

Appendix O

EC2 Chemical Model Results

To test the agreement between each model and observations, the ratio of the observed abundance relative to H_2 from Table 9.3 is compared to model predictions (or the inverse of that ratio if it was greater than 1) for that species. A weighting factor was applied for each molecule/transition, depending on how well determined it was thought its abundance should be (see section 12.1). Fig. O.1 compares the effect of varying the weighting factors. Tables O.1-O.6 list the agreement fit results for each model.

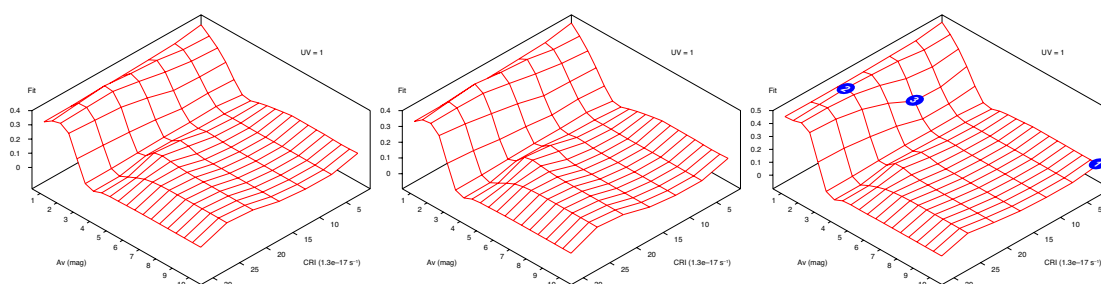


Figure O.1: Comparison of agreement factor for models with different weightings. Left: $\text{CO}=122$ $^{12}\text{CO}/^{13}\text{CO}/\text{C}^{18}\text{O}$ weighting factors = 1/2/2.

Centre: $\text{CO}=111$ $^{12}\text{CO}/^{13}\text{CO}/\text{C}^{18}\text{O}$ weighting factors = 1/1/1.

Right: $\text{All}=1$ All weighting factors = 1 (see section 12.1 for details).

(a) Agreement factor for models from Table O.1 with varying A_V (mag) and cosmic ray ionisation (CRI) in terms of the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, $T = 20 \text{ K}$, $n(\text{H}_2) = 1.2 \times 10^4 \text{ cm}^{-3}$, with a UV field set to the local ISM value, and most initial abundances reduced by a factor of 5 from typical local ISM values (see Table 12.6).

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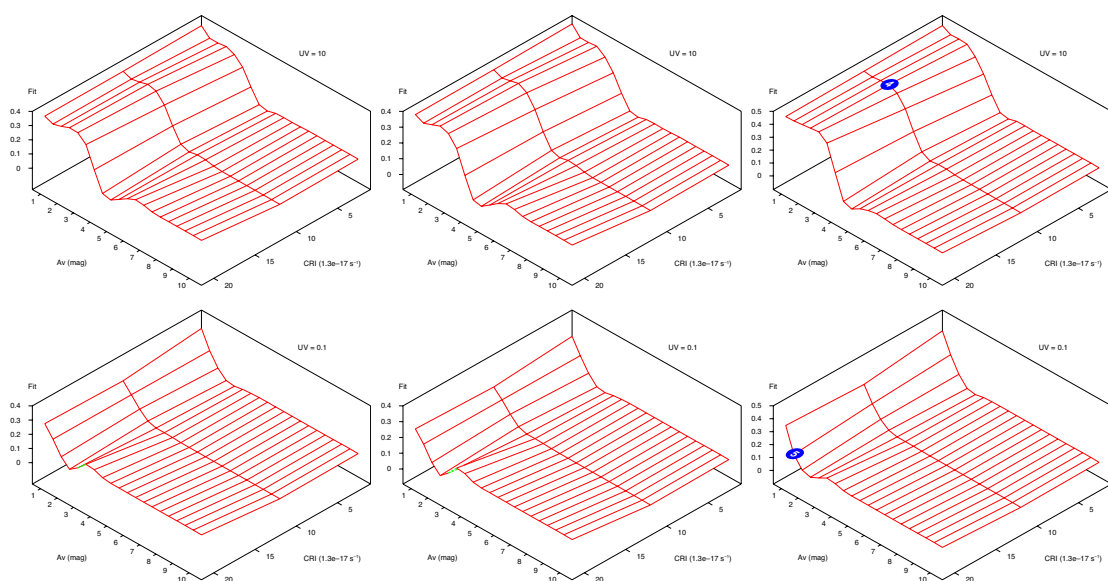


