



HAL
open science

Potential optimization for the calculation of shocked liquid nitromethane properties

Nicolas Desbiens, Emeric Bourasseau, Jean-Bernard Maillet

► **To cite this version:**

Nicolas Desbiens, Emeric Bourasseau, Jean-Bernard Maillet. Potential optimization for the calculation of shocked liquid nitromethane properties. *Molecular Simulation*, 2007, 33 (13), pp.1061-1070. 10.1080/08927020701589245 . hal-00515017

HAL Id: hal-00515017

<https://hal.science/hal-00515017>

Submitted on 4 Sep 2010

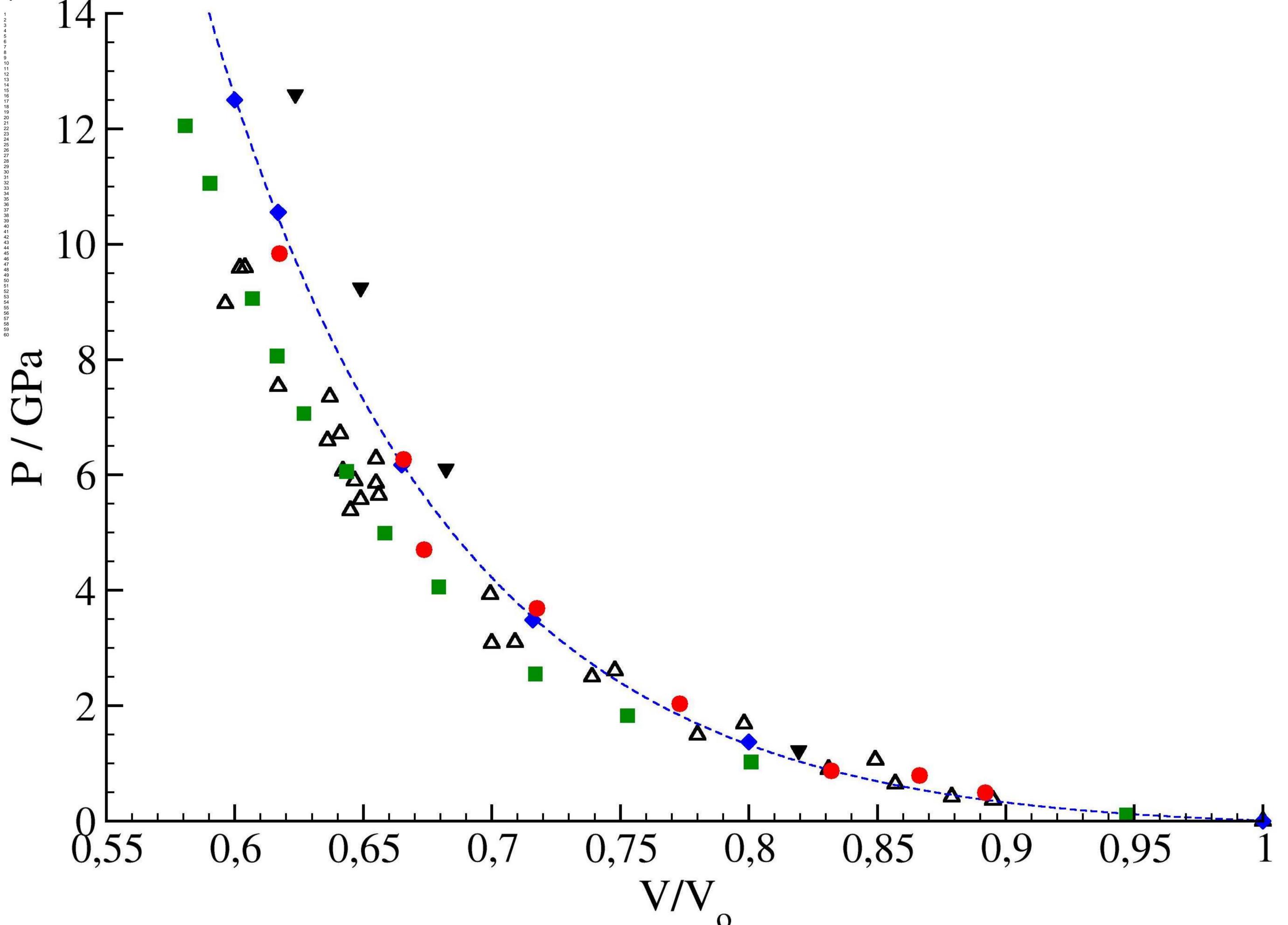
HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

