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Calculation of interaction mechanism for complex catalyst HF-BF_3 with p-methylstyrene in toluene with stoichiometric composition 1:1:1 by AB initio method

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Abstract: For the first time, a quantum-chemical study of initiation mechanism for monomer of *n*-methylstyrene cationic polymerization in the presence of a complex catalyst boron fluoride-hydrogen fluoride in toluene (with stoichiometric composition 1:1:1) was carried out by *ab initio* method. It was shown that activation energy of this reaction is 76 kJ/mol, and the thermal effect is 0 kJ/mol.

Keywords: *p*-methylstyrene, initiation mechanism, catalyst boron fluoride-hydrogen fluoride, toluene, reaction heat, *ab initio* method.

Introduction

Until now, a number of important fundamental questions remains unstudied, in particular, the questions, concerning the mechanisms of elementary acts of *n*-methylstyrene cationic polymerization, i.e initiation, growth and chain termination in the presence of a complex catalyst

$BF_3 \cdot HF$ in toluene. Therefore, the aim of this paper is to study the mechanism of *n*-methylstyrene initiation (within the framework of molecular model) in the presence of said complex catalyst by calculation of interaction reaction between monomer and initiator along the $R_{C1\text{-}H20}$ coordinate in toluene (with stoichiometric composition 1:1:1).

Methodical part

The initiation mechanism of monomer cationic polymerization for *n*-methylstyrene in the presence of a complex catalyst $BF_3 \cdot HF$ in toluene (with a stoichiometric mixture of 1:1:1) was studied. The distance between C(1) and H(20) atoms was chosen as a reaction coordinate. The calculation was carried out by *ab initio* RHF/6-311G** quantum chemical method [1] with geometry optimization for all parameters by gradient method incorporated into Firefly program [2] and based on GAMESS source code [1, 3]. This method was chosen due to the fact that it allows one to accurately calculate the energy barriers of a reaction and determine the active centers [3]. The calculations were performed within the framework of isolated molecule in toluene. The initiation mechanism of *n*-methylstyrene was realized according to the procedure described in detail in [4] and applied in papers [5-8]. The MacMolPlt program was used to visualize of molecule [9].

Calculation data

The calculation data for changes in bond lengths along the path of interaction, bond angles, atomic charges within molecular system during interaction of *n*-methylstyrene with $BF_3 \cdot HF$ catalyst in toluene (with stoichiometric composition 1:1:1) are presented in Table 1-3.

In Fig. 1 shows the geometric and electronic structure of initial model of *n*-methylstyrene, in Fig. 2 - the final structure of interaction of catalyst with *p*-methylstyrene, in Fig. 3 - the energy profile of this interaction, and in Fig. 4 – the change in atomic charges that directly involved in the interaction of complex catalyst $HF \cdot BF_3$ with *p*-methylstyrene.

Atoms C(1), C(2), H(20), F(21) and B(22) are directly involved in initiation of polymerization. Let us analyze the change in these atomic charges along selected reaction coordinate.

At the coordination stage (Stage 1, Steps 1-7), the atomic charge on C(1) changes from - 0.209 to - 0.245, at the stage of active center (AC) formation (Stage 2, Steps 8-17) - from - 0.257 to - 0.351, at the stage of final product formation (Stage 3, Steps 18-21) - from - 0.369 to - 0.245.

At the 1st stage, the atomic charge on C(2) changes from - 0.174 to - 0.178, at the 2nd stage - from - 0.173 to - 0.075, at the 3rd stage - from - 0.022 to - 0.110.

At the coordination stage, the atomic charge on H(20) changes from - 0.325 to - 0.329, at the AC formation stage - from - 0.366 to - 0.407, at the stage of final product formation - from 0.416 to 0.195.

At the 1st stage, the atomic charge on F(21) changes from - 0.334 to - 0.351, at the 2nd stage - from - 0.356 to - 0.440, at the 3rd stage - from - 0.441 to - 0.472.

At the coordination stage, the atomic charge on B(22) changes from - 0.816 to - 0.821, at the AC formation stage - from - 0.823 to - 0.847, and at the stage of final product formation - from 0.860 to 0.866.

The toluene atomic charges on (C(26)-C(32) and H(33)-H(40)) along the reaction coordinate varied in the following ranges: for C(26)-C(32) - from -0.175 to - 0.172 , for H(33)-H(40) - from 0.118 to 0.148. During this reaction, the F(21)-H(20) bonds are broken simultaneously, and the C(1)-C(2) double π-bond is transformed into a single σ-bond, a new bond C(1)-H(20) and a counter-ion $[BF_3 \cdot OH]^-$ (Fig. 2).

Calculated value of reaction activation energy was 76 kJ/mol, and the value of thermal effect was 0 kJ/mol.

Thus, the change in atomic charges, the behavior of reaction fragments, the breaking of old bonds and formation of new bonds in reaction studied indicate that it proceeds according to coordinated interactions scheme.

