Field modified spin-orbit potential curves of IBr. Preliminary dynamical results

Cristina Sanz Sanz[a], G. A. Worth[b]

[a] *Departamento de Química Física Aplicada, Módulo 14, Universidad Autónoma de Madrid, 28049 Madrid, Spain.*
[b] *Address: Dept. of Chemistry, University College London, 20, Gordon St., WC1H 0AJ, U.K.*

Potential Energy Curves

The data points for the potential curves and couplings for field-free IBR can be provided on request as a tarred archive PEC_SOC.1dspl. Each file, named sXX_YY.1dspl, provides the diabatic potential matrix elements at points from 4.2 to 10.0 bohr. XX and YY provide the state numbers. For details of how the curves were calculated as fits to quantum chemistry points, see Sec. 2.2.

Email addresses: cristina.sanz@uam.es (Cristina Sanz Sanz), g.a.worth@ucl.ac.uk (G. A. Worth)
URL: http://chemb125.ucl.ac.uk/worthgrp/ (G. A. Worth)

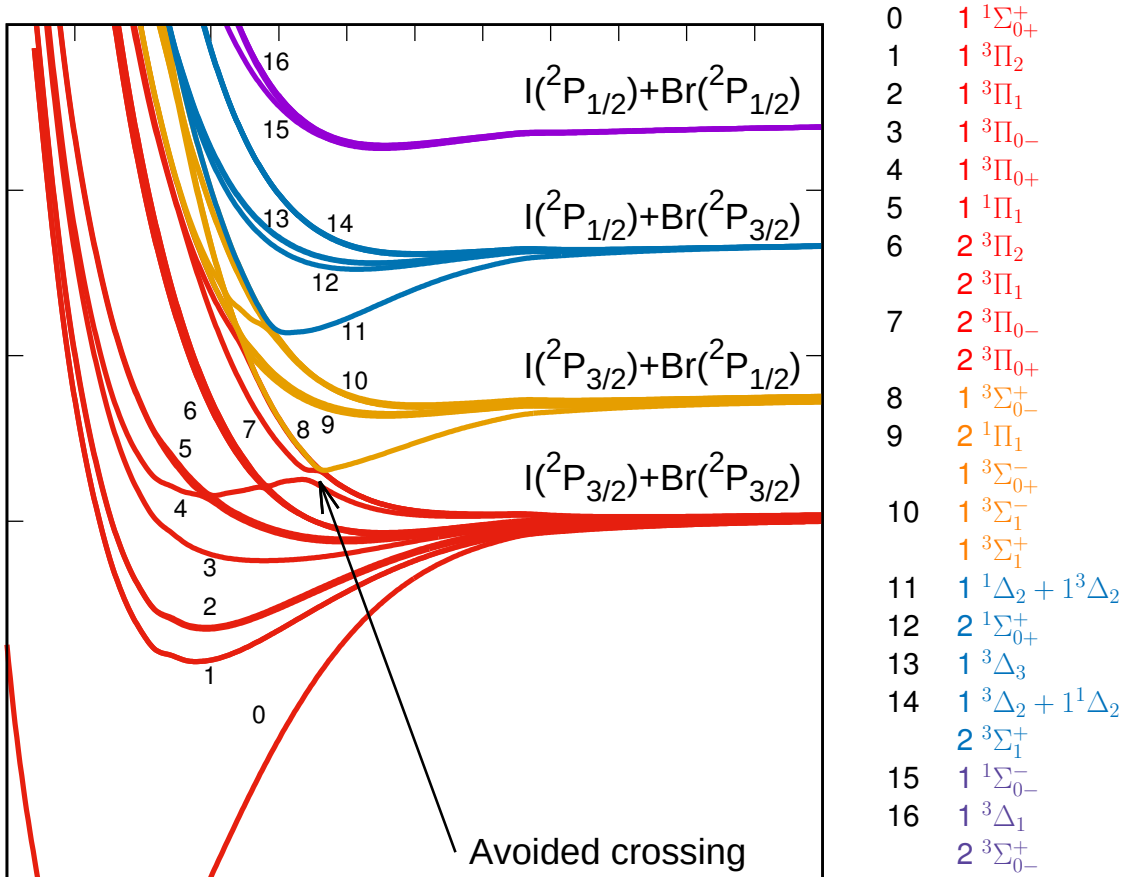

Figure S1: Assignments for the spin-coupled potential energy curves of IBr. The label for each PEC is the main spin-free configuration in the state at the Franck-Cpndon point.

