ESI for "An adaptive mutation simulated annealing based investigation on Coulombic explosion and identification of dissociation patterns in $(CO_2)_n^{2+}$ clusters"

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Keywords: Adaptive Mutation Simulated Annealing (AMSA), Molecular Cluster, $(CO_2)_n^{2+}$ cluster, Coulomb Explosion

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[80]See ESI for all the figures, all the fragmentation patterns and all the values of energies.

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FIGURES

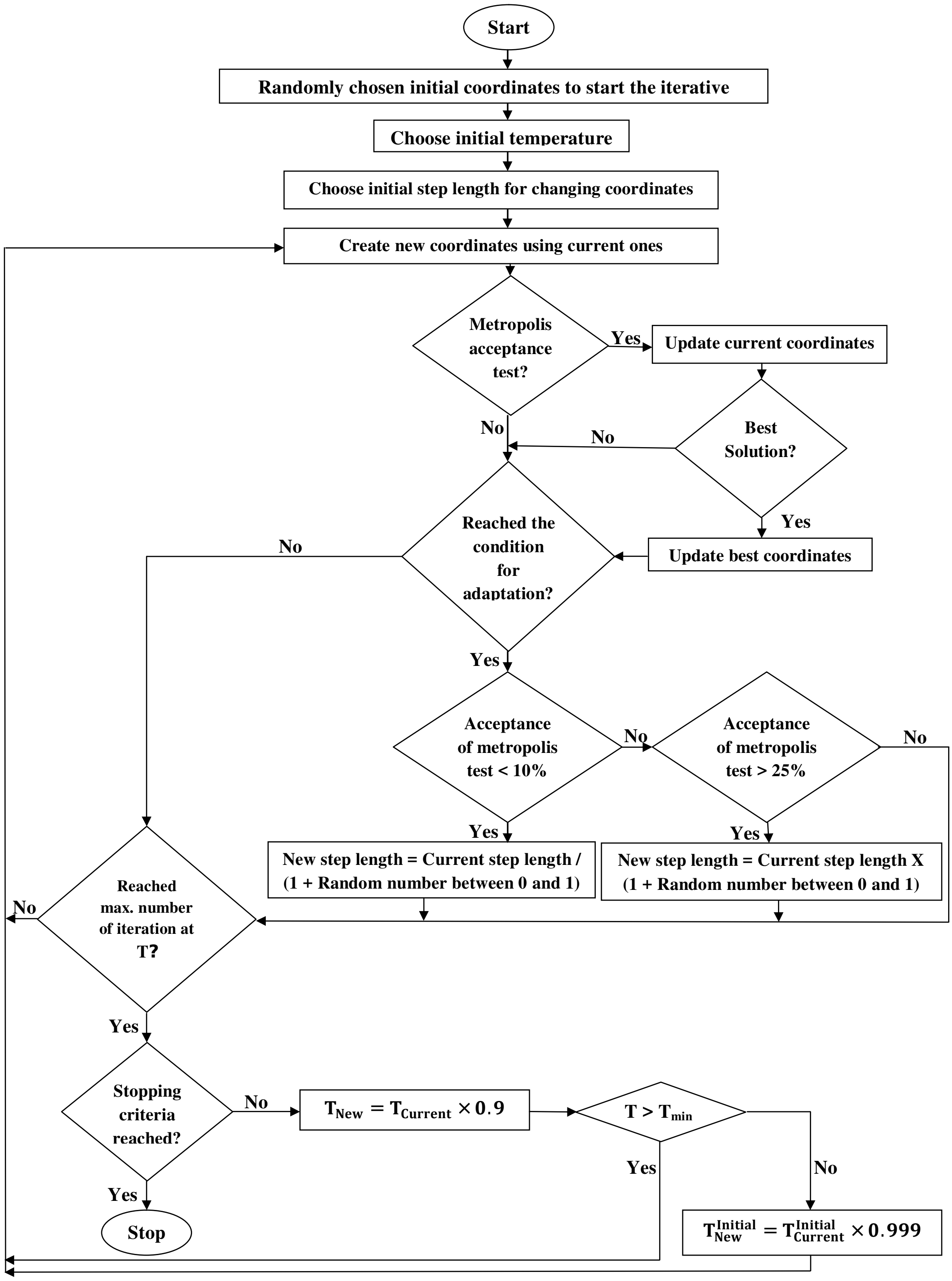
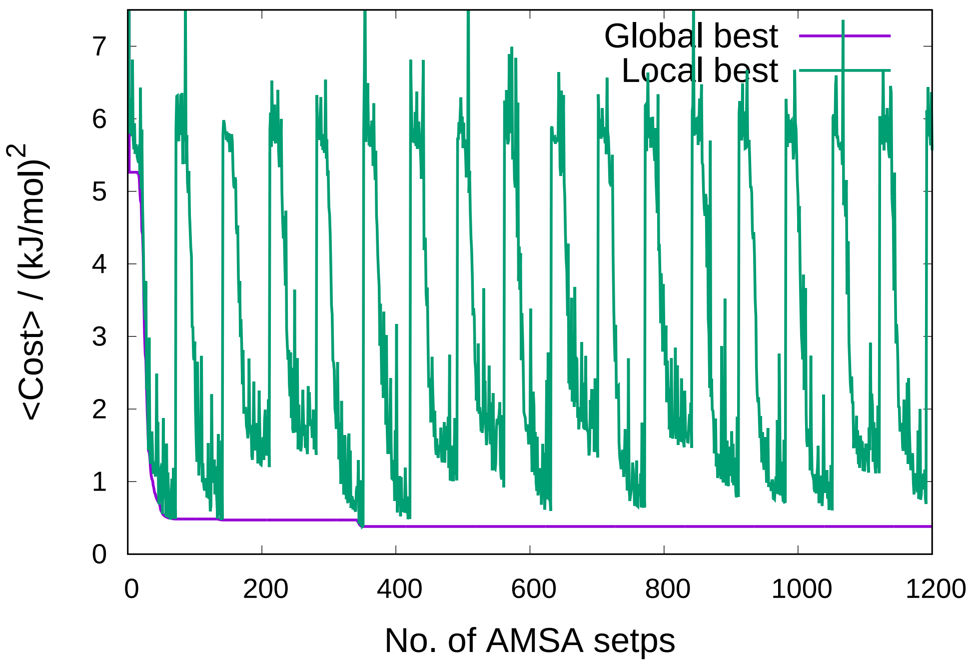
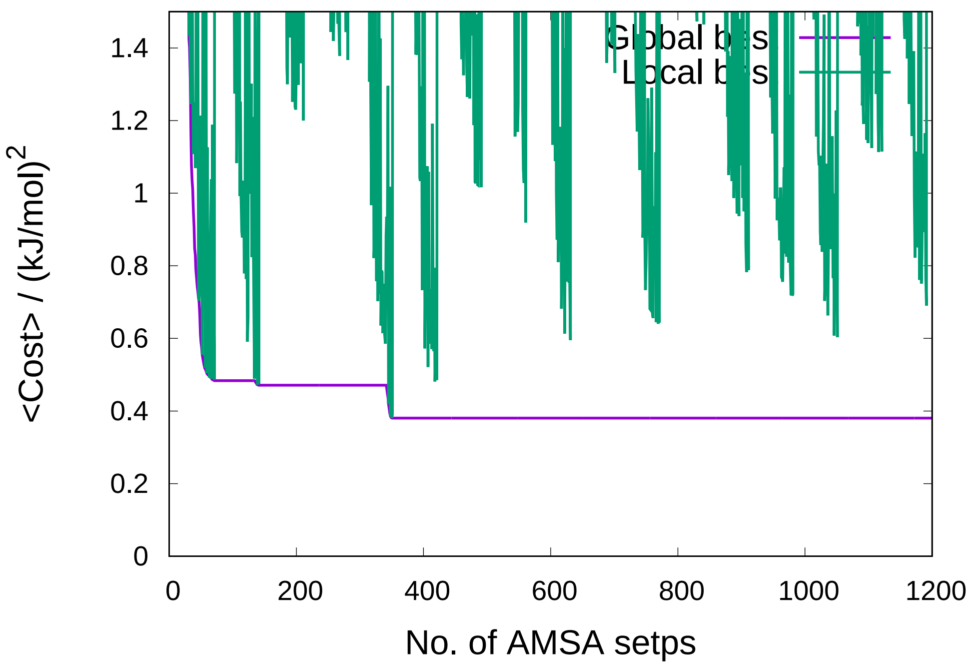