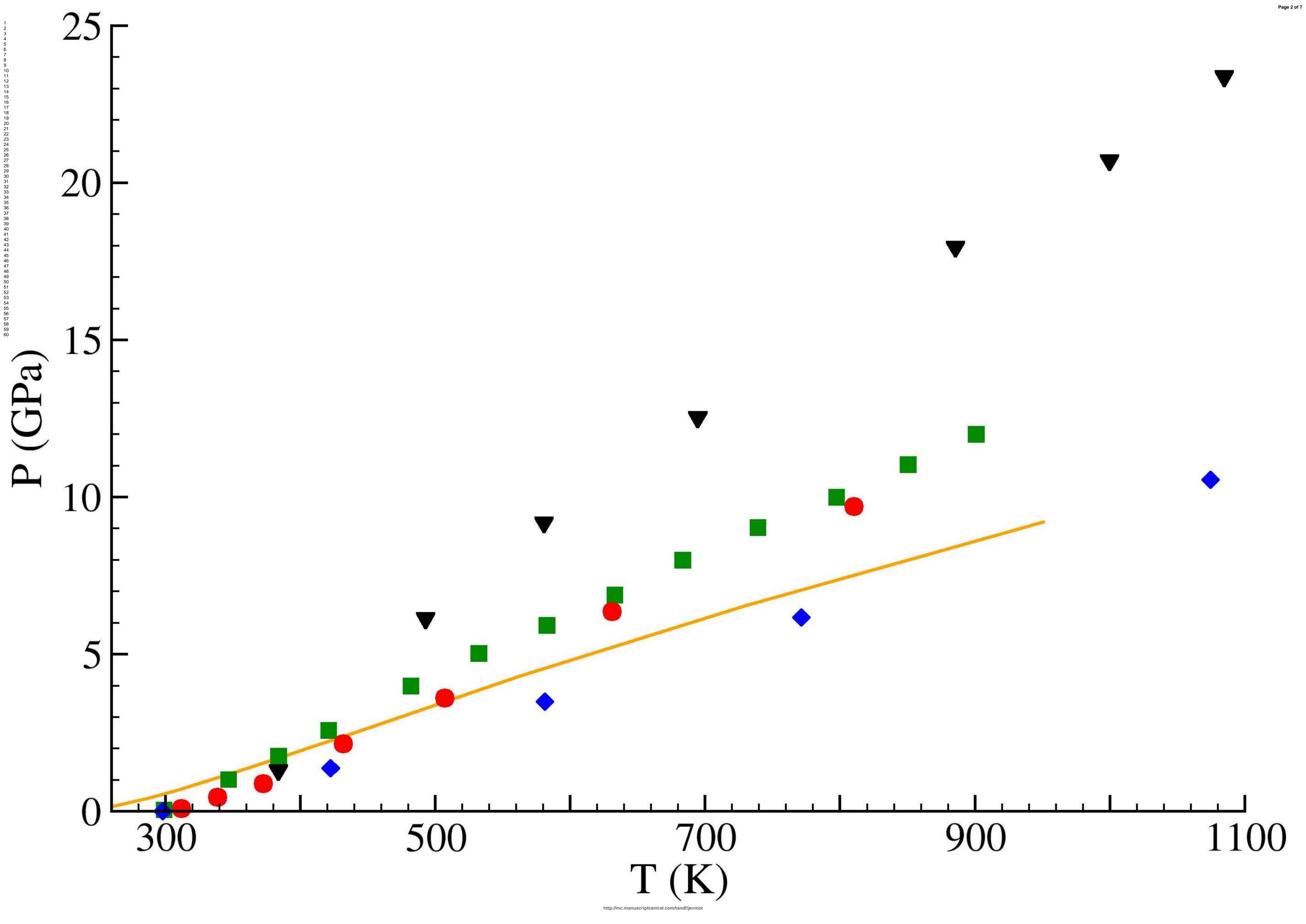
L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Potential optimization for the calculation of shocked liquid nitromethane properties