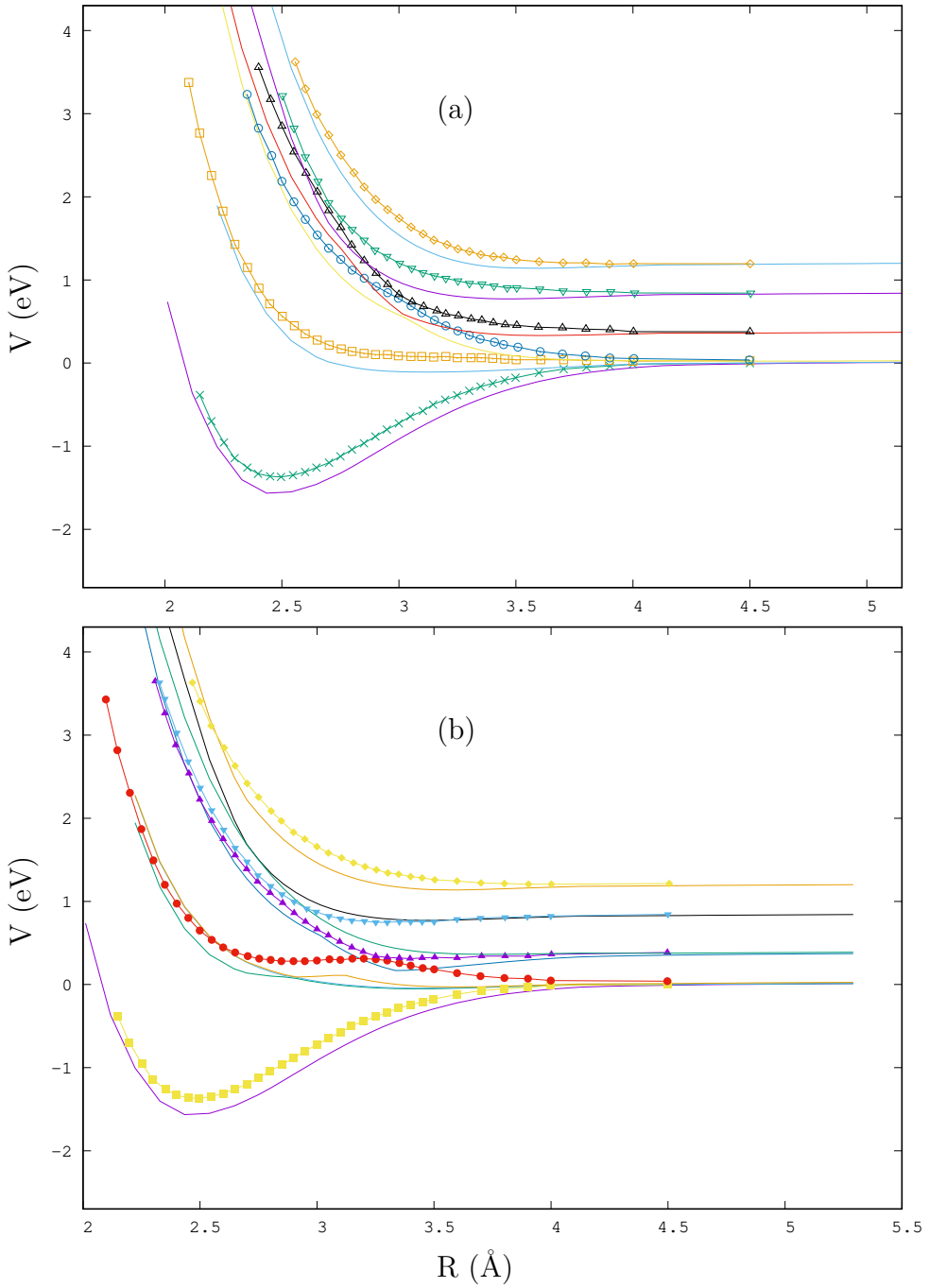

Figure S2: A comparison of the spin-coupled potential curves calculated in this work with the curves of Li *et al* [J. Quant. Spectrosc. and Radiat. Trans. (2014) **133**: 271]. (a) the $\Omega = 0^-$ and (b) the $\Omega = 0^+$ states. Solid lines are from the present work, and points are taken from the work of Li *et al*.