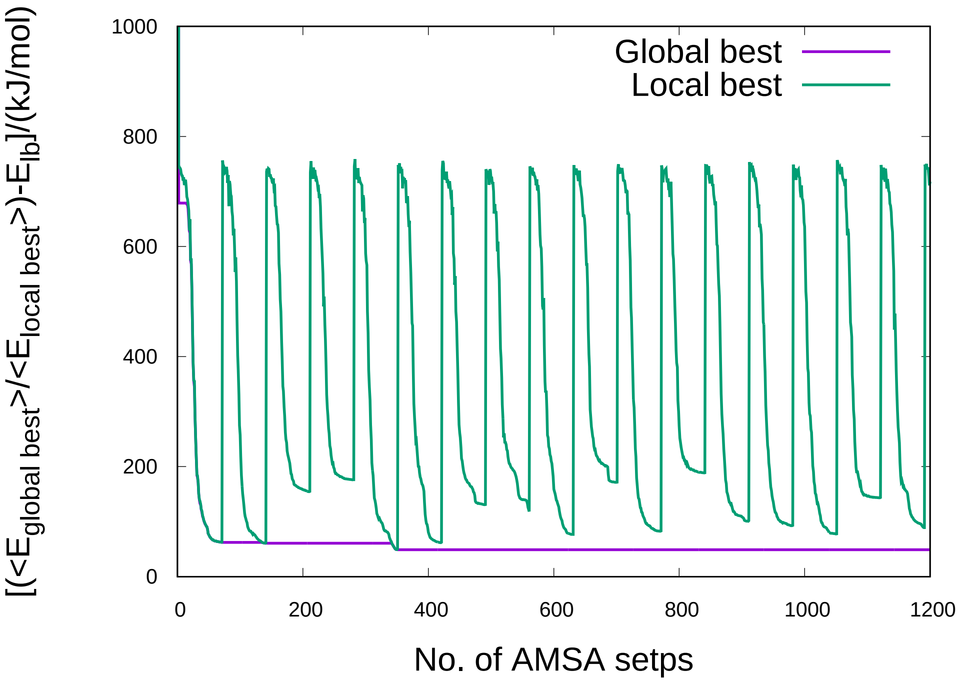
FIG. 1. Flowchart of adaptive mutation simulated annealing (AMSA) technique.



