J	$\nu\,(P_J)$	$\nu\,(R_J)$	m
29	1261.92		−29
28	1264.21		−28
27	1266.45		−27
26	1268.73		−26
25	1270.97		−25
24	1273.23		−24
23	1275.49		−23
22	1277.75		−22
21	1280.01		−21
20	1282.25		−20
19	1284.48		−19
18	1286.72		−18
17	1288.96		−17
16	1291.21		−16
15	1293.48		−15
14	1295.73		−14
13	1297.99		−13
12	1300.28		−12
11	1302.56		−11
10	1304.85		−10
9	1307.14		−9
8	1309.45		−8
7	1311.78		−7
6	1314.07		−6
5	1316.43		−5
4	1318.76		−4
3	1321.02		−3
2	1323.39		−2
1	1325.70		−1

J	$\nu\,(P_J)$	$\nu\,(R_J)$	m
0		1330.45	1
1		1332.84	2
2		1335.25	3
3		1337.65	4
4		1340.05	5
5		1342.37	6
6		1344.82	7
7		1347.19	8
8		1349.58	9
9		1351.99	10
10		1354.45	11
11		1356.82	12
12		1359.24	13
13		1361.67	14
14		1364.05	15
15		1366.55	16
16		1368.90	17
17		1371.45	18
18		1373.84	19
19		1376.28	20
20		1378.77	21
21		1381.19	22
22		1383.67	23
23		1386.21	24
24		1388.45	25
25		1390.90	26

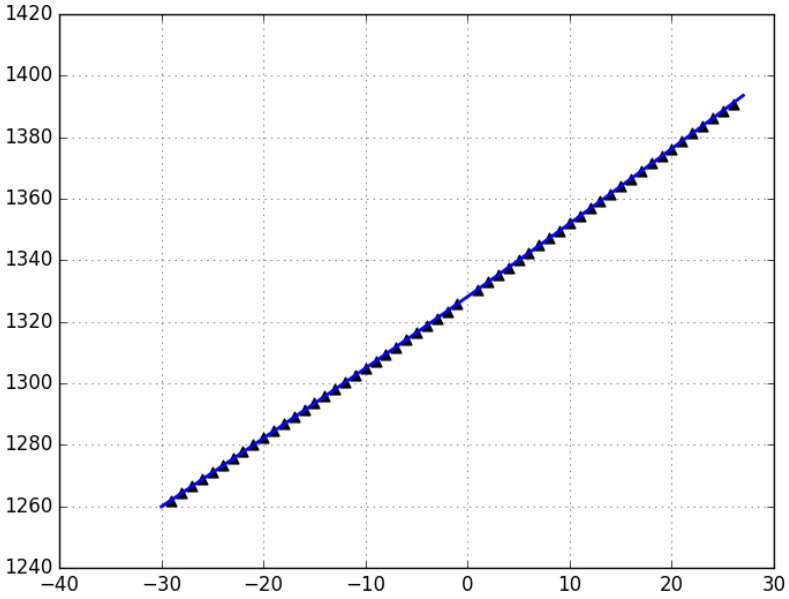

Рис. 1: Обработка результатов по ур. (I.2) полосы $\nu_4 + \nu_5$

	расчет	лит.
ν_0, см$^{-1}$	1328.17	1328.18
B_1, см$^{-1}$	1.178	
B_2, см$^{-1}$	1.175	
B_e, см$^{-1}$	1.174	1.1751
$\alpha_{e,eff}$, см$^{-1}$	-0.00257	-0.003586
I, г·см^2	$2.384 \cdot 10^{-39}$	$2.368 \cdot 10^{-39}$
r_{CC}, Å	1.213	1.2088 ± 0.0002
r_{CH}, Å	1.050	1.0566 ± 0.0003

$$\nu(J) = \nu_0 + (B' + B'')\, m + (B' - B'')\, m^2$$

$$\begin{aligned} B' &= B_e - \frac{1}{2}\alpha_e \\ B'' &= B_e - \frac{3}{2}\alpha_e \end{aligned} \quad \Longrightarrow \quad \begin{aligned} B_e &= \frac{1}{2}(3B'' - B') \\ \alpha_e &= B'' - B' \end{aligned}$$

$$\begin{aligned} I_H &= 2m_C R_C^2 + 2m_H R_H^2 \\ I_D &= 2m_C R_C^2 + 2m_D R_D^2 \end{aligned} \quad \Longrightarrow \quad \begin{aligned} R_H^2 &= \frac{I_D - I_H}{2(m_D - m_H)} \\ R_C^2 &= \frac{I_H}{2m_C} - \frac{m_H}{m_C} \cdot \frac{I_D - I_H}{2(m_D - m_H)} \end{aligned}$$

$$\begin{aligned} r_{CC} &= 2 \cdot R_C \\ r_{CH} &= R_H - R_C \end{aligned}$$