

## **Quantum Mechanical study for vibration Frequencies C -C bonds for Benzo [J] Fluoranthene molecule, positive and negative radical Ions.**

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### **Introduction**

The chemistry of polyaromatic hydrocarbons (PAHs) is gaining increasing importance due to their carcinogenic properties and their presence in interstellar spaces [1]. They could become potential starting materials for petrochemical industries, being a significant component of the heavy fractions of earth oils [2]. For these reasons considerable efforts were made to study their chemical and physical properties [1], e. g. IR spectroscopic studies also on their radical cations. Benzo [J] Fluoranthene (Fig. 2), is a prominent member of the PAH family, for which IR spectroscopic studies were done. Measurements were done for its radical cation and anion in the isolated matrix [3], as well as ab initio theoretical studies [4]. However a complete normal coordinate analysis on the symmetry and the valence basis of all its  $3N-6$  vibration modes is still missing. Benzo (J) fluoranthene is present as a component of polycyclic aromatic hydrocarbons (PAH) content in the environment usually resulting from the incomplete combustion or pyrolysis of organic matters, especially fossil fuels and tobacco. Insufficient data are available on the effect of this substance on human health, therefore utmost care must be taken[5]. The effects of benzo [J] fluoranthene on human health will depend mainly on the extent of exposure (length of time, etc), the amount one is exposed to (or concentration) [6]. PAHs can break down by reaction with sunlight and other chemicals in the air, over a period of days to weeks[7]. Some PAHs may cause cancer and may affect the eyes, kidneys, and liver[8]. These compounds require activation to electrophilic metabolites to exert their mutagenic or carcinogenic effects[9]. The DNA damages caused through the reactive metabolites of PAH is described involving the DNA covalent binding to form stable or depurinating adducts, the formation of apurinic sites, and the oxidative damage [10]. In former papers we applied the DFT method [11] for the calculation of molecular geometries, vibration frequencies and IR absorption intensities of planner aromatic hydrocarbon as well as their radical cations and anions. Both valence and symmetry assignments of the vibration modes could be accomplished, applying group theoretical considerations [12].

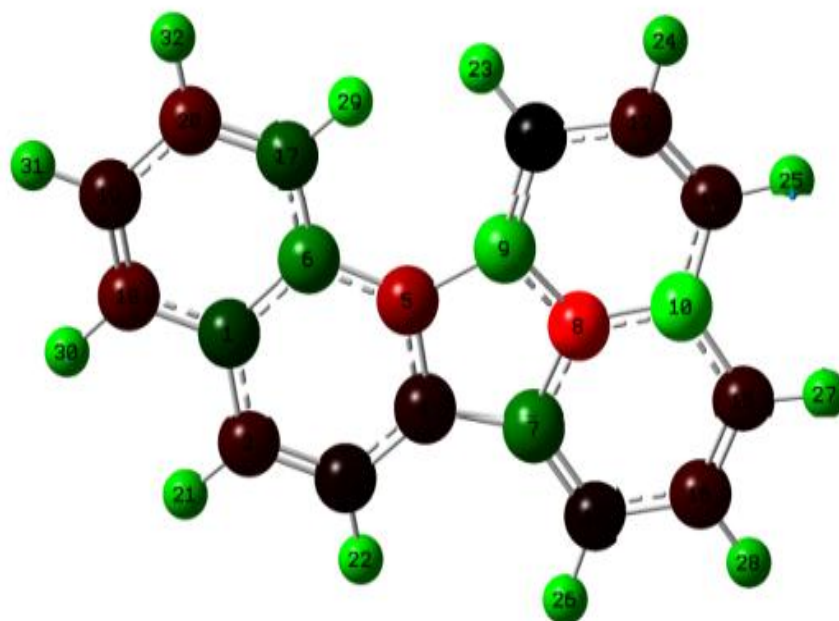
The present treatment enables calculating and assigning all  $(3N-6)$  vibration modes at once. Graphical representations of the vibration motion of the atoms for each mode could be obtained applying the Gaussian program[13]. The knowledge of the valence form of each vibration, as provided by the (DFT) values. (Fig. 3) allows a correlative comparison of the modes and consequently the force constants and bond strengths within the molecule. The physical and chemical properties of PAHs are determined by their conjugated electron systems, which are dependent on the number of aromatic rings and the molecular mass[14], [15].

### **Results.**

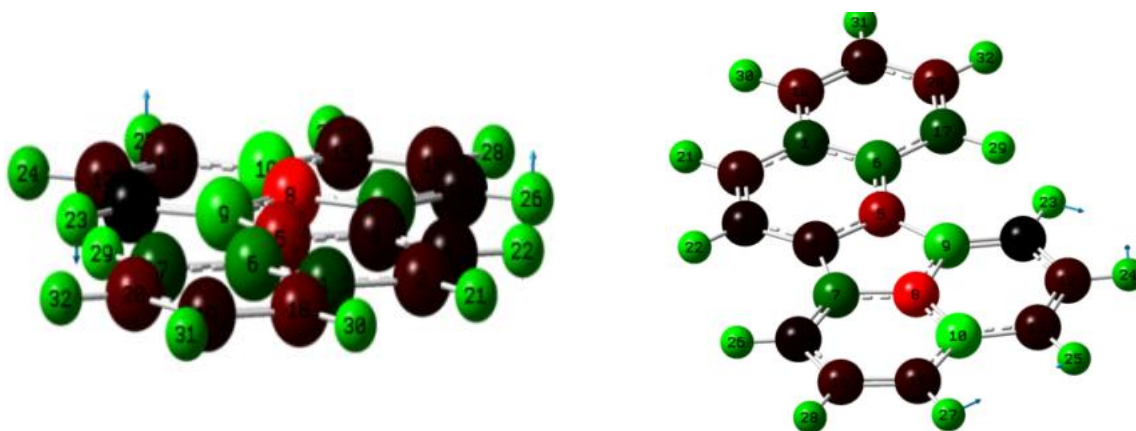
The ab initio quantum mechanical method was applied for the theoretical analysis of its vibration spectrum [16]. However, in this work only the basic and most prominent frequencies were discussed. As for Benzo [J] Fluoranthene [BJF] molecules the theoretical treatment were usually based on the ab initio [DFT] method and limited to the discussion of the most relevant vibrations with no full analyses of the  $[3N-6]$  normal coordinations [17]for the radical anion and cation, no experimental vibration frequencies were known. This method is used for evaluating vibration frequencies for the complete analysis of all vibration frequencies and normal coordinations of [BJF]. The reported vibration, IR. adsorption intensities are to be viewed cautiously, due to the quantum mechanical nature of [DFT] method by applied Gaussian03 program for our classification.

A B

Figure[1]: A description of the molecular vibrations motion of Benzo [J] Fluoranthene [BJF] is shown on this figure [1]; A-an in plane and B-an out of plane vibration mode.



Benzo[J]Fluoranthene shows Cs symmetry, The vibration Frequencies were calculated for the equilibrium geometry structure of the neutral and the two radical ions molecule (table-



1). Totally 90 modes of vibrations are expected for the molecule (3N-6). They are classified according to the character table[18], (61 $\hat{A}$ ) inplane, and (29 $''A$ ) out of-plane vibration modes (Figure-1). According to group theoretical considerations and a following irreducible representations :

$$\Gamma_{\text{tot.}} = 3N = 3 \times 32 = 96$$

$$\Gamma_{\text{vib}} = \Gamma_{\text{tot.}} - (\Gamma_{\text{rot.}} + \Gamma_{\text{tra.}})$$

$$\Gamma_{\text{tot.}} = 64\hat{A} + 32''A$$

$$\Gamma_{\text{vib}} = 3N - 6 = 96 - 6 = 90$$

$$\Gamma_{\text{vib}} = 61 \hat{A} + 29 ''A$$

(Fig-2): Structure of Benzo[J]Fluoranthene [BJF] showing the equilibrium geometry of the neutral molecule.