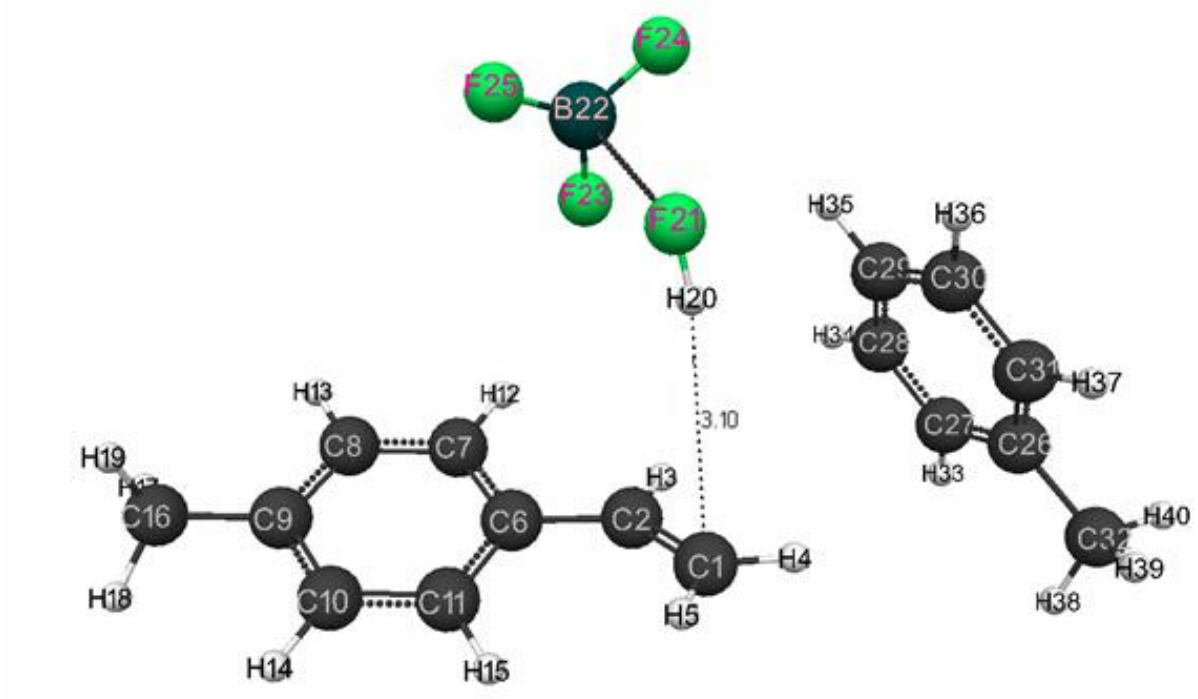

Figure 1. *The structure of initial model for complex catalyst HF·BF_3 with p-methylstyrene in toluene (the stoichiometric composition 1:1:1)*