Figure O.1 (continued): Agreement factor for models from Table O.2 with varying A_V (mag), CRI in terms of the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, and:
 (b) UV field increased by a factor of 10 compared to the local ISM value;
 (c) UV field reduced by a factor of 10 compared to the local ISM value.

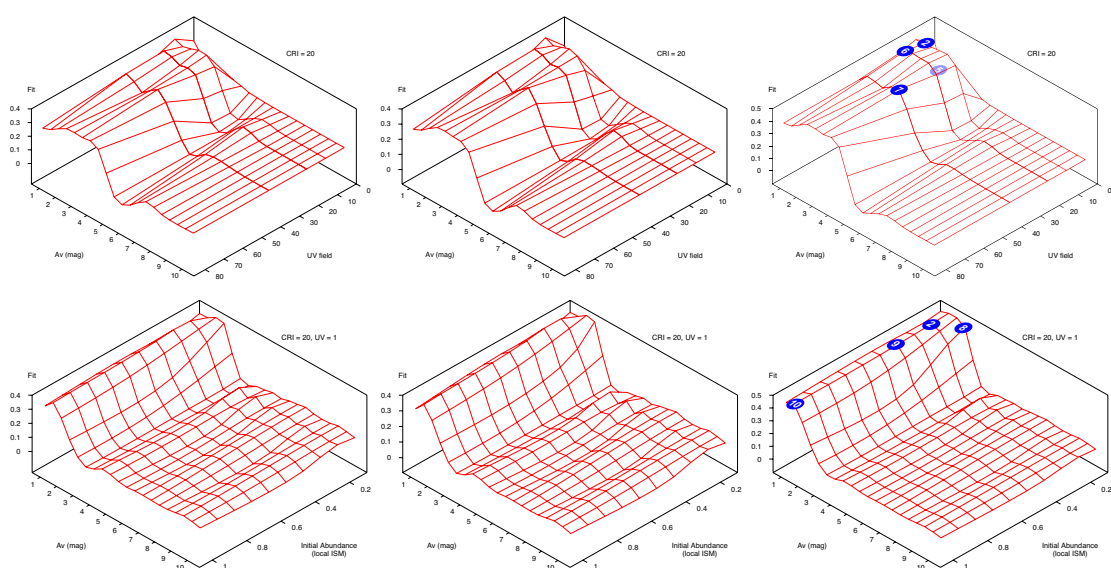


Figure O.1 (continued): Agreement factor for models with varying A_V (mag) and:
 (d) an increasing UV field compared to the local ISM value, and most initial abundances reduced by a factor of 5 (from Table O.3);
 (e) most initial abundances reducing relative to typical local ISM values, and a UV field set to the local ISM value (from Table O.4).