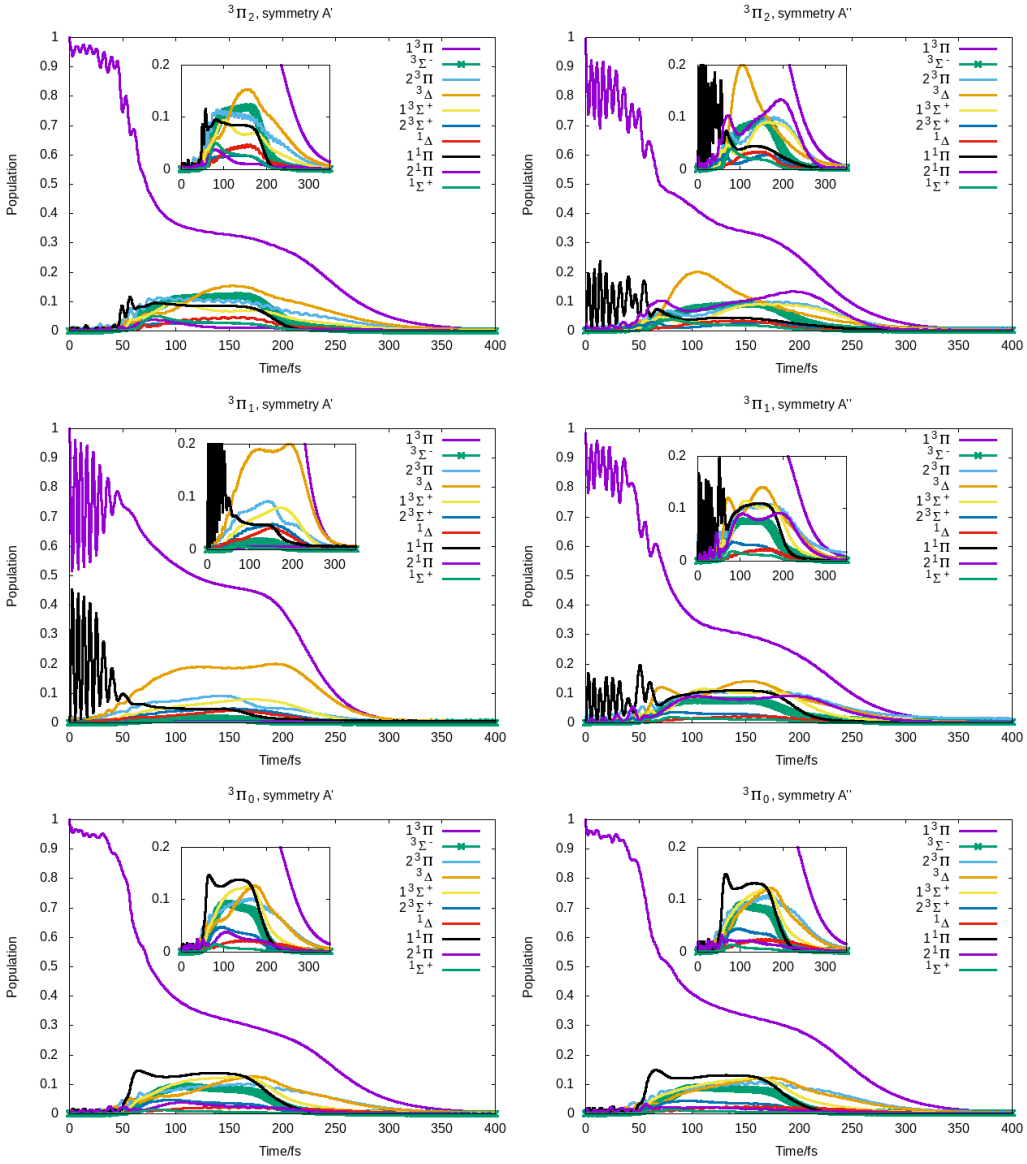

Figure S3: Population of non spin-orbit coupled states of IBr after a vertical excitation to the three m_s components (spin projections) of the state 1 $^3\Pi$ state in the two symmetries of the C_s group. Each line specifies the population of the sum of the components of each state. The energy of the initial wavepacket is 2.25 eV (18147 cm^{-1}).