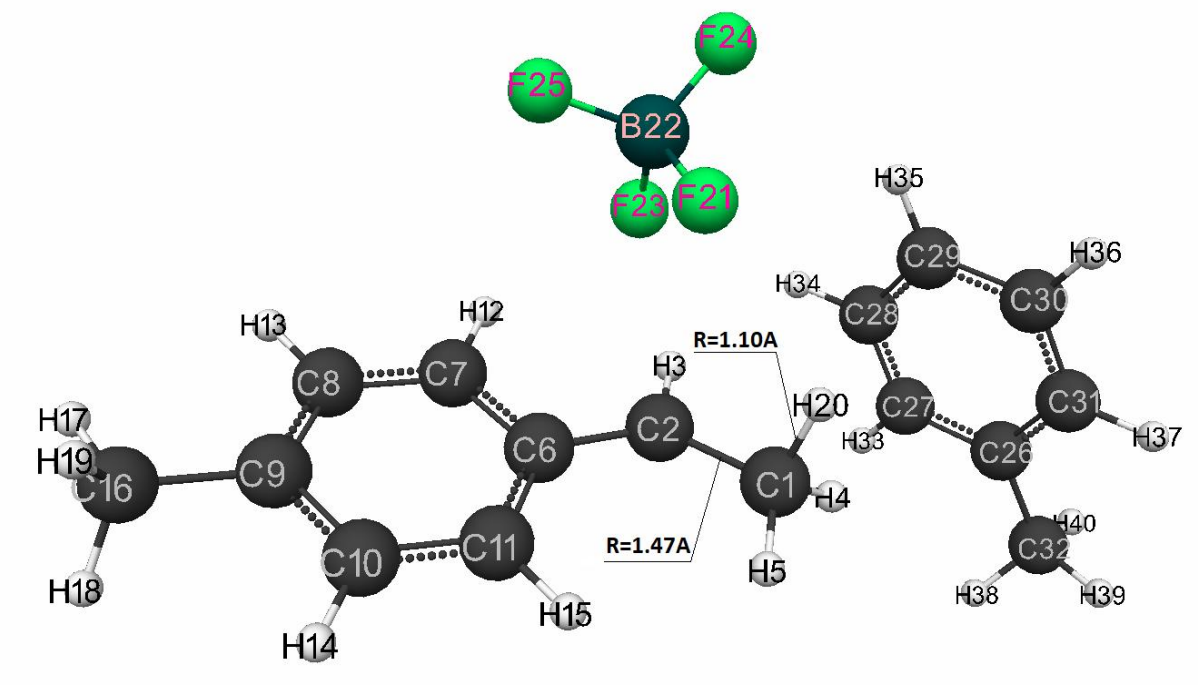

Figure 2. *The final interaction structure of complex catalyst $H_2O{\cdot}BF_3$ with p-methylstyrene in toluene (the stoichiometric composition 1:1:1)*

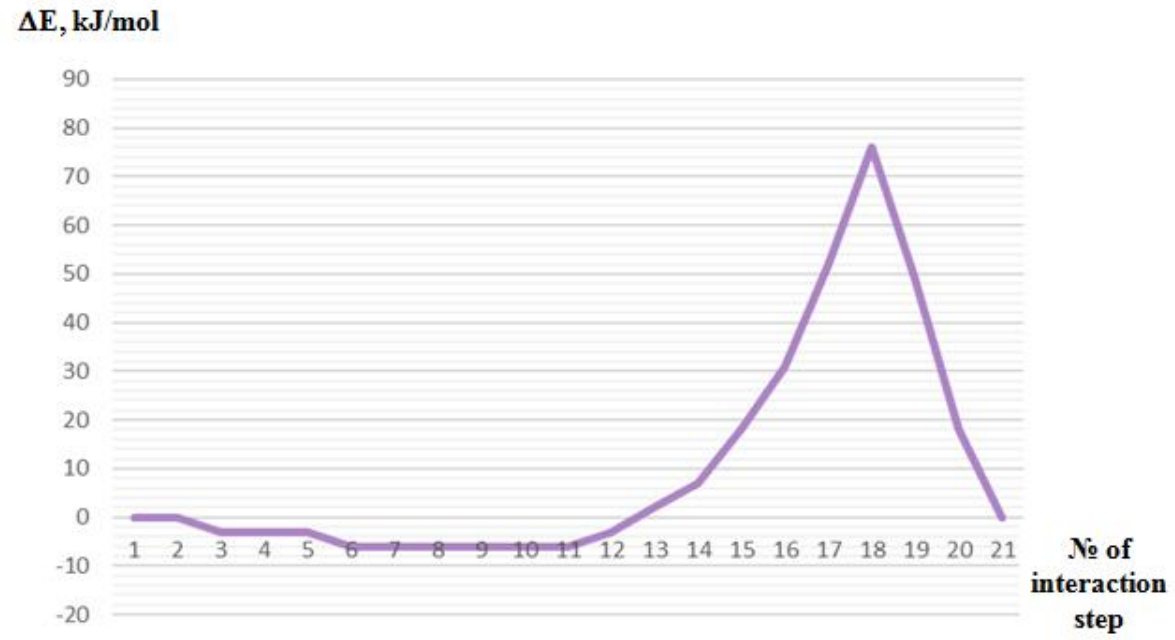

Figure 3. *Change in total energy (DE, kJ/mol) in the interaction process of the complex catalyst $H_2O{\cdot}BF_3$ with p-methylstyrene in toluene (the stoichiometric composition 1:1:1)*