Table (1): Calculated geometry structures of Benzo [J] Fluoranthene [BJF] neutral molecule, radical cation and anion by [DFT].

Bond length (Å) and Bond angles (deg.)	Neutral molecule (DFT) B3LYP/6-311G	Cation (DFT) B3LYP/6-311G	Anion (DFT) B3LYP/6-311G
C <sub>1</sub> -C <sub>2</sub>	1.419	1.429	1.433
C <sub>1</sub> -C <sub>6</sub>	1.445	1.440	1.449
C <sub>1</sub> -C <sub>18</sub>	1.425	1.409	1.417
C <sub>2</sub> -- C <sub>3</sub>	1.380	1.391	1.381
C <sub>2</sub> -H <sub>21</sub>	1.083	1.082	1.085
C <sub>3</sub> -- C <sub>4</sub>	1.404	1.392	1.407
C <sub>3</sub> -H <sub>22</sub>	1.080	1.080	1.085
C <sub>4</sub> -C <sub>5</sub>	1.422	1.468	1.451
C <sub>4</sub> -C <sub>7</sub>	1.475	1.456	1.447
C <sub>5</sub> -C <sub>6</sub>	1.432	1.450	1.430
C <sub>5</sub> -C <sub>9</sub>	1.488	1.451	1.454
C <sub>6</sub> -C <sub>17</sub>	1.428	1.418	1.424
C <sub>7</sub> -- C <sub>8</sub>	1.418	1.418	1.424
C <sub>7</sub> -- C <sub>14</sub>	1.388	1.385	1.408
C <sub>8</sub> -- C <sub>9</sub>	1.428	1.437	1.432
C <sub>8</sub> -- C <sub>10</sub>	1.403	1.403	1.412
C <sub>9</sub> -- C <sub>11</sub>	1.391	1.397	1.414
C <sub>10</sub> -- C <sub>13</sub>	1.425	1.427	1.427
C <sub>10</sub> -- C <sub>15</sub>	1.429	1.427	1.427
C <sub>11</sub> -- C <sub>12</sub>	1.423	1.412	1.408
C <sub>11</sub> -- H <sub>23</sub>	1.076	1.079	1.081
C <sub>12</sub> -- C <sub>13</sub>	1.382	1.395	1.401
C <sub>12</sub> -- H <sub>24</sub>	1.083	1.081	1.086
C <sub>13</sub> -- H <sub>25</sub>	1.083	1.082	1.085
C <sub>14</sub> -- C <sub>16</sub>	1.426	1.421	1.407
C <sub>14</sub> --H <sub>26</sub>	1.083	1.081	1.085
C <sub>15</sub> -C <sub>16</sub>	1.383	1.388	1.403
C <sub>15</sub> -- H <sub>27</sub>	1.083	1.082	1.085
C <sub>16</sub> -- H <sub>28</sub>	1.419	1.080	1.085
C <sub>17</sub> -C <sub>20</sub>	1.445	1.395	1.387
C <sub>17</sub> -- H <sub>29</sub>	1.425	1.07 <sup>^</sup>	1.0 <sup>^</sup>
C <sub>18</sub> -- C <sub>19</sub>	1.380	1.396	1.388
C <sub>18</sub> --H <sub>30</sub>	1.083	1.082	1.085
C <sub>19</sub> --- C <sub>20</sub>	1.404	1.399	1.409
C <sub>19</sub> --H <sub>31</sub>	1.080	1.082	1.084
C <sub>20</sub> H <sub>32</sub>	1.422	1.080	1.084
< C <sub>2</sub> C <sub>1</sub> C <sub>7</sub>	120.357	120.290	119.792
< C <sub>2</sub> C <sub>1</sub> C <sub>18</sub>	120.287	120.309	121.229
< C <sub>7</sub> C <sub>1</sub> C <sub>18</sub>	119.354	119.400	118.978
< C <sub>1</sub> C <sub>2</sub> C <sub>7</sub>	121.156	122.056	121.238
< C <sub>7</sub> C <sub>2</sub> H <sub>21</sub>	120.150	119.651	120.489
< C <sub>1</sub> C <sub>2</sub> H <sub>21</sub>	118.694	118.293	118.272
< C <sub>7</sub> C <sub>2</sub> C <sub>4</sub>	119.474	119.102	120.476
< C <sub>7</sub> C <sub>2</sub> H <sub>22</sub>	120.123	120.153	119.783
< C <sub>4</sub> C <sub>2</sub> H <sub>22</sub>	120.402	120.734	119.739

< C <sub>2</sub> C <sub>4</sub> C <sub>6</sub>	121.833	121.182	120.421
< C <sub>2</sub> C <sub>4</sub> C <sub>7</sub>	129.205	130.360	130.819
< C <sub>5</sub> C <sub>4</sub> C <sub>7</sub>	108.961	108.457	108.759
< C <sub>4</sub> C <sub>5</sub> C <sub>7</sub>	119.296	119.563	119.636
< C <sub>4</sub> C <sub>6</sub> C <sub>9</sub>	107.359	107.546	107.679
< C <sub>7</sub> C <sub>6</sub> C <sub>9</sub>	133.344	132.890	132.684
< C <sub>1</sub> C <sub>7</sub> C <sub>6</sub>	117.882	117.805	118.435
< C <sub>1</sub> C <sub>7</sub> C <sub>17</sub>	117.328	118.171	117.386
< C <sub>6</sub> C <sub>7</sub> C <sub>17</sub>	124.789	124.023	124.178
< C <sub>4</sub> C <sub>7</sub> C <sub>8</sub>	106.254	105.883	106.077
< C <sub>4</sub> C <sub>7</sub> C <sub>14</sub>	135.189	135.160	135.644
< C <sub>8</sub> C <sub>7</sub> C <sub>14</sub>	118.556	118.956	118.278
< C <sub>7</sub> C <sub>8</sub> C <sub>9</sub>	111.045	111.904	111.254
< C <sub>9</sub> C <sub>8</sub> C <sub>10</sub>	125.196	124.492	124.849
< C <sub>7</sub> C <sub>8</sub> C <sub>10</sub>	123.758	122.055	123.895
< C <sub>5</sub> C <sub>9</sub> C <sub>8</sub>	106.379	106.208	106.229
< C <sub>8</sub> C <sub>9</sub> C <sub>11</sub>	116.237	117.372	116.852
< C <sub>5</sub> C <sub>9</sub> C <sub>11</sub>	137.383	136.419	136.917
benzo[J]Fluoranethen	Molecular formula	C <sub>20</sub> H <sub>12</sub>	
Point Group	Cs	Cs	Cs
E (UB+HF-LYP)=	_769.36a. u.	_769.106. a.u	_769.399a. u
Dipole moment	0.4404 (debye)	1.3412 (debye)	1.7525 (debye)

Table (2) : Vibrational frequencies and IR absorption intensities of Benzo [J] Fluoranthene [BJF] neutral molecule.