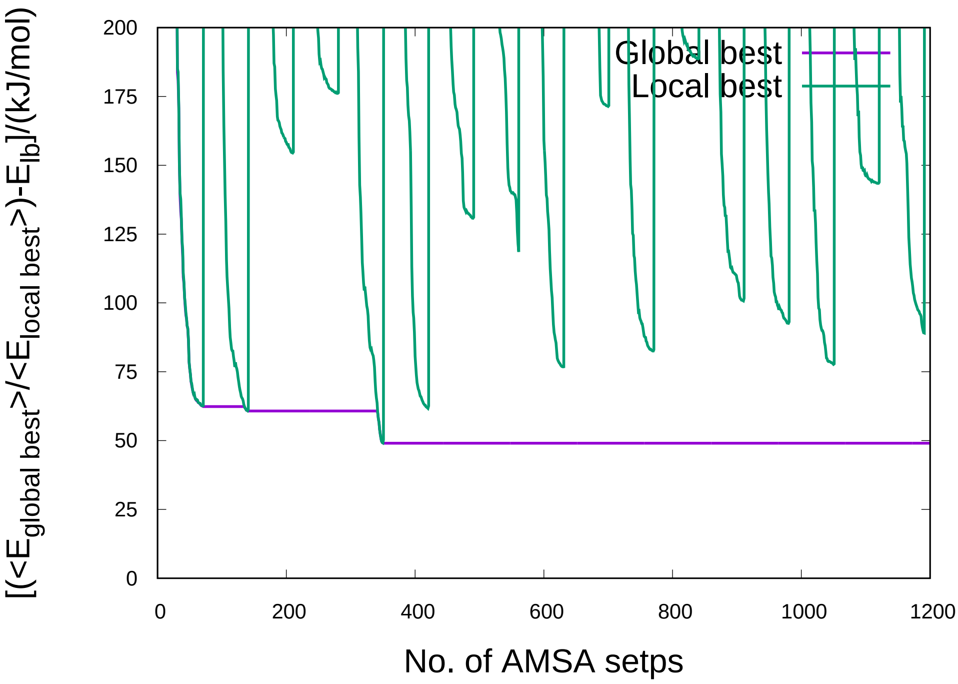
(a)Variation of Cost functional in AMSA



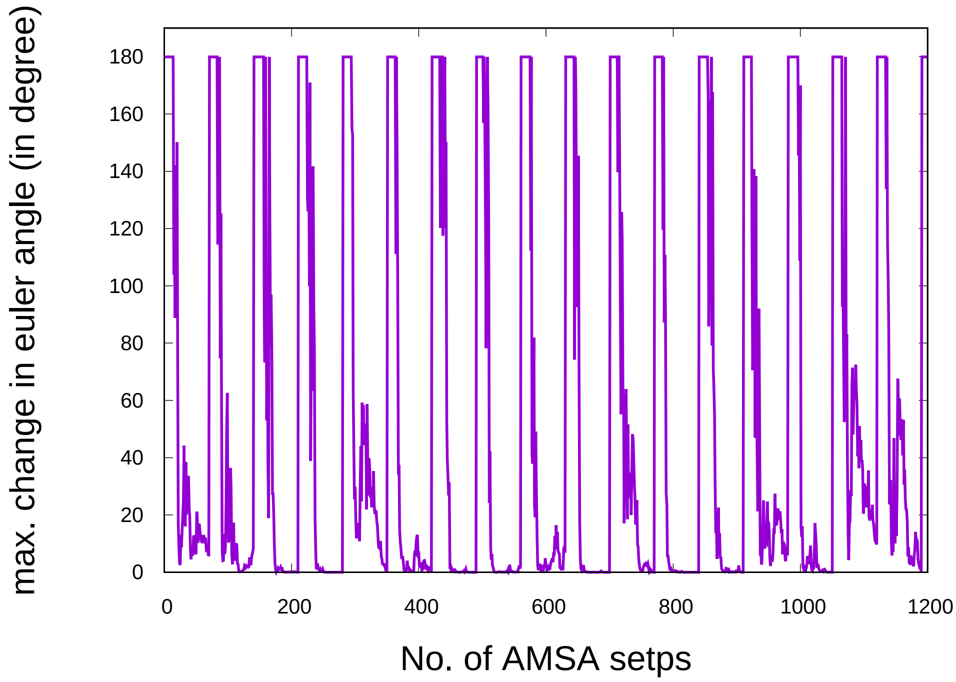
(b)Zoomed in profile of a portion of Fig. 2(a)