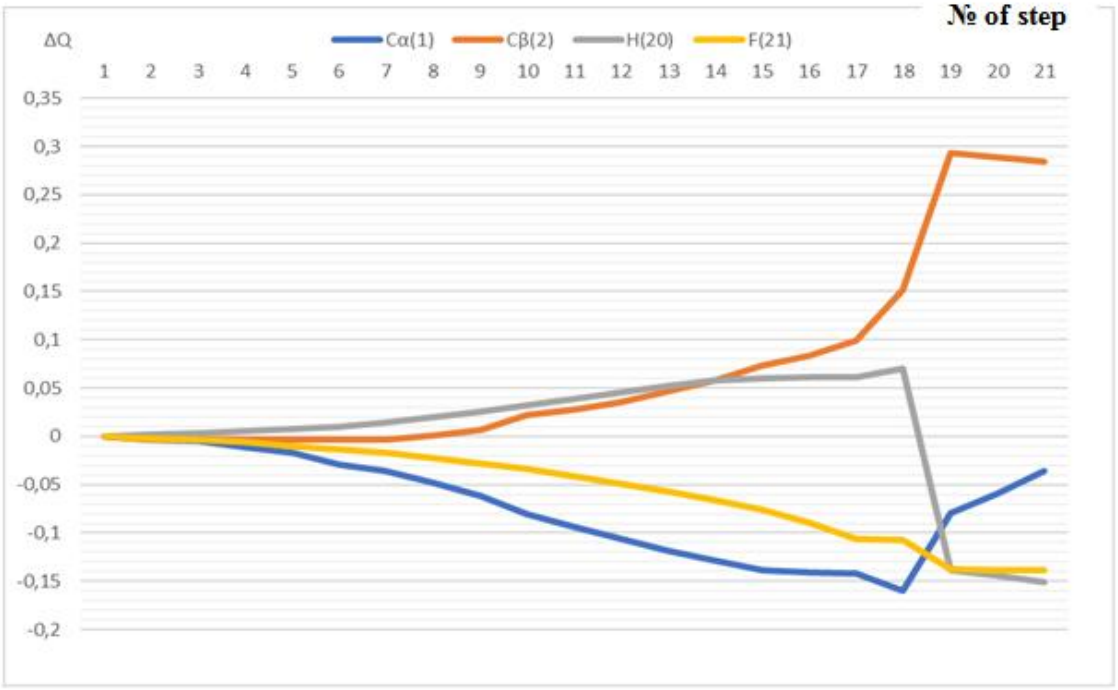

Figure 4. *Change in atomic charges (DQ) on C(1), C(2), H(20) and F(21) atoms along the coordinate of reaction studied (1-21 - № of step).*

Table 1. Change in bond lengths along the interaction pathway of complex catalyst HF BF_3 with *p*-methylstyrene in toluene (the stoichiometric composition of 1:1:1)

No of step	1	2	3	4	5	6	7	8	9	10
C(2)-C(1)	1,32	1,32	1,33	1,33	1,33	1,33	1,33	1,33	1,33	1,33
H(3)-C(2)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(4)-C(1)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(5)-C(1)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
C(6)-C(11)	1,39	1,39	1,40	1,40	1,40	1,40	1,40	1,40	1,40	1,40
C(6)-C(2)	1,48	1,48	1,48	1,48	1,48	1,48	1,48	1,48	1,48	1,48
C(7)-C(6)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(8)-C(7)	1,38	1,38	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(9)-C(8)	1,39	1,39	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38
C(10)-C(9)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(11)-C(10)	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38
H(12)-C(7)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(13)-C(8)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(14)-C(10)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(15)-C(11)	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07
C(16)-C(9)	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51

H(17)-C(16)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(18)-C(16)	1,08	1,08	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09
H(19)-C(16)	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09
H(20)-F(21)	0,90	0,90	0,90	0,90	0,90	0,90	0,91	0,91	0,91	0,91
H(20)-C(1)	3,10	3,00	2,90	2,80	2,70	2,60	2,50	2,40	2,30	2,20
B(22)-F(21)	2,43	2,42	2,41	2,41	2,40	2,41	2,39	2,38	2,37	2,36
F(23)-B(22)	1,30	1,30	1,30	1,30	1,30	1,31	1,31	1,31	1,31	1,31
F(24)-B(22)	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,30
F(25)-B(22)	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,30
C(26)-C(31)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(27)-C(26)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(28)-C(27)	1,38	1,38	1,38	1,38	1,38	1,39	1,39	1,39	1,39	1,39
C(29)-C(28)	1,39	1,39	1,39	1,39	1,39	1,38	1,38	1,38	1,38	1,38
C(30)-C(29)	1,38	1,38	1,38	1,38	1,38	1,39	1,39	1,39	1,39	1,39
C(31)-C(30)	1,39	1,39	1,39	1,39	1,39	1,38	1,38	1,38	1,38	1,39
C(32)-C(26)	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51
H(33)-C(27)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(34)-C(28)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(35)-C(29)	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07
H(36)-C(30)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,07
H(37)-C(31)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(38)-C(32)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(39)-C(32)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(40)-C(32)	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09

Continuation of ***Table 1.***

No of step	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**
C(2)-C(1)	1,33	1,33	1,33	1,33	1,33	1,33	1,33	1,34	1,46	1,47	1,47
H(3)-C(2)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,07	1,07	1,07
H(4)-C(1)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(5)-C(1)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
C(6)-C(11)	1,40	1,39	1,40	1,39	1,40	1,39	1,40	1,40	1,42	1,42	1,42
C(6)-C(2)	1,48	1,48	1,48	1,48	1,48	1,48	1,47	1,47	1,40	1,40	1,39
C(7)-C(6)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,41	1,41	1,41
C(8)-C(7)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,38	1,38	1,38	1,38
C(9)-C(8)	1,38	1,38	1,38	1,38	1,38	1,39	1,39	1,39	1,39	1,39	1,39
C(10)-C(9)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,40	1,41	1,41	1,41
C(11)-C(10)	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,36	1,36	1,36
H(12)-C(7)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,07	1,07	1,07