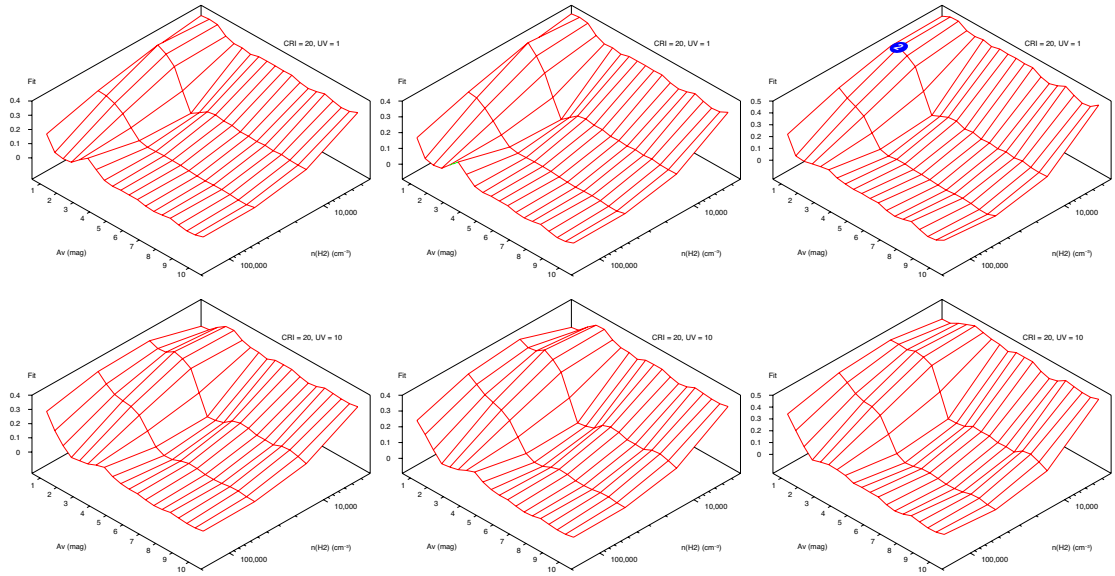


Figure O.1 (continued): Agreement factor from Table O.5 for models with varying A_V (mag) and $n(\text{H}_2)$ (cm^{-3}): (f) UV field set to the local ISM value; (g) UV field increased by a factor of 10 compared to the local ISM value. CRI rate = $20 \times 1.3 \times 10^{-17} \text{ s}^{-1}$, $T = 20 \text{ K}$, and most initial abundances reduced by a factor of 5.

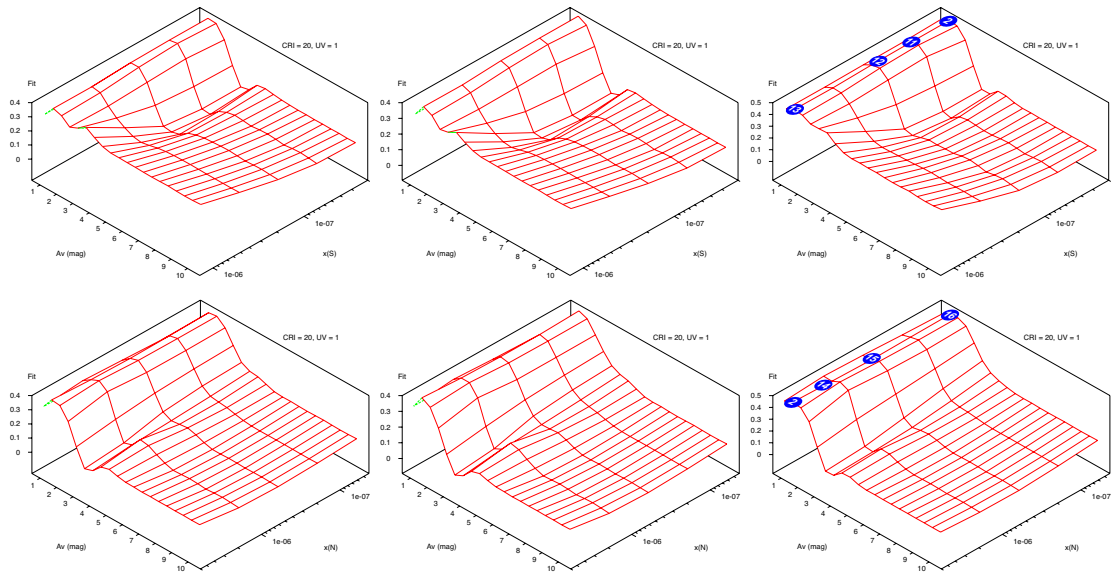


Figure O.1 (continued): Agreement factor from Table O.6 for models with varying A_V (mag) and initial abundances for: (h) sulphur, $x(\text{S})$; (i) nitrogen, $x(\text{N})$. CRI rate = $20 \times 1.3 \times 10^{-17} \text{ s}^{-1}$, $T = 20 \text{ K}$, $n(\text{H}_2) = 1.2 \times 10^4 \text{ cm}^{-3}$, with a UV field set to the local ISM value, and most other initial abundances reduced by a factor of 5.