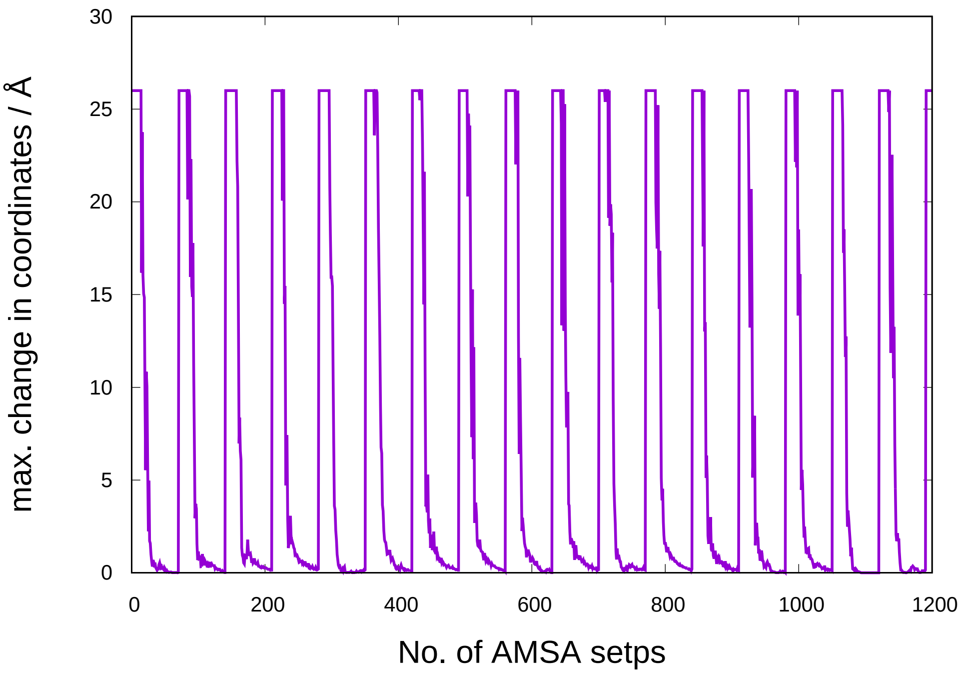
(c)Variation of energy in AMSA



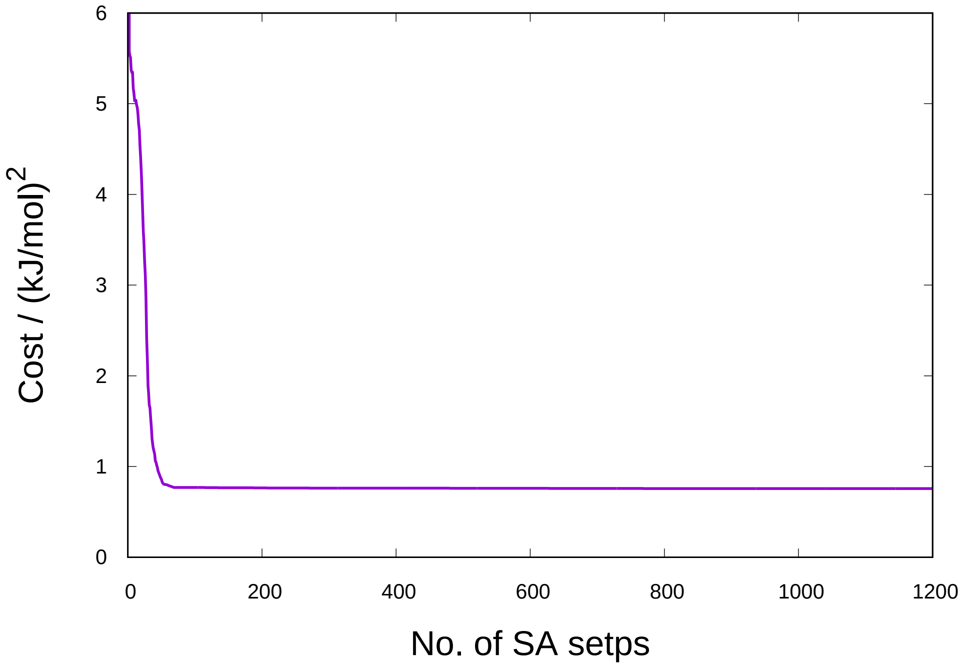
(d)Zoomed in profile of a portion of Fig. 2(c)



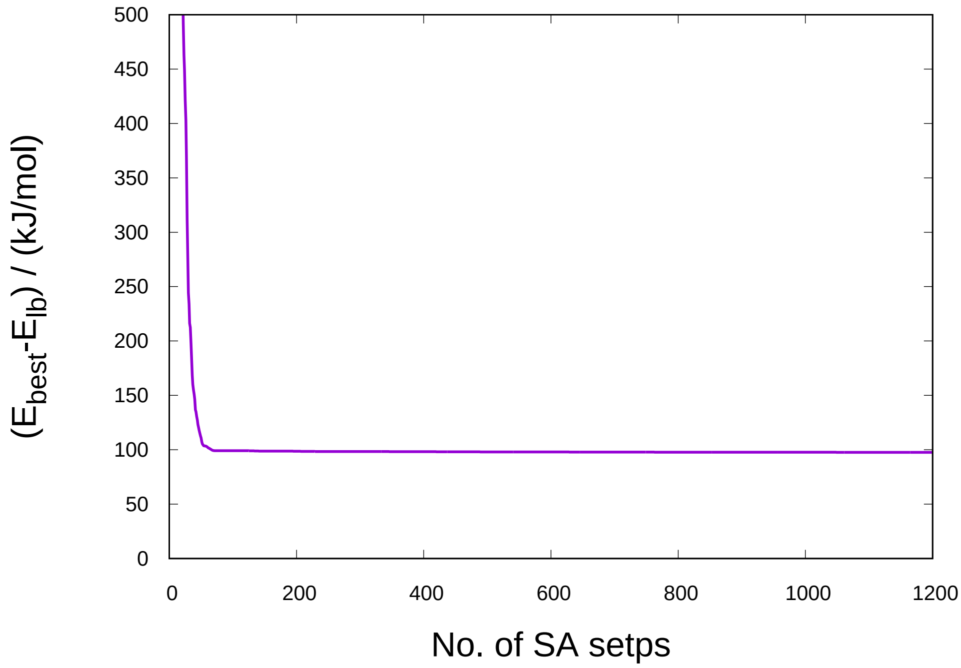
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