	Symmetry&description	(DFT) B3LYP/6-311G Frequency cm <sup>-1</sup>	Intensity km/mol
$\text{\AA}$			
v <sub>1</sub>	C H str.	3262	15.730
v <sub>2</sub>	C H str.	3228	12.090
v <sub>3</sub>	C H str.	3187	48.770
v <sub>4</sub>	C H str.	3185	68.670
v <sub>5</sub>	C H str.	3180	35.470
v <sub>6</sub>	C H str.	3179	51.007
v <sub>7</sub>	C H str.	3169	7.535
v <sub>8</sub>	C H str.	3169	31.490
v <sub>9</sub>	C H str.	3159	3.900
v <sub>10</sub>	C H str.	3158	3.040
v <sub>11</sub>	C H str.	3156	0.097
v <sub>12</sub>	C H str.	3155	2.920
v <sub>13</sub>	ring (CCC str.) + $\delta$ CH	1662	1.029
v <sub>14</sub>	ring (CCC str.) + $\delta$ CH	1655	2.750
v <sub>15</sub>	ring (CCC str.) + $\delta$ CH	1643	2.150
v <sub>16</sub>	ring (CCC str.) + $\delta$ CH	1632	0.197
v <sub>17</sub>	ring (CCC str.) + $\delta$ CH	1621	12.530

V <sub>18</sub>	ring (CCC str.) + $\delta$ CH	1593	2.400
V <sub>19</sub>	(CC str.) + $\delta$ CH	1568	11.260
V <sub>20</sub>	(CC str.) + $\delta$ CH	1531	11.270
V <sub>21</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1508	10.350
V <sub>22</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1491	15.520
V <sub>23</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1481	3.230
V <sub>24</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1475	6.780
V <sub>25</sub>	ring (CCC str.) + $\delta$ CH	1460	56.790
V <sub>26</sub>	ring (CCC str.) + $\delta$ CH	1416	0.897
V <sub>27</sub>	(CC str.) + $\delta$ CH	1407	3.679
V <sub>28</sub>	ring (CCC str.) + $\delta$ CH	1403	2.811
V <sub>29</sub>	ring (CCC str.) + $\delta$ CH	1385	1.686
V <sub>30</sub>	ring (CCC str.) + $\delta$ CH	1354	2.493
V <sub>31</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1319	7.250
V <sub>32</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1306	0.4558
V <sub>33</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1266	3.810
V <sub>34</sub>	$\delta$ CH+ $\delta$ ring ( $\delta$ CCC)	1254	4.654
V <sub>35</sub>	$\delta$ CH	1249	3.360
V <sub>36</sub>	$\delta$ CH	1233	2.270
V <sub>37</sub>	$\delta$ CH	1218	1.143
V <sub>38</sub>	$\delta$ CH	1204	2.163
V <sub>39</sub>	$\delta$ CH	1189	7.437
V <sub>40</sub>	$\delta$ CH	1187	3.044
V <sub>41</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1164	2.533
V <sub>42</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1097	2.413
V <sub>43</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1075	8.931
V <sub>44</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1057	4.587
V <sub>45</sub>	ring (CCC str.) + $\delta$ CH	1044	1.510
V <sub>46</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1002	0.1818
V <sub>47</sub>	$\delta$ ring ( $\delta$ CCC)+ $\delta$ CH	962	1.393
V <sub>48</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	854	1.183
V <sub>49</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	830	0.1539
V <sub>50</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	819	2.479
V <sub>51</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	732	0.836
V <sub>52</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	665	6.324
V <sub>53</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	628	0.451

Table (2) :cont.

	Symmetry&description	(DFT) B3LYP/6-311G Frequency cm <sup>-1</sup>	Intensity km/mol
v <sub>54</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	595	0.773
v <sub>55</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	566	5.084
v <sub>56</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	543	0.261
v <sub>57</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	501	2.473
v <sub>58</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	464	0.0762
v <sub>59</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	347	1.148
v <sub>60</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	292	0.055
v <sub>61</sub>	$\delta$ CH	150	0.235
"A			
v <sub>62</sub>	$\gamma$ CH	1020	0.066
v <sub>63</sub>	$\gamma$ CH	1016	1.406
v <sub>64</sub>	$\gamma$ CH	1004	0.026
v <sub>65</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	993	0.184
v <sub>66</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	976	0.633
v <sub>67</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	950	0.002
v <sub>68</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	933	0.031
v <sub>69</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	889	3.228
v <sub>70</sub>	$\gamma$ CH	852	21.200
v <sub>71</sub>	$\gamma$ CH	848	117.000
v <sub>72</sub>	$\gamma$ CH	817	9.956
v <sub>73</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	782	14.724
v <sub>74</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	781	11.013
v <sub>75</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	763	34.272
v <sub>76</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	714	3.072
v <sub>77</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	653	1.4955
v <sub>78</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	640	0.2744
v <sub>79</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	575	5.872
v <sub>80</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	534	7.555
v <sub>81</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	474	1.125
v <sub>82</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	466	2.558
v <sub>83</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	416	1.552
v <sub>84</sub>	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	338	0.437
v <sub>85</sub>	$\gamma$ CH	265	0.311
v <sub>86</sub>	$\gamma$ CH	203	1.015
v <sub>87</sub>	$\gamma$ CH	175	5.040
v <sub>88</sub>	$\gamma$ CH	157	0.395
v <sub>89</sub>	$\gamma$ CH	73	0.952
v <sub>90</sub>	$\gamma$ CH	60	0.0502

Table (3) : Vibrational frequencies and IR absorption intensities of Benzo [J] Fluoranthene [BJN] radical cation.

	Symmetry&description	(DFT) B3LYP/ 6-311G Frequency cm <sup>-1</sup>	Intensity km/mol
$\text{\AA}$			
v <sub>1</sub>	C H str.	3242	6.200
v <sub>2</sub>	C H str.	3220	9.000
v <sub>3</sub>	C H str.	3216	5.300
v <sub>4</sub>	C H str.	3211	13.800
v <sub>5</sub>	C H str.	3208	2.700
v <sub>6</sub>	C H str.	3204	6.500
v <sub>7</sub>	C H str.	3200	0.690
v <sub>8</sub>	C H str.	3193	3.360
v <sub>9</sub>	C H str.	3188	3.250
v <sub>10</sub>	C H str.	3188	0.160
v <sub>11</sub>	C H str.	3186	0.140
v <sub>12</sub>	C H str.	3185	0.021
v <sub>13</sub>	ring (CCC str.) + $\delta$ CH	1655	10.165
v <sub>14</sub>	ring (CCC str.) + $\delta$ CH	1629	13.600
v <sub>15</sub>	ring (CCC str.) + $\delta$ CH	1613	91.214
v <sub>16</sub>	ring (CCC str.) + $\delta$ CH	1611	147.117
v <sub>17</sub>	ring (CCC str.) + $\delta$ CH	1587	37.780
v <sub>18</sub>	ring (CCC str.) + $\delta$ CH	1568	16.799
v <sub>19</sub>	(CC str.) + $\delta$ CH	1542	52.001
v <sub>20</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1531	2.880
v <sub>21</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1493	53.798
v <sub>22</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1487	1.215
v <sub>23</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1481	201.400
v <sub>24</sub>	ring (CCC str.) + $\delta$ CH	1454	92.470
v <sub>25</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1445	76.727
v <sub>26</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1429	330.470
v <sub>27</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1406	17.810
v <sub>28</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1376	146.215
v <sub>29</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1369	3.135
v <sub>30</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1357	9.500
v <sub>31</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1328	70.990
v <sub>32</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1315	14.500
v <sub>33</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1272	29.700
v <sub>34</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1269	119.600
v <sub>35</sub>	$\delta$ CH	1249	2.400
v <sub>36</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1233	54.100
v <sub>37</sub>	$\delta$ CH	1223	2.180
v <sub>38</sub>	$\delta$ CH	1201	36.830
v <sub>39</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1182	20.100
v <sub>40</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1157	33.300

V41	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1127	37.600
V42	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1109	9.600
V43	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1081	33.200
V44	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1070	0.500
V45	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1049	9.420
V46	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1006	2.600
V47	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	955	2.300
V48	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	858	1.530
V49	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	821	1.700
V50	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	816	19.150
V51	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	732	1.700
V52	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	657	1.500

Table (3) :cont.