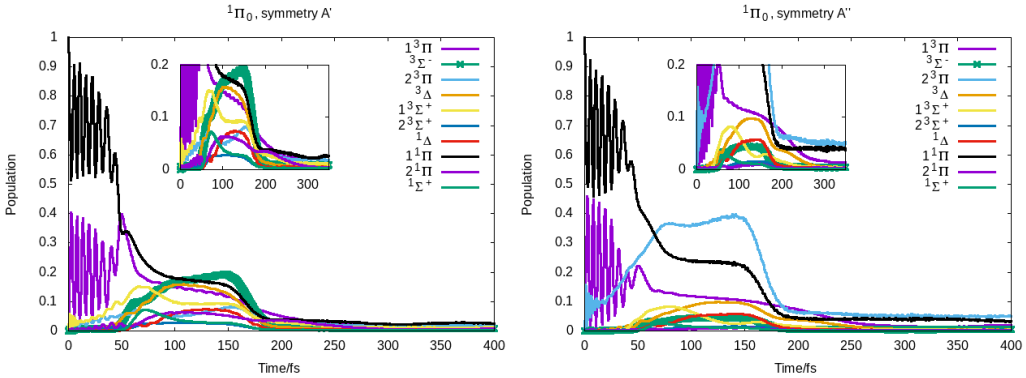

Figure S4: Population of non spin-orbit coupled states of IBr after a vertical excitation to the spin-orbit m_s components (spin projections) of the 1 $^1\Pi$ state in the two symmetries of the C_s group . Each line specifies the population of the sum of the components of each state. The energy of the initial wavepacket is 2.84 eV (22906 cm^{-1}).

Table S1: Final norm and flux absorbed in each of the channels after the excitation to every excited state of the system. States are numbered by excitation energy.

Excited state	**Final norm**	**Flux absorbed (%) in channel**			
		1	**2**	**3**	**4**
2	0.282	98.18	1.75	0.05	0.00
3	0.989	2.54	5.39	85.79	6.27
4	0.998	64.80	3.70	23.36	8.15
5	0.998	28.83	3.75	60.48	6.94
6	0.094	99.69	0.30	0.00	0.00
7	0.987	6.68	9.42	78.87	5.03
8	0.995	66.25	3.10	20.78	9.86
9	0.998	84.12	1.87	8.20	5.80
10	0.999	82.90	1.15	13.69	2.26
11	0.144	99.44	0.53	0.02	0.02
12	0.966	1.39	2.05	90.95	5.61
13	0.997	62.73	2.34	22.64	12.29
14	0.998	90.31	0.95	6.82	1.92
15	0.997	87.54	0.93	9.71	1.82
16	0.109	99.87	0.12	0.01	0.00
17	0.984	2.68	5.26	86.91	5.15
18	0.992	83.77	2.51	9.53	4.18
19	0.998	89.68	1.17	6.51	2.64
20	0.999	61.25	4.01	22.41	12.33
21	0.293	97.03	2.70	0.24	0.03
22	0.985	70.33	1.48	22.88	5.31
23	0.997	54.58	2.90	30.72	11.80
24	0.998	87.31	1.64	8.47	2.57
25	0.223	99.57	0.37	5.53	3.58
26	0.959	55.35	1.55	39.46	3.69
27	0.997	10.92	5.32	60.50	24.09
28	0.999	55.66	2.49	35.75	6.10
29	0.156	99.73	0.17	0.09	0.00
30	0.966	14.40	3.17	79.58	2.85
31	0.997	47.59	2.70	28.49	21.22
32	0.999	36.29	4.68	32.07	26.96
33	0.124	99.87	0.12	0.01	0.00
34	0.960	39.01	1.92	51.61	7.46
35	0.995	10.08	3.42	70.95	15.54
36	0.999	52.32	4.48	28.96	14.33