0083	-0.0026	-0.0146	
	73	c	0.0391	-0.0098	-0.0195	-0.0204	-0.0291	

74	С	0.0386	-0.0099	-0.0195	-0.0204	-0.0287	
75	С	-0.1209	-0.0049	0.0116	0.0111	0.0342	
76	С	0.0351	-0.0098	-0.0195	-0.0203	-0.0291	
77	С	0.0054	-0.0124	-0.0196	-0.0213	-0.0234	
78	С	-0.0376	-0.0083	-0.0154	-0.0225	-0.0416	
79	С	-0.0686	-0.0117	0.0084	0.0026	0.0153	
80	С	0.0190	-0.0123	-0.0147	-0.0180	-0.0163	
81	Sc	0.4269	0.3785	0.5106	1.0990	1.8638	1.87E+00
82	Sc	0.4286	0.3785	0.5107	1.0991	1.8637	1.87E+00
83	Sc	0.4259	0.3780	0.5101	1.0986	1.8643	1.86E+00
84	Ν	-1.3713	-0.2837	-0.5627	-1.2350	-2.1653	-1.82E+00
	F1(B39)	0.0899	-0.8512	-0.9692	-2.0622	-3.4265	0.0000
	F2(SC3N)	-0.0899	0.8512	0.9687	2.0617	3.4265	3.7720
	Total	0.0000	0.0000	-0.0005	-0.0005	0.0000	3.7720

Sc+N calibration curve constraction:

Charges on Sc3N		Sc 1s orbital energies	N 1s orbital energies
	-2	-161.91662	-14.30738
	-1	-161.95064	-14.31969
	0	-161.96970	-14.34887
	1	-161.96222	-14.34855
	2	-162.03197	-14.3908



 Orbital energies in Sc3N@C80 complex

 Sc 1s
 -161.9945

 N 1s
 -14.37341



 $Q_{predicted}^{Sc} = 1.226$

 $Q_{predicted}^{N} = 1.502$

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