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Table O.1: EC2 chemical model agreement results for varying CRI and A_V .

CRI	A_V	CO=122	CO=111	All=1	M	CRI	A_V	CO=122	CO=111	All=1	M
0.5	0.5	0.33	0.35	0.44		15	0.5	0.28	0.30	0.40	
0.5	1	0.28	0.29	0.38		15	1	0.34	0.36	0.42	
0.5	2	0.16	0.15	0.21		15	2	0.23	0.21	0.27	
0.5	3	0.00	0.00	0.00		15	3	0.00	0.00	0.00	
0.5	4	0.01	0.01	0.01		15	4	0.06	0.07	0.04	
0.5	5	0.03	0.04	0.02		15	5	0.03	0.03	0.01	
0.5	6	0.05	0.05	0.03		15	6	0.02	0.03	0.01	
0.5	7	0.05	0.05	0.03		15	7	0.02	0.02	0.01	
0.5	8	0.05	0.05	0.03		15	8	0.02	0.02	0.01	
0.5	10	0.05	0.05	0.03		15	10	0.02	0.02	0.01	
1	0.5	0.33	0.34	0.44		20	0.5	0.28	0.29	0.40	
1	1	0.29	0.30	0.39		20	1	0.36	0.37	0.43	2
1	2	0.18	0.17	0.23		20	2	0.27	0.24	0.34	
1	3	0.00	0.00	0.00		20	3	0.00	0.00	0.00	
1	4	0.01	0.01	0.00		20	4	0.08	0.08	0.06	
1	5	0.01	0.01	0.01		20	5	0.08	0.08	0.05	
1	6	0.01	0.02	0.01		20	6	0.07	0.07	0.04	
1	7	0.01	0.02	0.01		20	7	0.07	0.07	0.04	
1	8	0.01	0.02	0.01		20	8	0.07	0.07	0.04	
1	9	0.01	0.02	0.01		20	9	0.07	0.07	0.04	
1	10	0.01	0.02	0.01	1	20	10	0.07	0.07	0.04	
5	0.5	0.30	0.32	0.42		25	0.5	0.27	0.29	0.40	
5	1	0.31	0.32	0.40		25	1	0.33	0.35	0.42	
5	2	0.17	0.16	0.16		25	2	0.28	0.27	0.38	
5	3	0.01	0.01	0.01		25	3	0.00	0.00	0.00	
5	4	0.01	0.01	0.00		25	4	0.01	0.01	0.01	
5	5	0.00	0.00	0.00		25	5	0.06	0.07	0.05	
5	6	0.00	0.00	0.00		25	6	0.08	0.08	0.07	
5	7	0.00	0.00	0.00		25	7	0.08	0.09	0.07	
5	8	0.00	0.00	0.00		25	8	0.08	0.09	0.07	
5	10	0.00	0.00	0.00		25	10	0.08	0.09	0.07	
10	0.5	0.29	0.30	0.40		30	0.5	0.27	0.29	0.40	
10	1	0.34	0.36	0.43		30	1	0.31	0.33	0.41	
10	2	0.17	0.16	0.16	3	30	2	0.29	0.29	0.39	
10	3	0.01	0.01	0.00		30	3	0.00	0.00	0.00	
10	4	0.02	0.02	0.01		30	4	0.00	0.00	0.00	
10	5	0.01	0.01	0.00		30	5	0.01	0.01	0.01	
10	6	0.01	0.01	0.00		30	6	0.01	0.02	0.01	
10	7	0.01	0.01	0.00		30	7	0.02	0.02	0.01	
10	8	0.01	0.01	0.00		30	8	0.02	0.02	0.01	
10	10	0.01	0.01	0.00		30	9	0.02	0.02	0.01	
						30	10	0.02	0.02	0.01	

$T = 20$ K, $n(\text{H}_2) = 1.2 \times 10^4 \text{ cm}^{-3}$, CRI in terms of the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, most initial abundances reduced by a factor of 5 from typical local ISM values, UV field as local ISM.

Table O.2: EC2 chemical model agreement results for varying UV field, CRI and A_V .