	Symmetry&description	(DFT) B3LYP/ 6-311G Frequency $\text{cm}^{-1}$	Intensity km/mol
V53	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	627	0.520
V54	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	589	9.400
V55	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	562	7.420
V56	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	524	3.800
V57	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	497	6.437
V58	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	454	1.450
V59	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	346	4.170
V60	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	279	2.050
V61	$\delta$ CH	160	0.116
"A			
V62	$\gamma$ CH	1042	0.0167
V63	$\gamma$ CH	1039	0.690
V64	$\gamma$ CH	1029	0.050
V65	$\gamma$ CH	1013	0.030
V66	$\gamma$ CH	998	1.530
V67	$\gamma$ CH	978	0.990
V68	$\gamma$ CH	959	0.480
V69	$\gamma$ CH	913	2.912
V70	$\gamma$ CH	864	28.106
V71	$\gamma$ CH	850	122.700
V72	$\gamma$ CH	811	0.0002
V73	$\gamma$ CH	783	28.800
V74	$\gamma$ ring ( $\delta$ CCC)+ $\gamma$ CH	758	19.880
V75	$\gamma$ ring ( $\delta$ CCC)+ $\gamma$ CH	753	3.300
V76	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	699	3.338
V77	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	634	0.170
V78	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	615	0.550
V79	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	537	7.421



V80	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	512	11.998
V81	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	471	0.160
V82	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	445	2.955
V83	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	402	0.460
V84	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	339	0.127
V85	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	250	0.410
V86	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	192	1.601
V87	$\gamma\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	178	6.820
V88	$\text{CH} + \gamma \text{ ring } (\delta\text{CCC})$	153	152.900
V89	$\gamma\text{CH}$	71	71.400
V90	$\gamma\text{CH}$	48	47.980

Table (4): Vibrational frequencies and IR absorption intensities of Benzo [J] Fluoranthene [BJN] radical anion.

	Symmetry&description	(DFT) B3LYP/6-311G Frequency $\text{cm}^{-1}$	Intensity km/mol
$\bar{A}$			
V <sub>1</sub>	C H str.	3209	33.382
V <sub>2</sub>	C H str.	3174	29.154
V <sub>3</sub>	C H str.	3160	126.200
V <sub>4</sub>	C H str.	3153	205.171
V <sub>5</sub>	C H str.	3146	123.449
V <sub>6</sub>	C H str.	3143	127.246
V <sub>7</sub>	C H str.	3136	16.006
V <sub>8</sub>	C H str.	3135	43.923
V <sub>9</sub>	C H str.	3127	6.864
V <sub>10</sub>	C H str.	3119	4.432
V <sub>11</sub>	C H str.	3116	17.311
V <sub>12</sub>	C H str.	3113	27.260
V <sub>13</sub>	ring (CCC str.) + $\delta\text{CH}$	1627	28.295
V <sub>14</sub>	ring (CCC str.) + $\delta\text{CH}$	1614	81.822
V <sub>15</sub>	ring (CCC str.) + $\delta\text{CH}$	1586	25.276
V <sub>16</sub>	(CC str.) + $\delta\text{CH}$	1577	29.420
V <sub>17</sub>	ring (CCC str.) + $\delta\text{CH}$	1567	48.328
V <sub>18</sub>	(CC str.) + $\delta\text{CH}$	1559	26.365
V <sub>19</sub>	(CC str.) + $\delta\text{CH}$	1547	1.869
V <sub>20</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1514	7.205
V <sub>21</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1491	7.633
V <sub>22</sub>	$\delta \text{CH} + \delta \text{ ring } (\delta\text{CCC})$	1473	3.375
V <sub>23</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1471	50.462
V <sub>24</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1458	7.609
V <sub>25</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1429	138.850
V <sub>26</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1406	0.747
V <sub>27</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1398	11.517
V <sub>28</sub>	$\delta\text{ring } (\delta\text{CCC}) + \delta\text{CH}$	1389	20.081

V <sub>29</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1355	207.873
V <sub>30</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1346	29.274
V <sub>31</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1329	101.433
V <sub>32</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1308	2.377
V <sub>33</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1256	11.711
V <sub>34</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1248	5.679
V <sub>35</sub>	$\delta$ CH	1246	13.869
V <sub>36</sub>	$\delta$ CH	1217	93.424
V <sub>37</sub>	$\delta$ CH	1199	14.918
V <sub>38</sub>	$\delta$ CH	1193	0.752
V <sub>39</sub>	$\delta$ CH	1165	9.600
V <sub>40</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1161	3.440
V <sub>41</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1139	2.250
V <sub>42</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1094	3.662
V <sub>43</sub>	$\delta$ CH	1079	10.280
V <sub>44</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	1059	15.780
V <sub>45</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	1044	2.914
V <sub>46</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	996	12.258
V <sub>47</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	955	3.923
V <sub>48</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	849	0.274
V <sub>49</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	823	0.511
V <sub>50</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	811	14.55
V <sub>51</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	728	1.971
V <sub>52</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	662	3.607
V <sub>53</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	626	1.560

$\gamma$ : out of plane bending vibration.

$\delta$ : in- plane bending vibration

Table (4) :cont.

	Symmetry&description	(DFT) B3LYP/6-311G Frequency cm <sup>-1</sup>	Intensity km/mol
V <sub>54</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	590	4.821
V <sub>55</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	559	0.445
V <sub>56</sub>	$\delta$ ring ( $\delta$ CCC) + $\delta$ CH	538	6.305
V <sub>57</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	497	15.202
V <sub>58</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	461	1.227
V <sub>59</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	349	0.870
V <sub>60</sub>	$\delta$ CH + $\delta$ ring ( $\delta$ CCC)	293	1.090
V <sub>61</sub>	$\delta$ CH	156	0.685
"A			
V <sub>62</sub>	$\gamma$ CH	965	0.000
V <sub>63</sub>	$\gamma$ CH	946	0.442
V <sub>64</sub>	$\gamma$ CH	939	0.749
V <sub>65</sub>	$\gamma$ CH	931	1.278