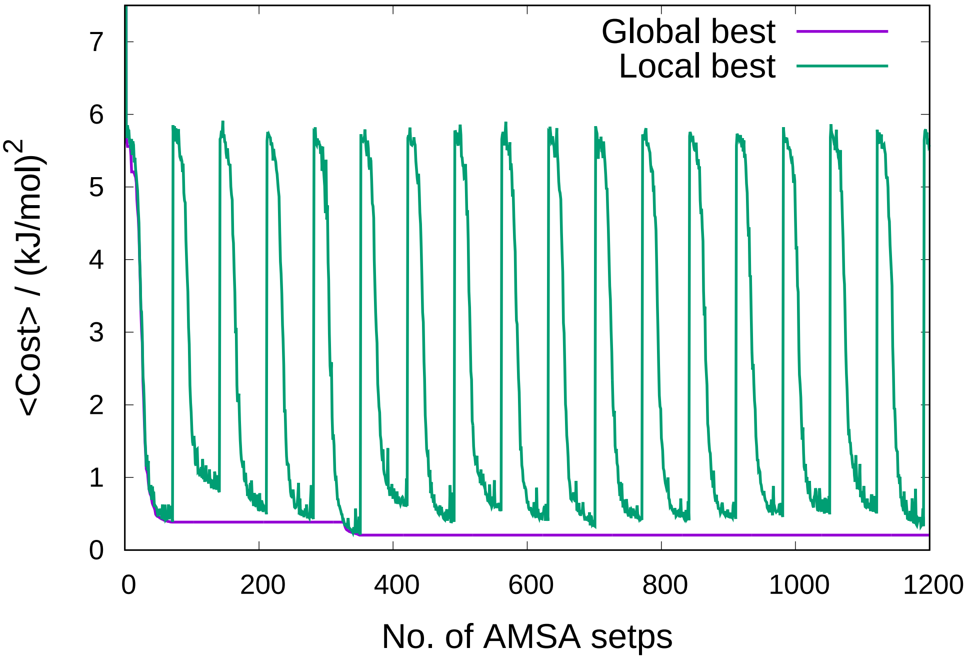


(g)Variation of Cost functional in SA

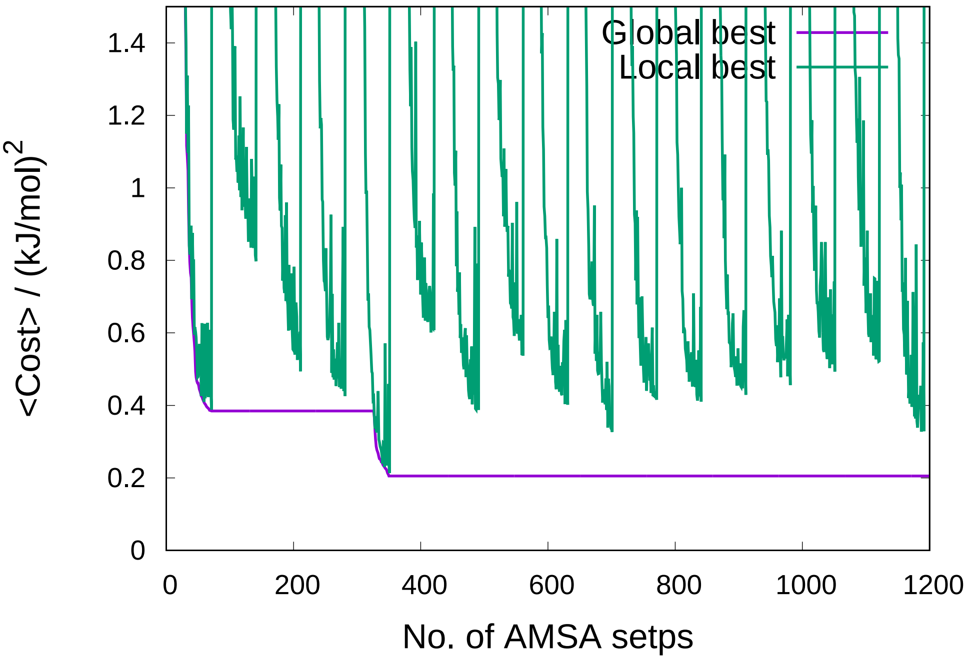


(h)Variation of energy in SA

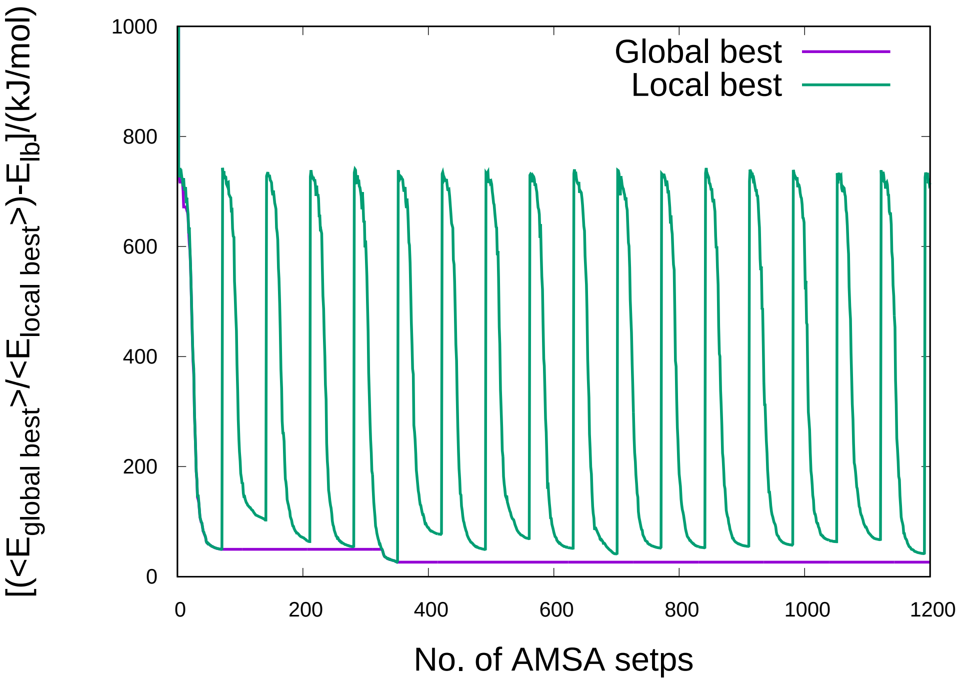
FIG. 2. Critical analysis of AMSA for $NOVER = 100$.