UV	CRI	A_V	CO=122	CO=111	All=1	M	UV	CRI	A_V	CO=122	CO=111	All=1	M
10	1	0.5	0.33	0.35	0.42		0.1	1	0.5	0.27	0.23	0.34	
10	1	1	0.27	0.29	0.39		0.1	1	1	0.15	0.14	0.19	
10	1	2	0.28	0.29	0.39		0.1	1	2	0.00	0.00	0.00	
10	1	3	0.20	0.19	0.23		0.1	1	3	0.01	0.01	0.00	
10	1	4	0.00	0.00	0.00		0.1	1	4	0.01	0.01	0.01	
10	1	5	0.01	0.01	0.01		0.1	1	5	0.01	0.02	0.01	
10	1	6	0.01	0.01	0.01		0.1	1	6	0.01	0.02	0.01	
10	1	7	0.01	0.02	0.01		0.1	1	7	0.01	0.02	0.01	
10	1	8	0.01	0.02	0.01		0.1	1	8	0.01	0.02	0.01	
10	1	10	0.01	0.02	0.01		0.1	1	10	0.01	0.02	0.01	
10	10	0.5	0.32	0.34	0.41		0.1	10	0.5	0.22	0.20	0.28	
10	10	1	0.28	0.30	0.40		0.1	10	1	0.15	0.15	0.14	
10	10	2	0.34	0.36	0.43	4	0.1	10	2	0.02	0.02	0.01	
10	10	3	0.27	0.25	0.33		0.1	10	3	0.01	0.02	0.01	
10	10	4	0.00	0.00	0.00		0.1	10	4	0.01	0.01	0.00	
10	10	5	0.03	0.04	0.02		0.1	10	5	0.01	0.01	0.00	
10	10	6	0.01	0.01	0.00		0.1	10	6	0.01	0.01	0.00	
10	10	7	0.01	0.01	0.00		0.1	10	7	0.01	0.01	0.00	
10	10	8	0.01	0.01	0.00		0.1	10	8	0.01	0.01	0.00	
10	10	10	0.01	0.01	0.00		0.1	10	10	0.01	0.01	0.00	
10	20	0.5	0.32	0.33	0.41		0.1	20	0.5	0.23	0.21	0.29	
10	20	1	0.29	0.31	0.41		0.1	20	1	0.15	0.14	0.11	5
10	20	2	0.33	0.35	0.42		0.1	20	2	0.00	0.00	0.00	
10	20	3	0.28	0.27	0.38		0.1	20	3	0.10	0.11	0.07	
10	20	4	0.00	0.00	0.00		0.1	20	4	0.08	0.08	0.04	
10	20	5	0.03	0.03	0.02		0.1	20	5	0.07	0.07	0.04	
10	20	6	0.09	0.10	0.05		0.1	20	6	0.07	0.07	0.04	
10	20	7	0.07	0.07	0.04		0.1	20	7	0.07	0.07	0.04	
10	20	8	0.07	0.07	0.04		0.1	20	8	0.07	0.07	0.04	
10	20	10	0.07	0.07	0.04		0.1	20	10	0.07	0.07	0.04	

$T = 20$ K, $n(\text{H}_2) = 1.2 \times 10^4 \text{ cm}^{-3}$, CRI in terms of the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, most initial abundances reduced by a factor of 5 from typical local ISM values, UV field in terms of the local ISM.

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Table O.3: EC2 chemical model agreement results for varying UV field and A_V .