V66	$\gamma$ CH	923	3.300
V67	$\gamma$ CH	877	0.210
V68	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	842	8.470
V69	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	832	8.260
V70	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	816	24.294
V71	$\gamma$ CH	799	14.780
V72	$\gamma$ CH	788	56.340
V73	$\gamma$ CH	748	100.200
V74	$\gamma$ CH	741	6.836
V75	$\gamma$ CH	729	0.413
V76	$\gamma$ CH	690	5.930
V77	$\gamma$ CH	638	1.078
V78	$\gamma$ ring (CCC) + $\gamma$ CH	619	0.0369
V79	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	569	3.076
V80	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	534	3.510
V81	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	504	0.130
V82	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	442	4.603
V83	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	392	0.332
V84	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	328	0.499
V85	$\gamma$ CH + $\gamma$ ring ( $\delta$ CCC)	256	0.371
V86	$\gamma$ CH	204	0.841
V87	$\gamma$ CH	184	3.915
V88	$\gamma$ CH	158	0.077
V89	$\gamma$ CH	73	0.434
V90	$\gamma$ CH	56	0.068

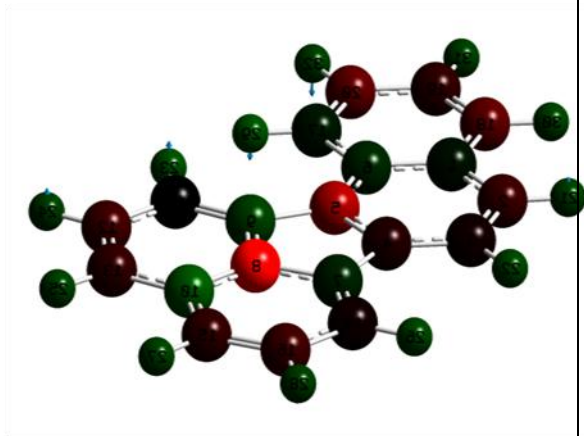
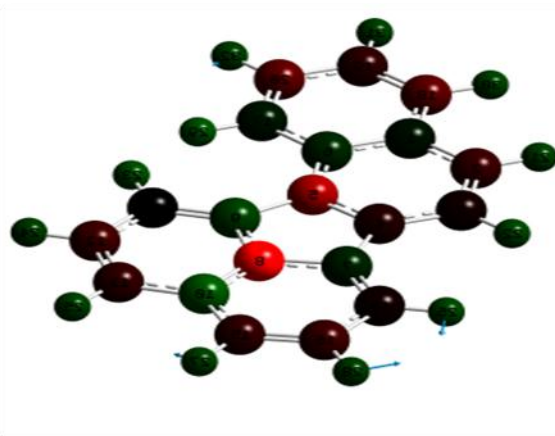
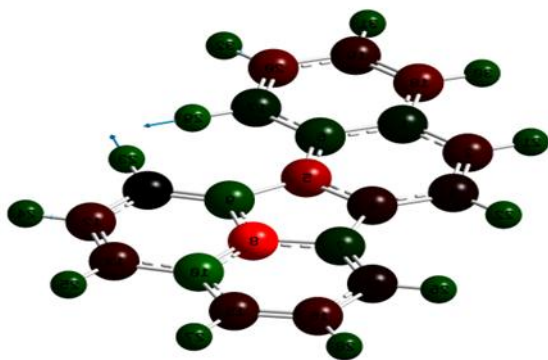
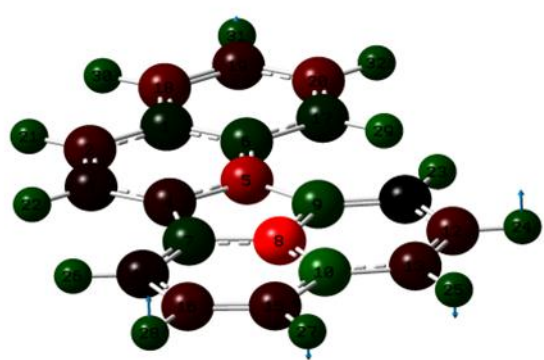
V<sub>21</sub> out plane (neutral)V<sub>29</sub> inplane (neutral)V<sub>80</sub> CH stretching (neutral).V<sub>45</sub> ring bending (neutral)

Fig-3: some vibration modes of the Benzo [J] Fluoranthene neutral molecule as drawn by Gaussian program.

Classification of vibration frequencies of [BJF]neutral molecule.

1- In-plane modes of vibrations

1-The CH stretching vibration

Totally twelve (C-H) Vibration frequencies are calculated and included in (table-2) the motion of these modes is localized completely on the H atoms (Fig-3). The calculated vibrations frequencies values were about (3262 - 3155 cm<sup>-1</sup>). The IR. Absorption intensities values were about (68.61-0.097)Km mol<sup>-1</sup> as shown in (table- 2).

2 - Ring CC stretching vibration

The calculated vibrations frequencies values were about (1662 – 1354 cm<sup>-1</sup>). The IR. Absorption intensities values were about (56.79– 0.197)Km mol<sup>-1</sup> as shown in (table- 2).

3- The in-plane deformation vibrations frequencies (δCH).

Totally twelve (δCH) vibrations frequencies are calculated , The motion of these modes is localized completely on the (H) atoms (Fig-3). The calculated vibrations frequencies values

were about  $(1319 - 150 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(15.52 - 0.055) \text{ Km mol}^{-1}$  as shown in (table - 2).

4- The in-plane deformation vibrations frequencies ( $\delta\text{CCC}$ ).

The calculated vibrations frequencies values were about  $(1002 - 292 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(2.479 - 0.153) \text{ Km mol}^{-1}$  as shown in (table- 2).

#### Out -plane modes of vibrations

1-The Out -plane deformation vibrations frequencies ( $\gamma\text{CH}$ ).

The calculated vibrations frequencies values were about  $(1020-60 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(117- 0.023) \text{ Km mol}^{-1}$  as shown in (table - 2).

2-Out-plane modes deformation vibrations frequencies ( $\gamma\text{CC}$ ).

The calculated vibrations frequencies values were about  $(852-338 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(117-0.27) \text{ Km mol}^{-1}$  as shown in (table-2).

#### Classification of vibration frequencies of [BJF] cation radical.

For both ions of [BJF] ,The (DFT) treatment yielded bond distances of minor changes from those of neutral molecule (table-1) , radical cation shows (Cs) symmetry, similar to the neutral molecule. For the changes which occurred in bond lengths and bond angles of (neutral, cation, anion)[BJF] molecule. as shown in (table -1).The different is the change of the vibration frequencies values of (C C) bonds due to the change in the charge of the molecule (Fig.7).

#### In-plane modes of vibrations

1-The CH stretching vibration

Totally twelve (C-H) Vibration frequencies are calculated and included in (table-٣) the motion of these modes is localized completely on the H atoms (Fig-4). The calculated vibrations frequencies values were about  $(3241.9 - 3185.4 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(9.00 - 0.021) \text{ Km mol}^{-1}$  as shown in (table - ٣).

2 - Ring CC stretching vibration

The calculated vibrations frequencies values were about  $(1655.3 - 1453.8 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(147.11- 10.165) \text{ Km mol}^{-1}$  as shown in (table-3).

3- The in-plane deformation vibrations frequencies ( $\delta\text{CH}$ ).

Totally twelve ( $\delta\text{CH}$ ) vibrations frequencies are calculated , The motion of these modes is localized completely on the (H) atoms (Fig-4). The calculated vibrations frequencies values were about  $(1531.4 -160.00 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(15.52- 0.055) \text{ Km mol}^{-1}$  as shown in (table -3).

4- The in-plane deformation vibrations frequencies ( $\delta\text{CCC}$ ).

The calculated vibrations frequencies values were about  $(1480.8- 346.2 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(330.47- 0.5) \text{ Km mol}^{-1}$  as shown in (table-3).