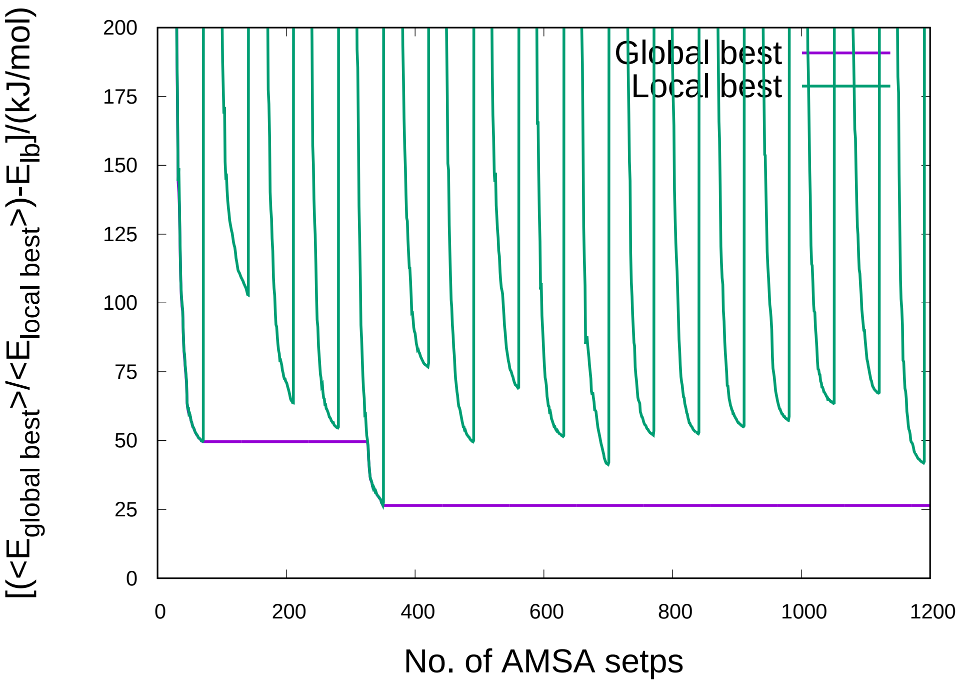
(a)Variation of Cost functional in AMSA



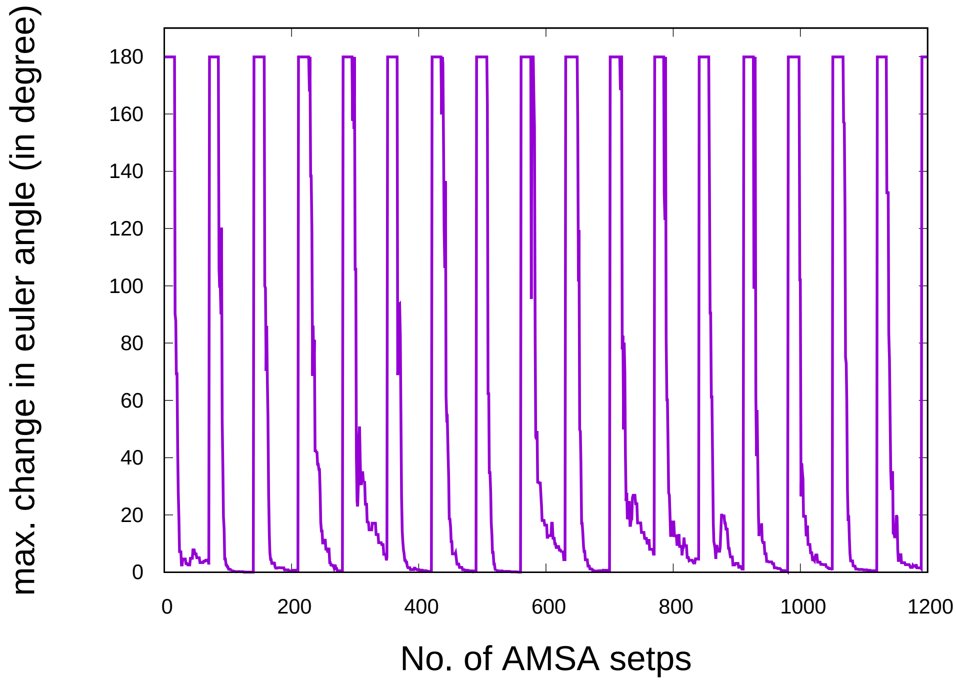
(b)Zoomed in profile of a portion of Fig. 3(a)