UV	A_V	CO=122	CO=111	All=1	M	UV	A_V	CO=122	CO=111	All=1	M
0.1	0.5	0.23	0.21	0.29		20	0.5	0.27	0.28	0.37	
0.1	1	0.15	0.14	0.11	5	20	1	0.34	0.36	0.43	6
0.1	2	0.00	0.00	0.00		20	2	0.30	0.32	0.44	
0.1	3	0.10	0.11	0.07		20	3	0.30	0.31	0.39	
0.1	4	0.08	0.08	0.04		20	4	0.01	0.01	0.01	
0.1	5	0.07	0.07	0.04		20	5	0.00	0.00	0.00	
0.1	6	0.07	0.07	0.04		20	6	0.11	0.12	0.07	
0.1	7	0.07	0.07	0.04		20	7	0.07	0.08	0.04	
0.1	8	0.07	0.07	0.04		20	8	0.07	0.07	0.04	
0.1	10	0.07	0.07	0.04		20	10	0.07	0.07	0.04	
1	0.5	0.28	0.29	0.40		40	0.5	0.22	0.23	0.34	
1	1	0.36	0.37	0.43	2	40	1	0.33	0.35	0.40	
1	2	0.27	0.24	0.34		40	2	0.26	0.27	0.38	
1	3	0.00	0.00	0.00		40	3	0.35	0.36	0.44	7
1	4	0.08	0.08	0.06		40	4	0.18	0.17	0.16	
1	5	0.08	0.08	0.05		40	5	0.00	0.00	0.00	
1	6	0.07	0.07	0.04		40	6	0.07	0.07	0.05	
1	7	0.07	0.07	0.04		40	7	0.08	0.09	0.05	
1	8	0.07	0.07	0.04		40	8	0.07	0.07	0.04	
1	9	0.07	0.07	0.04		40	9	0.07	0.07	0.04	
1	10	0.07	0.07	0.04		40	10	0.07	0.07	0.04	
10	0.5	0.32	0.33	0.41		80	0.5	0.21	0.22	0.33	
10	1	0.29	0.31	0.41		80	1	0.23	0.25	0.35	
10	2	0.33	0.35	0.42		80	2	0.31	0.32	0.43	
10	3	0.28	0.27	0.38		80	3	0.31	0.32	0.42	
10	4	0.00	0.00	0.00		80	4	0.29	0.28	0.39	
10	5	0.03	0.03	0.02		80	5	0.00	0.00	0.00	
10	6	0.09	0.10	0.05		80	6	0.01	0.01	0.00	
10	7	0.07	0.07	0.04		80	7	0.10	0.11	0.06	
10	8	0.07	0.07	0.04		80	8	0.07	0.08	0.04	
10	10	0.07	0.07	0.04		80	10	0.07	0.07	0.04	

$T = 20$ K, $n(\text{H}_2) = 1.2 \times 10^4 \text{ cm}^{-3}$, CRI 20 times the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, most initial abundances reduced by a factor of 5 from typical local ISM values, UV field in terms of the local ISM.

Table O.4: EC2 chemical model agreement results for varying IA and A_V .

IA	A_V	CO=122	CO=111	All=1	M
0.1	0.5	0.31	0.32	0.41	
0.1	1	0.31	0.33	0.43	
0.1	2	0.34	0.35	0.40	8
0.1	3	0.01	0.01	0.01	
0.1	4	0.02	0.02	0.01	
0.1	5	0.04	0.04	0.02	
0.1	6	0.05	0.05	0.02	
0.1	8	0.05	0.05	0.02	
0.1	10	0.05	0.05	0.02	
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0.2	0.5	0.28	0.29	0.40	
0.2	1	0.36	0.37	0.43	2
0.2	2	0.27	0.24	0.34	
0.2	3	0.00	0.00	0.00	
0.2	4	0.08	0.08	0.06	
0.2	5	0.08	0.08	0.05	
0.2	6	0.07	0.07	0.04	
0.2	7	0.07	0.07	0.04	
0.2	8	0.07	0.07	0.04	
0.2	9	0.07	0.07	0.04	
0.2	10	0.07	0.07	0.04	
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0.4	0.5	0.29	0.31	0.41	
0.4	1	0.35	0.36	0.42	9
0.4	2	0.16	0.16	0.18	
0.4	3	0.00	0.00	0.00	
0.4	4	0.04	0.04	0.02	
0.4	5	0.02	0.02	0.01	
0.4	6	0.02	0.02	0.01	
0.4	8	0.02	0.02	0.01	
0.4	10	0.02	0.02	0.01	
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1	0.5	0.27	0.27	0.39	
1	1	0.33	0.32	0.41	10
1	2	0.13	0.13	0.16	
1	3	0.00	0.00	0.00	
1	4	0.05	0.06	0.03	
1	5	0.03	0.03	0.02	
1	6	0.03	0.03	0.02	
1	7	0.03	0.03	0.02	
1	8	0.03	0.03	0.02	
1	10	0.03	0.03	0.02	

$T = 20$ K, $n(\text{H}_2) = 1.2 \times 10^4 \text{ cm}^{-3}$, CRI 20 times the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, most initial abundances (IA) reduced by factor indicated from typical local ISM values, UV field as local ISM.