#### Out -plane modes of vibrations

1-The Out -plane deformation vibrations frequencies ( $\gamma\text{CH}$ ).

The calculated vibrations frequencies values were about  $(1042.14- 47.98) \text{ cm}^{-1}$ . The IR. Absorption intensities values were about  $(28.8- 0.0092) \text{ Km mol}^{-1}$  as shown in (table-3).

2- Out -plane deformation vibrations frequencies ( $\gamma\text{CC}$ ).

The calculated vibrations frequencies values were about  $(758.2- 152.9 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(19.88- 0.042) \text{ Km mol}^{-1}$  as shown in (table-3).

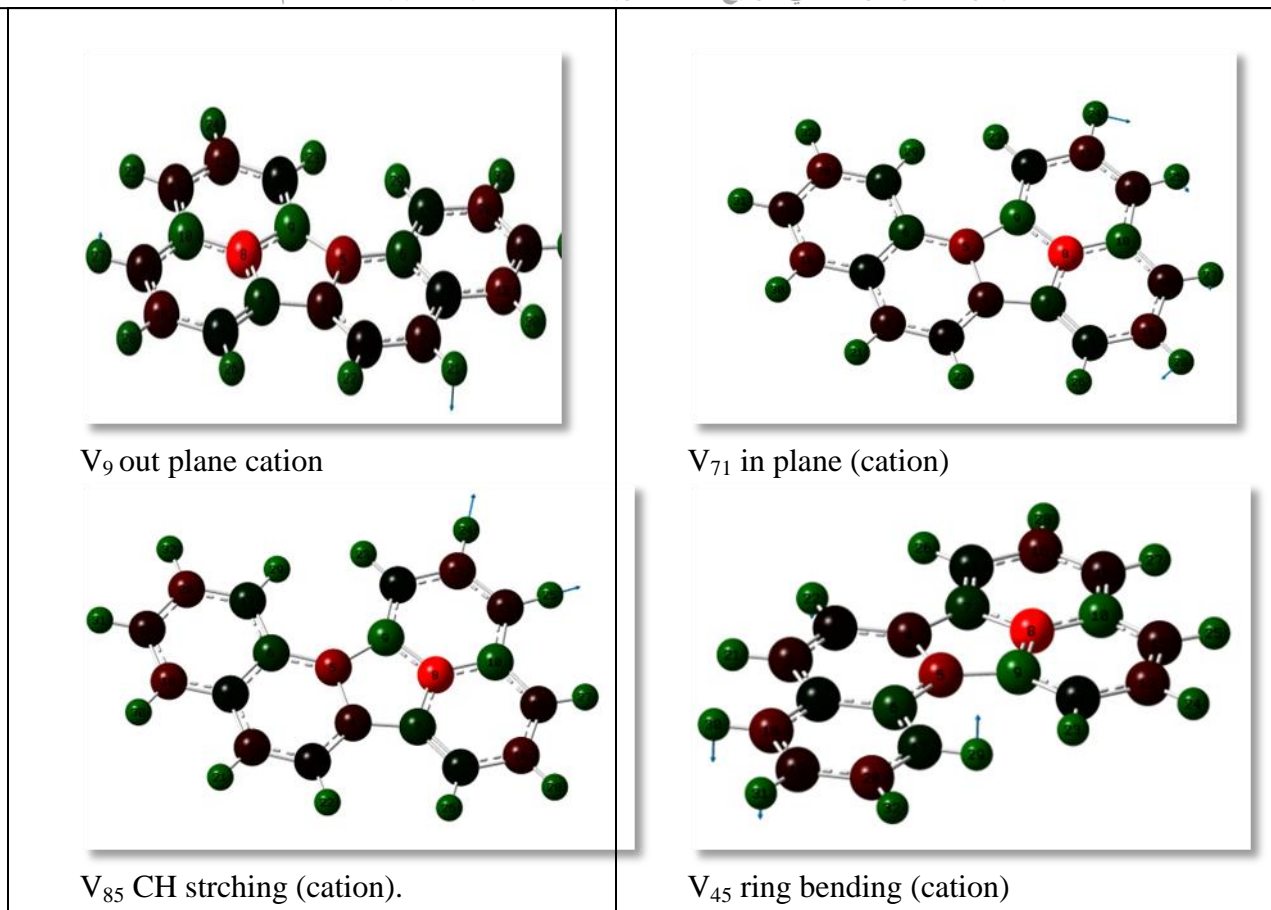


Fig-4: pictures of some vibration modes of the Benzo [J] Fluoranthene radical cation as drawn by Gaussian program.

Classification of vibration frequencies of [BJF] ] radical anion.

### In-plane modes of vibrations

#### 1-The CH stretching vibration

Totally twelve (C-H) Vibration frequencies are calculated and included in (table-4) the motion of these modes is localized completely on the H atoms (Fig.5). The calculated vibrations frequencies values were about  $(3208.7 - 3113.3) \text{ cm}^{-1}$ . The IR. Absorption intensities values were about  $(205.171-4.432) \text{ Km mol}^{-1}$  as shown in (table - 4).

#### 2 - Ring CC stretching vibration

The calculated vibrations frequencies values were about  $(1627.4 - 1547.03 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(81.82- 1.869) \text{ Km mol}^{-1}$  as shown in (table - 4).

#### 3- The in-plane deformation vibrations frequencies ( $\delta\text{CH}$ ).

Totally twelve ( $\delta\text{CH}$ ) vibrations frequencies are calculated (Fig.5), The motion of these modes is localized completely on the (H) atoms. The calculated vibrations frequencies values were about  $(1473.23 - 156.2 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(93.42- 0.27) \text{ Km mol}^{-1}$  as shown in (table - 4).

#### 4- The in-plane deformation vibrations frequencies ( $\delta\text{CCC}$ )

The calculated vibrations frequencies values were about  $(1514.23 - 538.13 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(207.87- 0.445) \text{ Km mol}^{-1}$  as shown in (table-4).

### Out -plane modes of vibrations

#### 1-The Out -plane deformation vibrations frequencies ( $\gamma\text{CH}$ ) modes.

The calculated vibrations frequencies values were about  $(964.7- 55.588 \text{ cm}^{-1})$ . The IR. Absorption intensities values were about  $(100.20- 0.00) \text{ Km mol}^{-1}$  as shown in (table - 4).

#### 2-Out-plane deformation vibrations frequencies ( $\gamma\text{CC}$ ) modes.

The calculated vibrations frequencies values were about (876.5-328.44)  $\text{cm}^{-1}$ . The IR. Absorption intensities values were about (4.603-0.0369)  $\text{Km mol}^{-1}$  as shown in (table-4).

#### Discussion

A study, of title compounds, was undertaken to investigate the possible use of quantum chemical molecular orbital calculations, which predict the preferred site or sites of electrophilic substitution, as a predictor of complete carcinogenic potential. These data were the basis for the development of rules of molecular geometry for predicting the center or centers of highest electron density in the molecule (Fig.8). Using these rules, the complete carcinogenic potentials of the hydrocarbons were predicted. These predictions were compared to the available carcinogenicity data base for this series of compounds. It is concluded that a knowledge of the center or centers of highest electron density is useful in making predictions of complete carcinogenic potential of unsubstituted title compounds. The compounds studied were fluoranthene, benzo[j]fluoranthene molecule ,positive and negative Radical Ions.The present study reveals that there are electronic determinants of carcinogenicity.