H(13)-C(8)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,07	1,07	1,07
H(14)-C(10)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,07	1,07	1,07
H(15)-C(11)	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07
C(16)-C(9)	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,50	1,50	1,50
H(17)-C(16)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(18)-C(16)	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,08	1,09	1,09
H(19)-C(16)	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09
H(20)-F(21)	0,91	0,92	0,92	0,93	0,94	0,95	0,97	1,06	2,51	2,52	2,51
H(20)-C(1)	2,10	2,00	1,90	1,80	1,70	1,60	1,50	1,40	1,30	1,20	1,10
B(22)-F(21)	2,34	2,33	2,30	2,29	2,26	2,22	2,15	1,72	1,41	1,41	1,41
F(23)-B(22)	1,31	1,31	1,31	1,31	1,31	1,31	1,31	1,34	1,42	1,42	1,42
F(24)-B(22)	1,30	1,30	1,30	1,30	1,30	1,30	1,31	1,33	1,36	1,36	1,36
F(25)-B(22)	1,30	1,30	1,30	1,30	1,30	1,30	1,30	1,32	1,37	1,37	1,37
C(26)-C(31)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(27)-C(26)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(28)-C(27)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39
C(29)-C(28)	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,39	1,39	1,39
C(30)-C(29)	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,39	1,38	1,38	1,38
C(31)-C(30)	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,38	1,39	1,39	1,39
C(32)-C(26)	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51	1,51
H(33)-C(27)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(34)-C(28)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,07	1,07	1,07
H(35)-C(29)	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07
H(36)-C(30)	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,07	1,08	1,08	1,08
H(37)-C(31)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(38)-C(32)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,09	1,09	1,09
H(39)-C(32)	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08	1,08
H(40)-C(32)	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09	1,09

Table 2. *Change in valence angles along the interaction pathway of complex catalyst HF BF_3 with p-methylstyrene in toluene (the stoichiometric composition of 1:1:1)*

No of step	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
H(3)-C(2)-C(1)	118	118	118	118	118	118	118	118	118	118
H(4)-C(1)-C(2)	121	121	121	120	120	120	121	121	121	121
H(5)-C(1)-C(2)	123	123	123	123	123	123	123	123	122	123
C(6)-C(11)-C(10)	121	121	121	121	121	121	121	121	121	121
C(6)-C(2)-C(1)	127	127	127	127	127	127	127	127	127	127
C(7)-C(6)-C(11)	118	118	118	118	118	118	118	118	118	118
C(8)-C(7)-C(6)	121	121	121	121	121	121	121	121	121	121

C(9)-C(8)-C(7)	121	121	121	121	121	121	121	121	121	121
C(10)-C(9)-C(8)	118	118	118	118	118	118	118	118	118	118
C(11)-C(10)-C(9)	121	121	121	121	121	121	121	121	121	121
H(12)-C(7)-C(6)	120	120	120	120	120	120	120	120	120	120
H(13)-C(8)-C(7)	119	119	119	119	119	119	119	119	119	119
H(14)-C(10)-C(9)	120	120	119	119	119	119	119	119	119	119
H(15)-C(11)-C(10)	119	119	119	119	119	119	119	119	119	119
C(16)-C(9)-C(8)	121	121	122	122	122	122	122	122	122	122
H(17)-C(16)-C(9)	111	111	111	111	111	111	111	111	111	111
H(18)-C(16)-C(9)	111	111	111	111	111	111	111	111	111	111
H(19)-C(16)-C(9)	111	111	111	111	111	111	111	111	111	111
H(20)-F(21)-B(22)	123	123	122	122	123	122	122	122	122	122
H(20)-C(1)-C(2)	69	69	70	72	72	74	74	75	77	79
F(23)-B(22)-F(21)	91	91	91	91	91	91	91	91	91	91
F(24)-B(22)-F(21)	92	92	92	92	92	92	92	92	93	93
F(25)-B(22)-F(21)	94	94	94	94	94	94	94	94	94	94
C(26)-C(31)-C(30)	121	121	121	121	121	121	121	121	121	121
C(27)-C(26)-C(31)	118	118	118	118	118	118	118	118	118	118
C(28)-C(27)-C(26)	121	121	121	121	121	121	121	121	121	121
C(29)-C(28)-C(27)	120	120	120	120	120	120	120	120	120	120
C(30)-C(29)-C(28)	119	119	119	119	119	119	119	119	119	119
C(31)-C(30)-C(29)	120	120	120	120	120	120	120	120	120	120
C(32)-C(26)-C(31)	121	121	121	121	121	121	121	121	121	121
H(33)-C(27)-C(26)	120	120	120	120	120	120	120	120	120	120
H(34)-C(28)-C(27)	120	120	120	120	120	120	120	120	120	120
H(35)-C(29)-C(28)	120	120	120	120	120	120	121	121	121	121
H(36)-C(30)-C(29)	120	120	120	120	120	120	120	120	120	120
H(37)-C(31)-C(30)	119	119	119	119	119	120	119	119	119	119
H(38)-C(32)-C(26)	111	111	111	111	111	111	111	111	111	111
H(39)-C(32)-C(26)	111	111	111	111	111	111	111	111	111	111
H(40)-C(32)-C(26)	111	111	111	111	111	111	111	111	111	111