Journal:	<i>Molecular Simulation</i> / <i>Journal of Experimental Nanoscience</i>
Manuscript ID:	GMOS-2007-0056.R1
Journal:	Molecular Simulation
Date Submitted by the Author:	22-Jun-2007
Complete List of Authors:	Desbiens, Nicolas; CEA Bourasseau, Emeric; CEA Maillet, Jean-Bernard; CEA
Keywords:	parameter optimization, nitromethane, shock hugoniot, Monte Carlo simulations
Note: The following files were submitted by the author for peer review, but cannot be converted to PDF. You must view these files (e.g. movies) online.	
biblio.bib introduction.tex methods.tex results.tex conclusion.tex phjcp_mod.bst	

SCHOLARONE™
Manuscripts

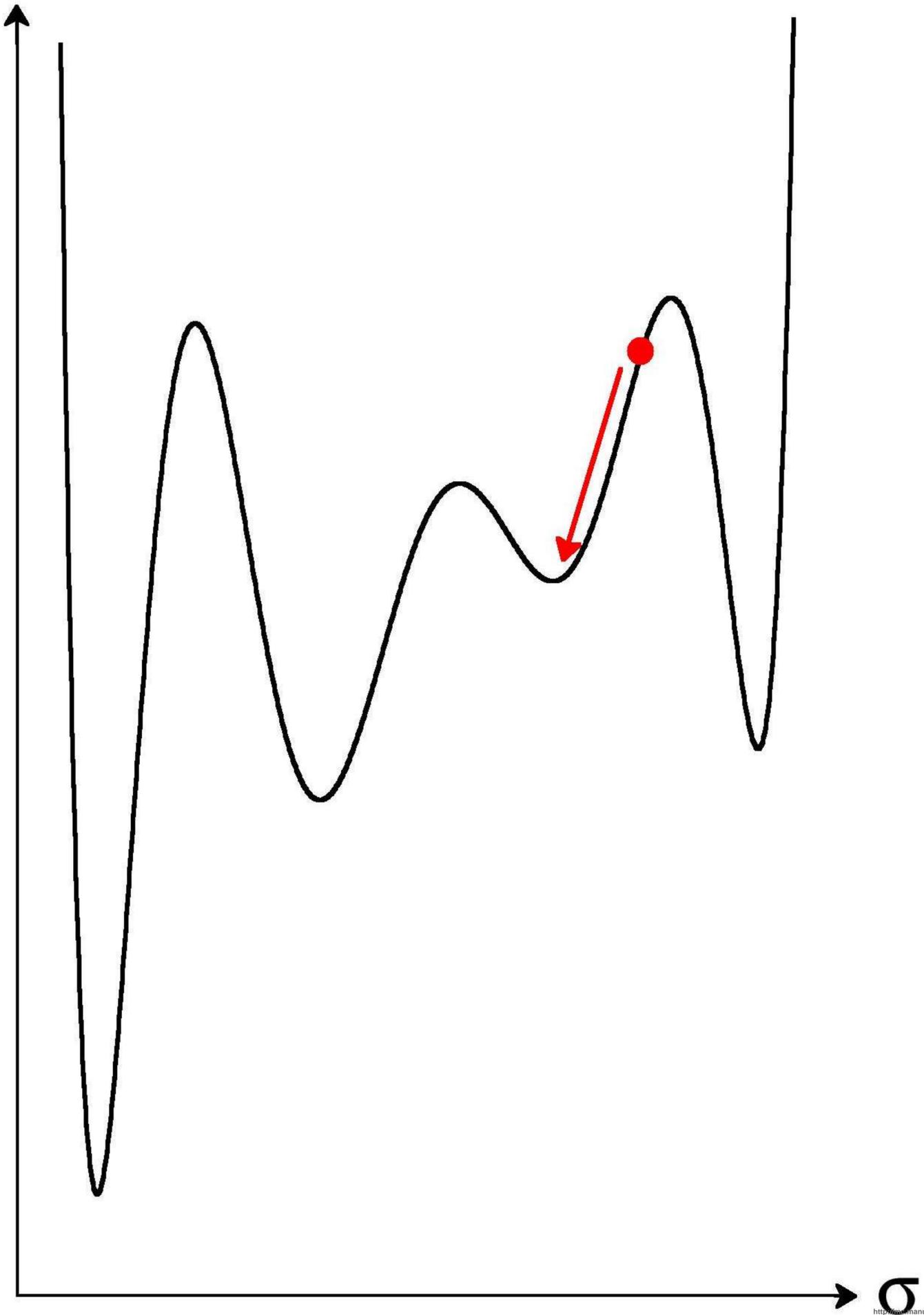