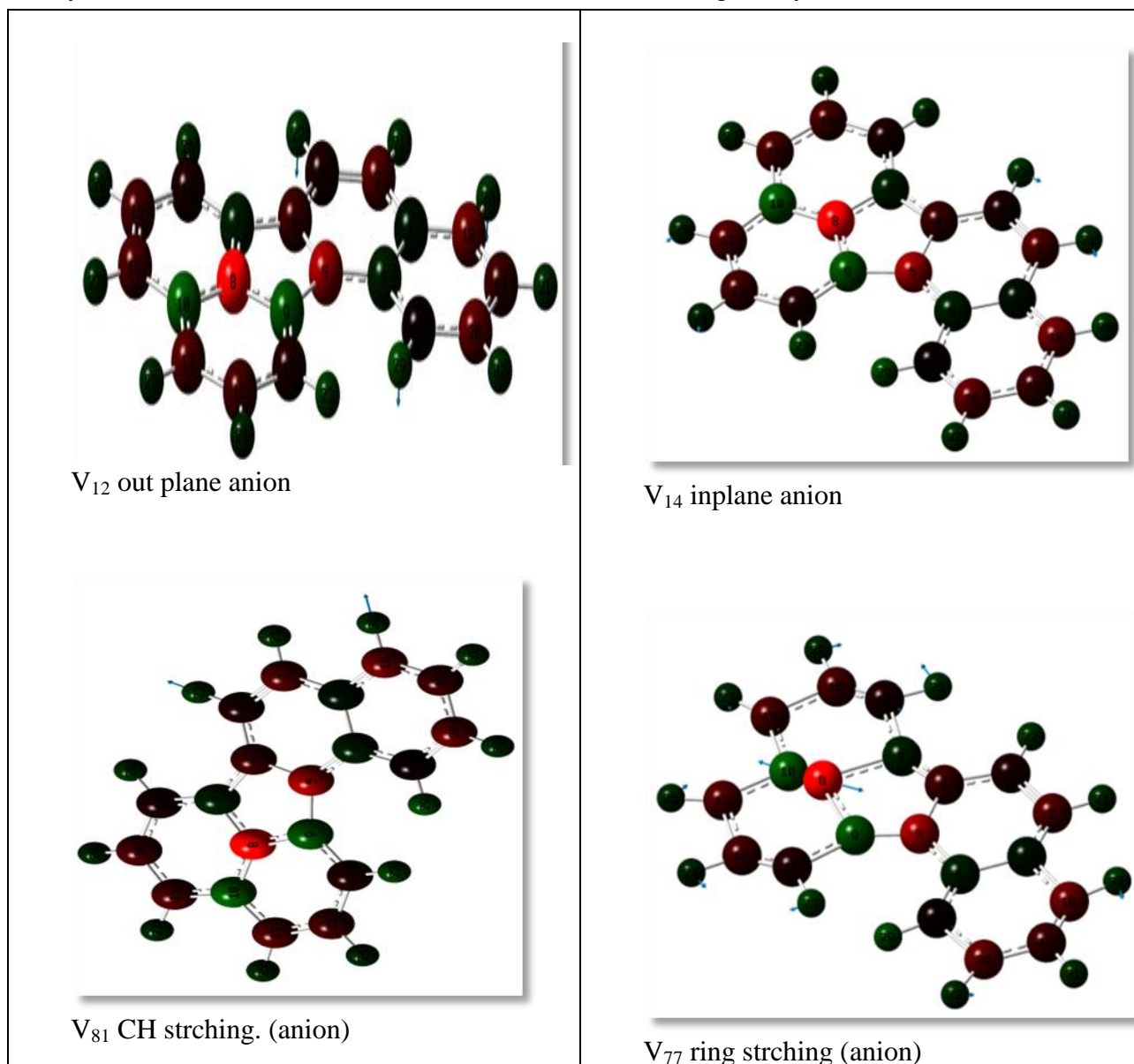
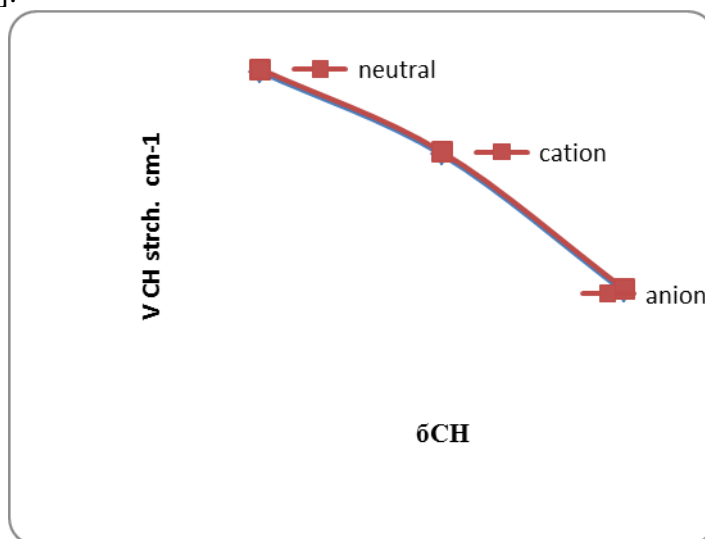


Fig-5: pictures of some vibration modes of the Benzo [J] Fluoranthene radical anion as drawn by Guassian program.

Molecular modeling; predicting carcinogenicity; sites of electrophilic substitution [19]. Most PAHs are also fluorescent, emitting characteristic wavelengths of light when they are excited (when the molecules absorb light). The extended pi-electron electronic structures of PAHs (Fig.8), lead to these spectra, as well as to certain large PAHs also exhibiting semi-conducting and other behaviors[20].



(Fig. 6). Graphical correlation of the calculated  $\sigma\rho C$  at different carbon atoms with the corresponding C-H vibration frequencies, for each carbon atom in the (BJF) radical anion, neutral molecule and cation  $(C_{20}H_{12})^-$ ,  $(C_{20}H_{12})$ ,  $(C_{20}H_{12})^+$

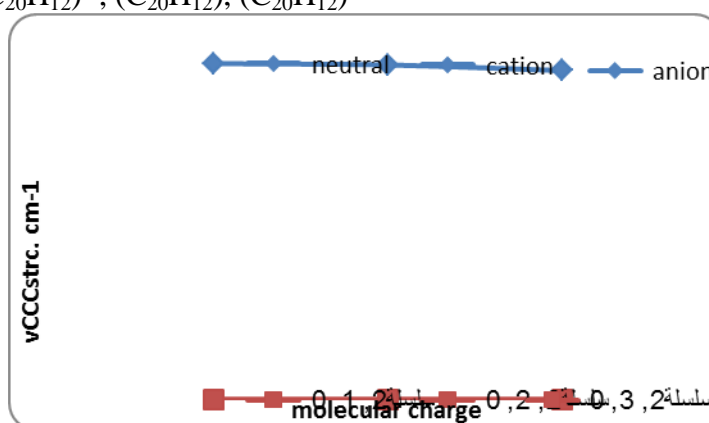


Fig.7: Graphical correlation of the change in the vibrations frequencies values of C C bond in (BJF) molecule due to the change in the charge of the molecule.

#### The CH and C-C stretching vibration for radical anion and cation of (BJF) molecule.

For both ions of the planner (BJF) molecule yielded bond distances of minor changes from those of the neutral molecule (Table-1), but retained the  $C_s$  symmetry. As for the stretching C- H and C- C vibration are appeared in the symmetric modes only in the (anion, cation, neutral) (BJF) molecule (Fig6, 7).