Continuation of ***Table 2.***

No of step	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**
H(3)-C(2)-C(1)	118	118	118	118	118	118	118	117	115	115	116
H(4)-C(1)-C(2)	121	121	120	121	120	120	120	120	112	111	110
H(5)-C(1)-C(2)	122	122	123	122	122	122	122	122	117	116	115
C(6)-C(11)-C(10)	121	121	121	121	121	121	121	121	120	120	120
C(6)-C(2)-C(1)	127	127	127	127	127	127	127	128	128	128	128

C(7)-C(6)-C(11)	118	118	118	118	118	118	118	119	119	119	119
C(8)-C(7)-C(6)	121	121	121	121	121	121	121	121	120	120	120
C(9)-C(8)-C(7)	121	121	121	121	121	121	121	121	120	120	120
C(10)-C(9)-C(8)	118	118	118	118	118	118	118	118	120	120	120
C(11)-C(10)-C(9)	121	121	121	121	121	121	121	121	121	121	120
H(12)-C(7)-C(6)	120	120	120	120	120	120	120	120	119	119	119
H(13)-C(8)-C(7)	119	119	119	119	119	119	119	119	120	120	120
H(14)-C(10)-C(9)	119	120	119	119	119	120	120	120	119	119	119
H(15)-C(11)-C(10)	119	119	119	119	119	119	119	119	119	120	120
C(16)-C(9)-C(8)	122	122	122	122	122	121	121	121	121	121	121
H(17)-C(16)-C(9)	111	111	111	111	111	111	111	111	112	112	112
H(18)-C(16)-C(9)	111	111	111	111	111	111	111	111	111	110	110
H(19)-C(16)-C(9)	111	111	111	111	111	111	111	111	110	110	110
H(20)-F(21)-B(22)	122	122	122	123	123	123	124	123	148	148	148
H(20)-C(1)-C(2)	80	81	83	85	87	89	90	88	99	102	103
F(23)-B(22)-F(21)	92	92	92	92	93	93	94	100	106	106	106
F(24)-B(22)-F(21)	93	93	93	93	94	94	95	101	110	110	110
F(25)-B(22)-F(21)	94	94	94	94	94	95	95	102	109	109	109
C(26)-C(31)-C(30)	121	121	121	121	121	121	121	121	121	121	121
C(27)-C(26)-C(31)	118	118	118	118	118	118	118	118	118	118	118
C(28)-C(27)-C(26)	121	121	121	121	121	121	121	121	121	121	121
C(29)-C(28)-C(27)	120	120	120	120	120	120	120	120	120	120	120
C(30)-C(29)-C(28)	119	119	119	119	119	119	119	119	119	119	119
C(31)-C(30)-C(29)	120	120	120	120	120	120	120	120	120	120	120
C(32)-C(26)-C(31)	121	121	121	121	121	121	121	121	121	121	121
H(33)-C(27)-C(26)	120	120	120	120	120	120	120	120	119	119	119
H(34)-C(28)-C(27)	120	120	120	120	120	120	120	120	120	120	120
H(35)-C(29)-C(28)	121	121	121	121	121	121	121	121	120	120	120
H(36)-C(30)-C(29)	120	120	120	120	120	120	120	120	120	120	120
H(37)-C(31)-C(30)	119	119	119	119	119	119	119	119	120	120	120
H(38)-C(32)-C(26)	111	111	111	111	111	111	111	111	111	111	111
H(39)-C(32)-C(26)	111	111	111	111	111	111	111	111	111	111	111
H(40)-C(32)-C(26)	111	111	111	111	111	111	111	111	111	111	111

Table 3.*Change in atomic charges along the interaction pathway of complex catalyst HF BF_3 with p-methylstyrene in toluene (the stoichiometric composition of 1:1:1)*

Atom	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
C(1)	-0,209	-0,212	-0,214	-0,220	-0,226	-0,238	-0,245	-0,257	-0,270	-0,290
C(2)	-0,174	-0,178	-0,177	-0,177	-0,178	-0,177	-0,178	-0,173	-0,168	-0,152