Table O.5: EC2 chemical model agreement results for varying $n(\text{H}_2)$ and A_V .

UV	$n(\text{H}_2)$	A_V	CO=122	CO=111	All=1	M	UV	$n(\text{H}_2)$	A_V	CO=122	CO=111	All=1
1	3.2e3	0.5	0.33	0.35	0.41		10	3.2e3	0.5	0.21	0.22	0.33
1	3.2e3	1	0.33	0.35	0.44		10	3.2e3	1	0.22	0.23	0.34
1	3.2e3	2	0.28	0.30	0.40		10	3.2e3	2	0.31	0.33	0.41
1	3.2e3	3	0.26	0.28	0.41		10	3.2e3	3	0.28	0.29	0.42
1	3.2e3	4	0.27	0.28	0.41		10	3.2e3	4	0.26	0.27	0.40
1	3.2e3	5	0.27	0.28	0.41		10	3.2e3	5	0.27	0.28	0.41
1	3.2e3	6	0.27	0.28	0.41		10	3.2e3	6	0.27	0.28	0.41
1	3.2e3	8	0.27	0.28	0.41		10	3.2e3	8	0.27	0.28	0.41
1	3.2e3	10	0.27	0.28	0.41		10	3.2e3	10	0.27	0.28	0.41
1	1.2e4	0.5	0.28	0.29	0.40		10	1.2e4	0.5	0.32	0.33	0.41
1	1.2e4	1	0.36	0.37	0.43	2	10	1.2e4	1	0.29	0.31	0.41
1	1.2e4	2	0.27	0.24	0.34		10	1.2e4	2	0.33	0.35	0.42
1	1.2e4	3	0.00	0.00	0.00		10	1.2e4	3	0.28	0.27	0.38
1	1.2e4	4	0.08	0.08	0.06		10	1.2e4	4	0.00	0.00	0.00
1	1.2e4	5	0.08	0.08	0.05		10	1.2e4	5	0.03	0.03	0.02
1	1.2e4	6	0.07	0.07	0.04		10	1.2e4	6	0.09	0.10	0.05
1	1.2e4	7	0.07	0.07	0.04		10	1.2e4	7	0.07	0.07	0.04
1	1.2e4	8	0.07	0.07	0.04		10	1.2e4	8	0.07	0.07	0.04
1	1.2e4	9	0.07	0.07	0.04		10	1.2e4	9	0.07	0.07	0.04
1	1.2e4	10	0.07	0.07	0.04		10	1.2e4	10	0.07	0.07	0.04
1	1.4e5	0.5	0.11	0.12	0.15		10	1.4e5	0.5	0.23	0.19	0.27
1	1.4e5	1	0.01	0.01	0.01		10	1.4e5	1	0.13	0.13	0.17
1	1.4e5	2	0.01	0.01	0.02		10	1.4e5	2	0.00	0.00	0.00
1	1.4e5	3	0.10	0.11	0.05		10	1.4e5	3	0.02	0.02	0.04
1	1.4e5	4	0.01	0.01	0.01		10	1.4e5	4	0.06	0.07	0.03
1	1.4e5	5	0.01	0.01	0.00		10	1.4e5	5	0.02	0.02	0.01
1	1.4e5	6	0.01	0.01	0.00		10	1.4e5	6	0.01	0.01	0.00
1	1.4e5	8	0.01	0.01	0.00		10	1.4e5	8	0.01	0.01	0.00
1	1.4e5	10	0.01	0.01	0.00		10	1.4e5	10	0.01	0.01	0.00

$T = 20$ K, CRI 20 times the standard ISM rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, most initial abundances reduced by a factor of 5 from typical local ISM values, UV field in terms of the local ISM.

Table O.6: EC2 chemical model agreement results for varying $x(S)$, $x(N)$ and A_V .