1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

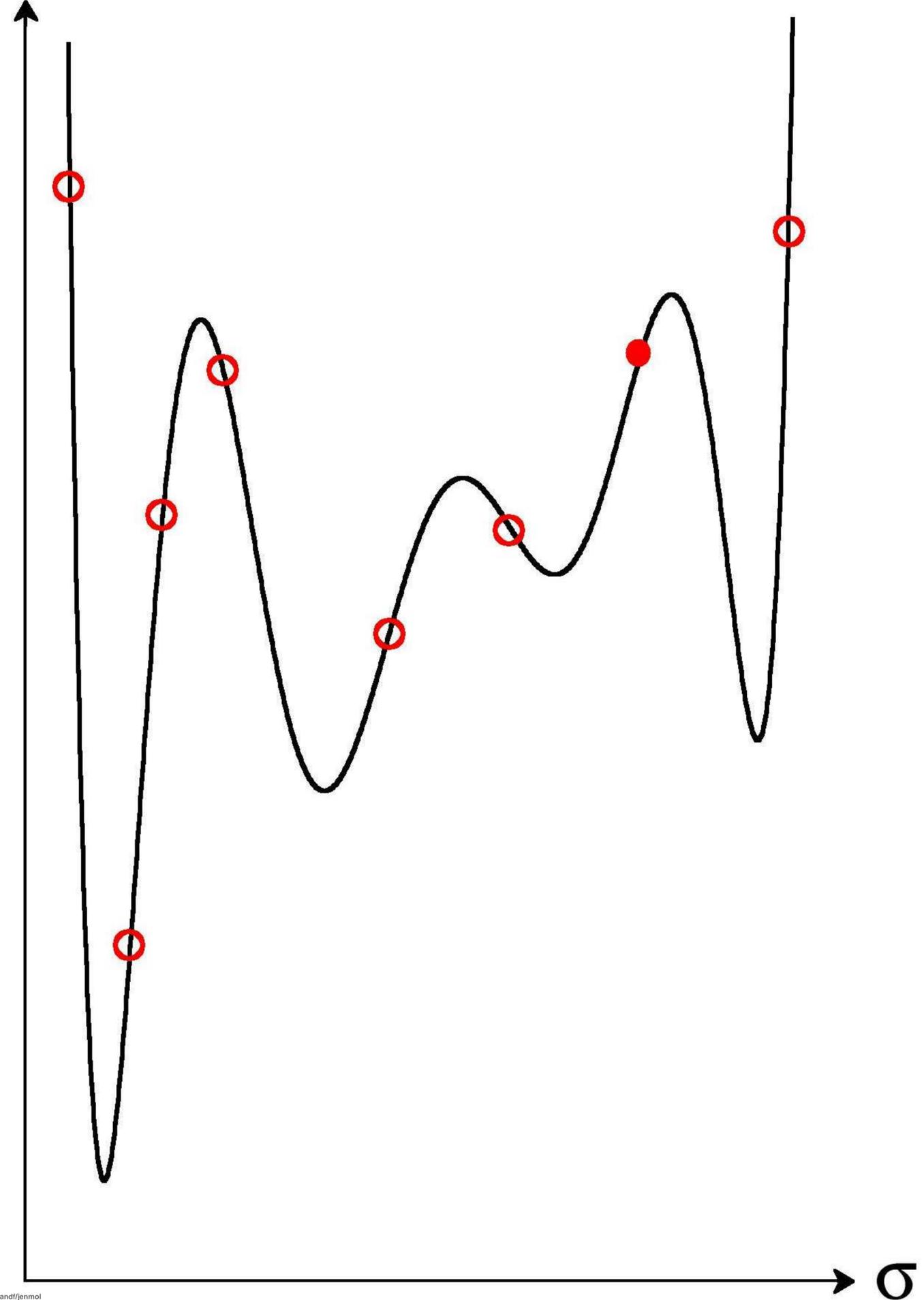
f_{tot}

Local minimization



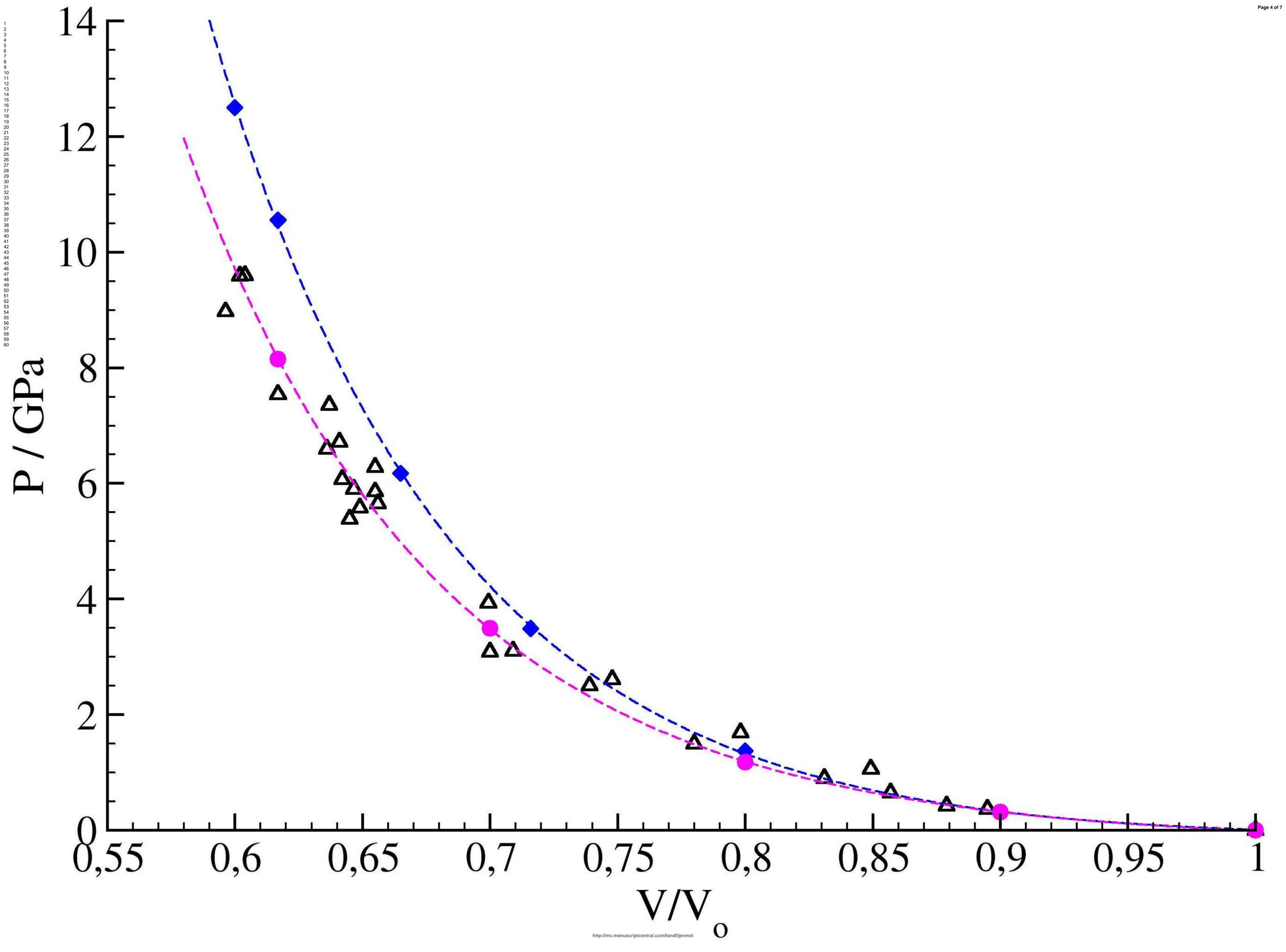
f_{tot}

Random exploration

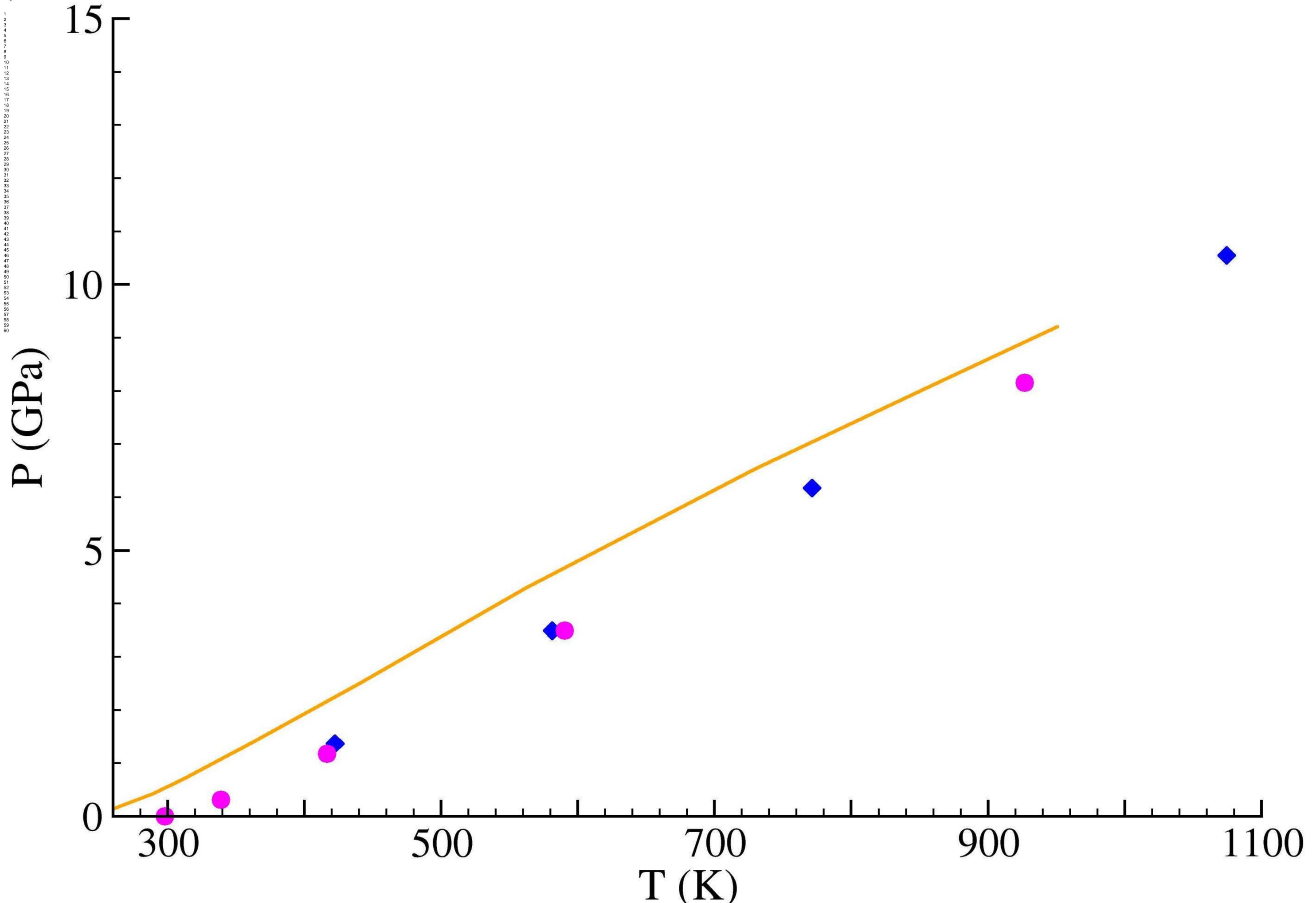