H(3)	0,119	0,120	0,118	0,119	0,121	0,121	0,123	0,124	0,124	0,122
H(4)	0,134	0,136	0,143	0,144	0,146	0,156	0,157	0,159	0,161	0,167
H(5)	0,105	0,106	0,105	0,107	0,108	0,108	0,110	0,112	0,114	0,116
C(6)	-0,054	-0,053	-0,062	-0,059	-0,058	-0,061	-0,060	-0,060	-0,061	-0,065
C(7)	-0,068	-0,067	-0,056	-0,056	-0,056	-0,055	-0,054	-0,052	-0,051	-0,046
C(8)	-0,090	-0,090	-0,084	-0,084	-0,084	-0,084	-0,083	-0,083	-0,083	-0,084
C(9)	-0,120	-0,120	-0,123	-0,122	-0,122	-0,122	-0,122	-0,122	-0,121	-0,121
C(10)	-0,084	-0,084	-0,086	-0,086	-0,086	-0,086	-0,086	-0,086	-0,086	-0,086
C(11)	-0,064	-0,064	-0,060	-0,061	-0,061	-0,060	-0,060	-0,060	-0,060	-0,057
H(12)	0,104	0,105	0,100	0,101	0,102	0,103	0,104	0,104	0,104	0,100
H(13)	0,088	0,088	0,087	0,087	0,088	0,088	0,088	0,088	0,088	0,089
H(14)	0,086	0,086	0,086	0,086	0,087	0,087	0,087	0,088	0,088	0,088
H(15)	0,092	0,092	0,091	0,092	0,092	0,092	0,093	0,093	0,094	0,094
C(16)	-0,177	-0,177	-0,177	-0,177	-0,177	-0,177	-0,177	-0,177	-0,177	-0,177
H(17)	0,100	0,099	0,095	0,095	0,095	0,095	0,095	0,095	0,096	0,096
H(18)	0,098	0,098	0,106	0,106	0,106	0,107	0,107	0,107	0,108	0,108
H(19)	0,114	0,114	0,110	0,110	0,111	0,110	0,110	0,110	0,111	0,110
H(20)	0,346	0,348	0,349	0,351	0,354	0,356	0,360	0,366	0,372	0,378
F(21)	-0,334	-0,336	-0,338	-0,340	-0,344	-0,347	-0,351	-0,356	-0,362	-0,368
B(22)	0,816	0,818	0,815	0,817	0,818	0,820	0,821	0,823	0,825	0,822
F(23)	-0,288	-0,288	-0,288	-0,288	-0,289	-0,290	-0,291	-0,292	-0,293	-0,292
F(24)	-0,273	-0,274	-0,274	-0,275	-0,275	-0,274	-0,274	-0,275	-0,276	-0,278
F(25)	-0,263	-0,263	-0,263	-0,263	-0,264	-0,264	-0,265	-0,265	-0,266	-0,266
C(26)	-0,123	-0,124	-0,123	-0,123	-0,123	-0,118	-0,118	-0,118	-0,118	-0,116
C(27)	-0,098	-0,098	-0,098	-0,099	-0,100	-0,100	-0,100	-0,100	-0,101	-0,100
C(28)	-0,088	-0,088	-0,087	-0,087	-0,087	-0,087	-0,087	-0,087	-0,087	-0,083
C(29)	-0,130	-0,130	-0,126	-0,126	-0,125	-0,126	-0,126	-0,125	-0,124	-0,127
C(30)	-0,100	-0,100	-0,100	-0,099	-0,096	-0,097	-0,095	-0,093	-0,091	-0,093
C(31)	-0,099	-0,099	-0,104	-0,104	-0,105	-0,108	-0,108	-0,109	-0,110	-0,114
C(32)	-0,175	-0,175	-0,174	-0,174	-0,174	-0,175	-0,175	-0,174	-0,174	-0,174
H(33)	0,089	0,089	0,088	0,088	0,088	0,087	0,087	0,087	0,087	0,087
H(34)	0,099	0,098	0,098	0,097	0,097	0,096	0,096	0,096	0,096	0,095
H(35)	0,118	0,118	0,117	0,118	0,117	0,115	0,115	0,115	0,114	0,110
H(36)	0,105	0,105	0,106	0,106	0,106	0,106	0,106	0,107	0,107	0,112
H(37)	0,088	0,088	0,088	0,088	0,088	0,088	0,088	0,088	0,087	0,088
H(38)	0,100	0,100	0,100	0,100	0,099	0,098	0,098	0,097	0,097	0,097
H(39)	0,096	0,096	0,096	0,096	0,096	0,097	0,097	0,097	0,097	0,097
H(40)	0,114	0,114	0,114	0,114	0,114	0,113	0,113	0,113	0,113	0,113