#### General Correlation.

As for the C-H stretching vibrations, it is found on specting the frequency values of (table-2 ,3, 4) that, the vibrations frequencies values of the neutral are higher than those for the cation and these are higher than the frequencies values of the radical anion.

$$\nu_{sym. CH\ str.} (C_{20}H_{12}) > \nu_{sym. CH\ str.} (C_{20}H_{12})^+ > \nu_{sym. CH\ str.} (C_{20}H_{12})^-$$

#### The C-C stretching vibrations

Different is the change of the vibration frequencies values of the C-C bonds due to the change in the charge of the molecule. It is appeared only the symmetric modes only in the (anion, cation, neutral) (BJF) molecule.

$$\nu_{sym. CCC\ str.} (C_{20}H_{12}) > \nu_{sym. CCC\ str.} (C_{20}H_{12})^+ > \nu_{sym. CCC\ str.} (C_{20}H_{12})^-$$



The calculated vibrations frequencies values of the neutral are higher than those for the radical cation and these are higher than the frequencies values of the radical anion. The reason for this change in the vibration frequencies values is the change in bond orders of the related bonds due to the radical ion formation. According to the pairing theorem, adding an electron to the neutral molecules, forming the radical anion, where as removing an electron, to form a radical cation, the difference in the MO coefficient changes, bond order of C C bonds and consequently their vibrations frequencies values. As for the in plane deformations the following correlation were found

$$\delta_{\text{sym. CH}} (\text{C}_{20}\text{H}_{12})^+ > \delta_{\text{sym. CH}} (\text{C}_{20}\text{H}_{12})^- > \delta_{\text{sym. CH}} (\text{C}_{20}\text{H}_{12})$$

$$\delta_{\text{sym. CCC}} (\text{C}_{20}\text{H}_{12})^- > \delta_{\text{sym. CCC}} (\text{C}_{20}\text{H}_{12}) > \delta_{\text{sym. CCC}} (\text{C}_{20}\text{H}_{12})^+$$

And for the out of plane modes of vibrations.

$$\gamma_{\text{CH}} (\text{C}_{20}\text{H}_{12})^- > \gamma_{\text{CH}} (\text{C}_{20}\text{H}_{12}) > \gamma_{\text{CH}} (\text{C}_{20}\text{H}_{12})^+$$

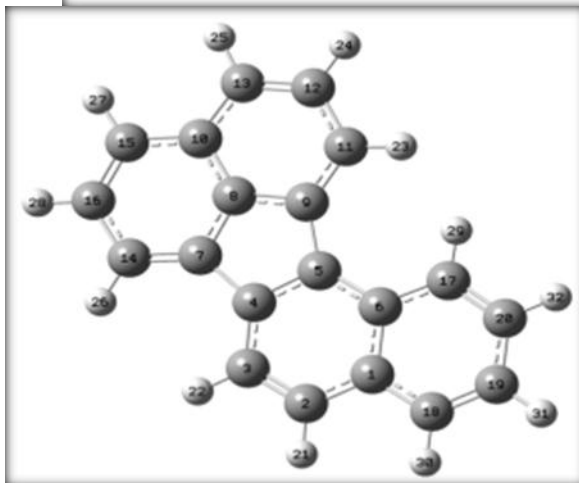
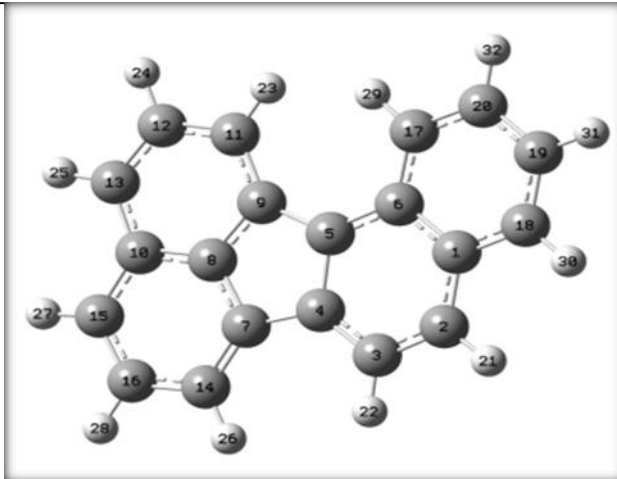
$$\gamma_{\text{CCC}} (\text{C}_{20}\text{H}_{12}) > \gamma_{\text{CCC}} (\text{C}_{20}\text{H}_{12})^+ > \gamma_{\text{CCC}} (\text{C}_{20}\text{H}_{12})^-$$

### Conclusion

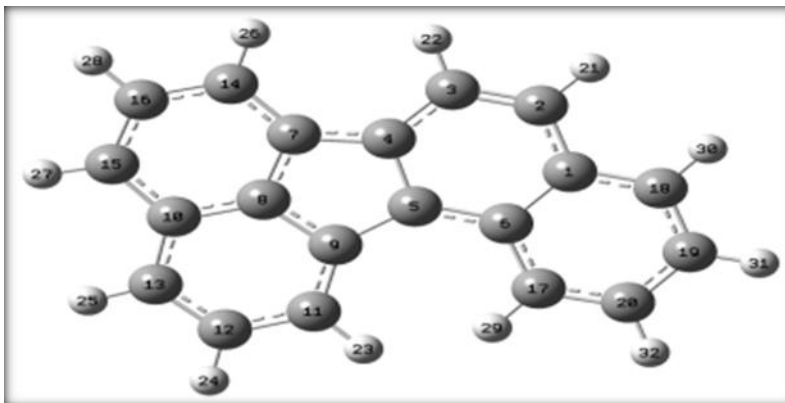
The complete analysis of all vibration frequencies and normal coordinates of (BJF) molecule and its radical cation and anion, yielded good frequency values by applying Gaussian 3 Program. The change in vibration frequencies of CC bond is due to the change in the charge, bond order, force constant and bond lengths, of the planner (BJF) molecule. According to the pairing theorem, adding an electron to the neutral molecules, forming the radical anion, where as removing an electron, to form a radical cation, the difference in the MO coefficient changes, bond order of C C bonds and consequently their vibrations frequencies values, change bonds length, and bond charge. A relation is found between Total Energy and the vibration frequencies values for the three types of planner (BJF) molecule. The Total Energy **of cation is higher** than the neutral and this is higher than Total Energy values of the radical anion (table-1).

$$E (\text{C}_{20}\text{H}_{12})^+ > E (\text{C}_{20}\text{H}_{12}) > E (\text{C}_{20}\text{H}_{12})^-$$

Calculating the electron charge densities of the  $\sigma$  electrons for two charged and neutral planner (BJF) molecule, and inspecting their correlation with the corresponding CH stretching frequencies an almost linear correlation is found (Fig. 6).  $\rho_{\text{CH str.}} (\text{C}_{20}\text{H}_{12})^- > \rho_{\text{CH str.}} (\text{C}_{20}\text{H}_{12}) > \rho_{\text{CH str.}} (\text{C}_{20}\text{H}_{12})^+$



BJF cation BJF neutral



BJF anion

Fig.8: The equilibrium geometry of (BJF) radical cation, anion and neutral molecule compared with each other by distribution with electron densities charge on carbon atoms.

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