σ

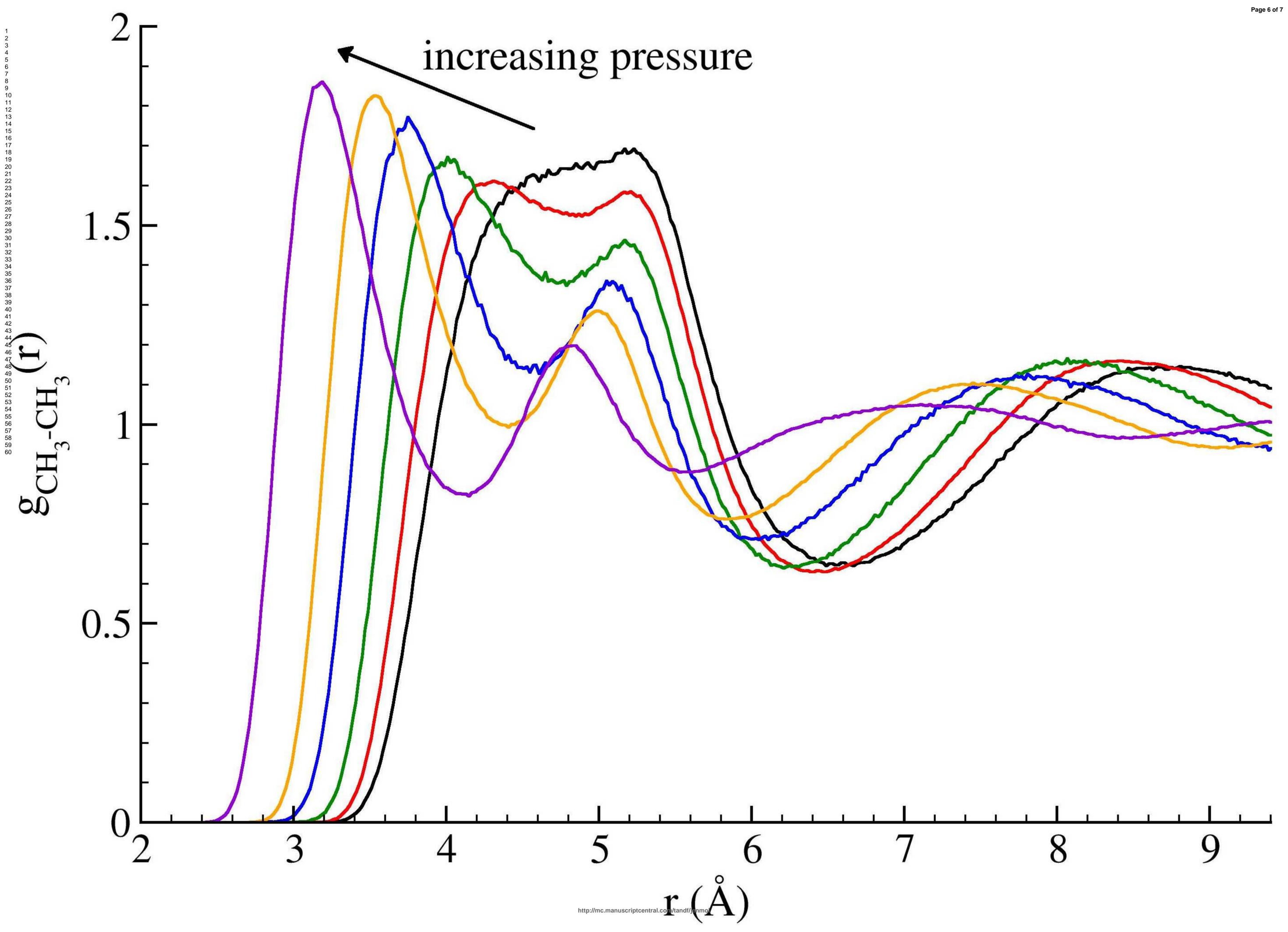
σ



1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60



1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60



1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