Continuation of ***Table 3.***

Atom	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**
C(1)	-0,303	-0,315	-0,328	-0,338	-0,347	-0,350	-0,351	-0,369	-0,288	-0,268	-0,245
C(2)	-0,146	-0,138	-0,127	-0,116	-0,101	-0,090	-0,075	-0,022	0,119	0,115	0,110
H(3)	0,124	0,125	0,124	0,125	0,124	0,126	0,129	0,147	0,242	0,239	0,237
H(4)	0,168	0,170	0,174	0,174	0,176	0,176	0,177	0,186	0,181	0,172	0,165
H(5)	0,118	0,121	0,123	0,126	0,128	0,130	0,132	0,138	0,118	0,112	0,106
C(6)	-0,067	-0,070	-0,075	-0,080	-0,086	-0,091	-0,099	-0,133	-0,213	-0,211	-0,211
C(7)	-0,046	-0,044	-0,042	-0,040	-0,038	-0,035	-0,031	-0,008	0,067	0,069	0,069
C(8)	-0,083	-0,084	-0,084	-0,084	-0,084	-0,085	-0,085	-0,088	-0,113	-0,111	-0,110
C(9)	-0,120	-0,120	-0,119	-0,118	-0,117	-0,116	-0,114	-0,105	-0,054	-0,054	-0,053
C(10)	-0,086	-0,086	-0,086	-0,087	-0,087	-0,088	-0,088	-0,092	-0,114	-0,114	-0,115
C(11)	-0,057	-0,057	-0,054	-0,054	-0,050	-0,049	-0,046	-0,032	0,021	0,022	0,023
H(12)	0,101	0,101	0,100	0,101	0,100	0,101	0,103	0,112	0,181	0,178	0,178
H(13)	0,089	0,090	0,090	0,090	0,091	0,091	0,092	0,097	0,119	0,119	0,119
H(14)	0,088	0,089	0,089	0,090	0,090	0,091	0,092	0,095	0,108	0,108	0,108
H(15)	0,095	0,095	0,096	0,096	0,097	0,098	0,099	0,103	0,120	0,122	0,123
C(16)	-0,178	-0,178	-0,178	-0,178	-0,178	-0,178	-0,178	-0,180	-0,186	-0,186	-0,186
H(17)	0,096	0,096	0,096	0,096	0,097	0,097	0,098	0,101	0,118	0,118	0,118
H(18)	0,108	0,108	0,109	0,109	0,110	0,110	0,111	0,113	0,122	0,124	0,125
H(19)	0,111	0,111	0,111	0,112	0,112	0,113	0,114	0,118	0,136	0,135	0,135
H(20)	0,385	0,392	0,398	0,404	0,406	0,407	0,407	0,416	0,207	0,202	0,195
F(21)	-0,375	-0,383	-0,391	-0,400	-0,410	-0,423	-0,440	-0,441	-0,471	-0,472	-0,472
B(22)	0,825	0,828	0,829	0,832	0,834	0,839	0,847	0,860	0,866	0,866	0,866
F(23)	-0,294	-0,295	-0,297	-0,299	-0,301	-0,305	-0,311	-0,364	-0,471	-0,470	-0,470
F(24)	-0,278	-0,279	-0,280	-0,282	-0,283	-0,285	-0,290	-0,326	-0,389	-0,389	-0,389
F(25)	-0,267	-0,268	-0,269	-0,270	-0,272	-0,274	-0,278	-0,316	-0,412	-0,412	-0,411
C(26)	-0,117	-0,117	-0,116	-0,116	-0,115	-0,115	-0,116	-0,117	-0,122	-0,121	-0,121
C(27)	-0,101	-0,101	-0,101	-0,101	-0,101	-0,101	-0,102	-0,103	-0,124	-0,121	-0,121
C(28)	-0,084	-0,085	-0,084	-0,085	-0,085	-0,086	-0,087	-0,090	-0,113	-0,111	-0,112
C(29)	-0,125	-0,126	-0,128	-0,128	-0,128	-0,129	-0,130	-0,132	-0,123	-0,124	-0,124
C(30)	-0,089	-0,088	-0,089	-0,088	-0,088	-0,087	-0,086	-0,094	-0,093	-0,093	-0,093
C(31)	-0,114	-0,114	-0,115	-0,115	-0,115	-0,115	-0,115	-0,114	-0,109	-0,110	-0,109
C(32)	-0,174	-0,174	-0,175	-0,174	-0,175	-0,175	-0,175	-0,174	-0,171	-0,172	-0,172
H(33)	0,086	0,086	0,086	0,086	0,086	0,086	0,085	0,085	0,084	0,084	0,084
H(34)	0,095	0,095	0,095	0,095	0,095	0,094	0,094	0,094	0,125	0,125	0,125
H(35)	0,109	0,108	0,107	0,107	0,107	0,107	0,108	0,115	0,150	0,148	0,148
H(36)	0,112	0,112	0,114	0,115	0,115	0,116	0,118	0,125	0,100	0,099	0,099
H(37)	0,088	0,088	0,088	0,088	0,088	0,088	0,088	0,088	0,084	0,083	0,083

H(38)	0,097	0,097	0,096	0,096	0,096	0,096	0,096	0,095	0,092	0,092	0,092
H(39)	0,097	0,097	0,098	0,098	0,098	0,098	0,098	0,097	0,092	0,092	0,092
H(40)	0,113	0,113	0,113	0,113	0,113	0,113	0,113	0,113	0,114	0,114	0,114

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