$x(S)$	A_V	CO=122	CO=111	All=1	M	$x(N)$	A_V	CO=122	CO=111	All=1	M
2e-8	0.5	0.28	0.29	0.40		4.3e-6	0.5	0.28	0.29	0.40	
2e-8	1	0.36	0.37	0.43	2	4.3e-6	1	0.36	0.37	0.43	2
2e-8	2	0.27	0.24	0.34		4.3e-6	2	0.27	0.24	0.34	
2e-8	3	0.00	0.00	0.00		4.3e-6	3	0.00	0.00	0.00	
2e-8	4	0.08	0.08	0.06		4.3e-6	4	0.08	0.08	0.06	
2e-8	5	0.08	0.08	0.05		4.3e-6	5	0.08	0.08	0.05	
2e-8	6	0.07	0.07	0.04		4.3e-6	6	0.07	0.07	0.04	
2e-8	7	0.07	0.07	0.04		4.3e-6	7	0.07	0.07	0.04	
2e-8	8	0.07	0.07	0.04		4.3e-6	8	0.07	0.07	0.04	
2e-8	9	0.07	0.07	0.04		4.3e-6	9	0.07	0.07	0.04	
2e-8	10	0.07	0.07	0.04		4.3e-6	10	0.07	0.07	0.04	
5e-8	0.5	0.27	0.29	0.39		2.1e-6	0.5	0.30	0.32	0.42	
5e-8	1	0.36	0.37	0.43	11	2.1e-6	1	0.34	0.36	0.42	14
5e-8	2	0.29	0.27	0.39		2.1e-6	2	0.32	0.29	0.41	
5e-8	3	0.00	0.00	0.00		2.1e-6	3	0.00	0.00	0.00	
5e-8	4	0.05	0.05	0.04		2.1e-6	4	0.12	0.13	0.09	
5e-8	5	0.09	0.09	0.04							
5e-8	6	0.08	0.08	0.04		2.1e-6	6	0.04	0.04	0.02	
5e-8	8	0.07	0.08	0.03		2.1e-6	8	0.04	0.04	0.02	
5e-8	10	0.07	0.08	0.03		2.1e-6	10	0.04	0.04	0.02	
1e-7	0.5	0.27	0.28	0.39		4.3e-7	0.5	0.29	0.30	0.41	
1e-7	1	0.36	0.38	0.43	12	4.3e-7	1	0.34	0.35	0.41	15
1e-7	2	0.29	0.27	0.38		4.3e-7	2	0.30	0.27	0.40	
1e-7	3	0.00	0.00	0.00		4.3e-7	3	0.09	0.09	0.08	
1e-7	4	0.03	0.03	0.03		4.3e-7	4	0.07	0.07	0.05	
1e-7	5	0.09	0.10	0.04							
1e-7	6	0.10	0.11	0.05		4.3e-7	6	0.02	0.02	0.01	
1e-7	8	0.10	0.10	0.04		4.3e-7	8	0.02	0.02	0.01	
1e-7	10	0.10	0.10	0.04		4.3e-7	10	0.02	0.02	0.01	
1e-6	0.5	0.27	0.28	0.38		4.3e-8	0.5	0.26	0.27	0.38	
1e-6	1	0.34	0.36	0.42	13	4.3e-8	1	0.34	0.36	0.42	16
1e-6	2	0.27	0.27	0.37		4.3e-8	2	0.30	0.27	0.40	
1e-6	3	0.34	0.31	0.38		4.3e-8	3	0.12	0.13	0.18	
1e-6	4	0.27	0.25	0.29		4.3e-8	4	0.09	0.09	0.09	
1e-6	5	0.25	0.24	0.28		4.3e-8	5	0.05	0.05	0.06	
1e-6	6	0.25	0.24	0.28		4.3e-8	6	0.05	0.05	0.06	
1e-6	8	0.25	0.24	0.28		4.3e-8	8	0.05	0.05	0.06	
1e-6	10	0.25	0.24	0.28		4.3e-8	10	0.05	0.05	0.06	

$T = 20$ K, $n(H_2) = 1.2 \times 10^4$ cm $^{-3}$, CRI 20 times the standard ISM rate of 1.3×10^{-17} s $^{-1}$, most other initial abundances reduced by a factor of 5 from typical local ISM values, UV field as local ISM.