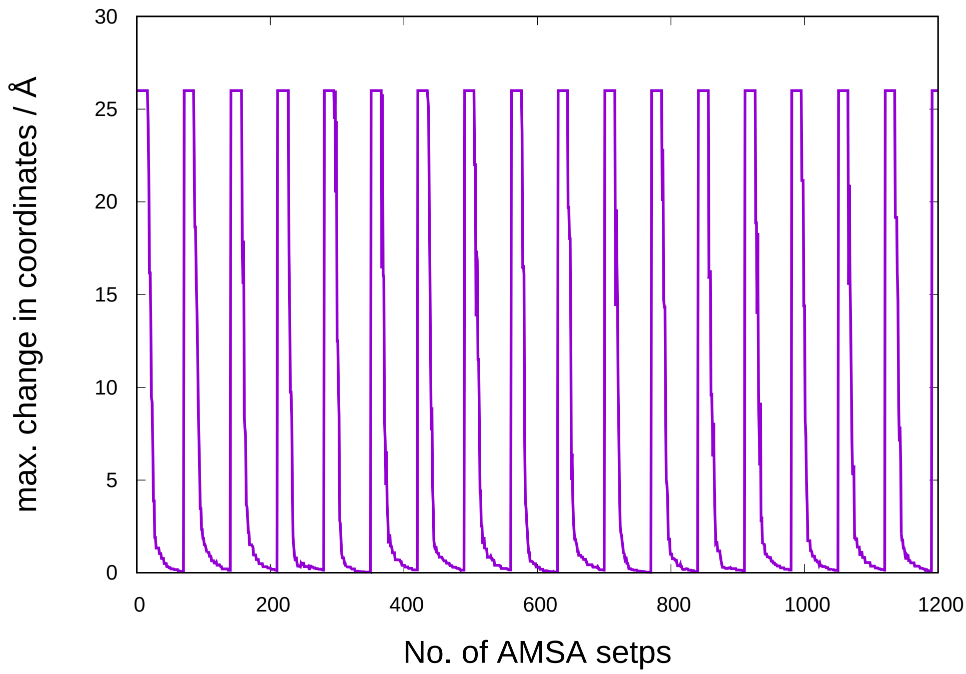
(c)Variation of energy in AMSA



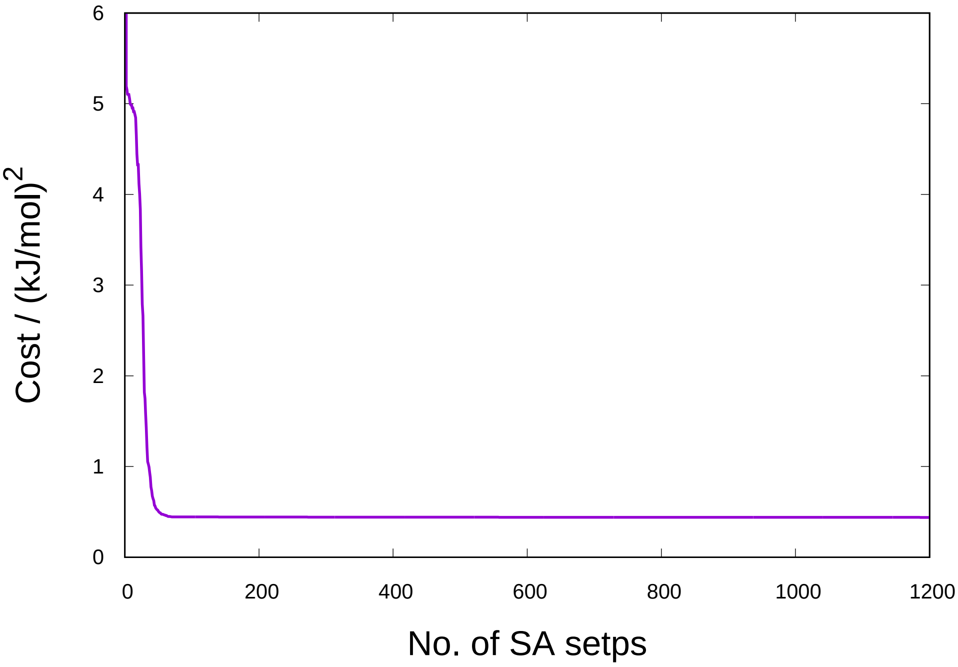
(d)Zoomed in profile of a portion of Fig. 3(c)



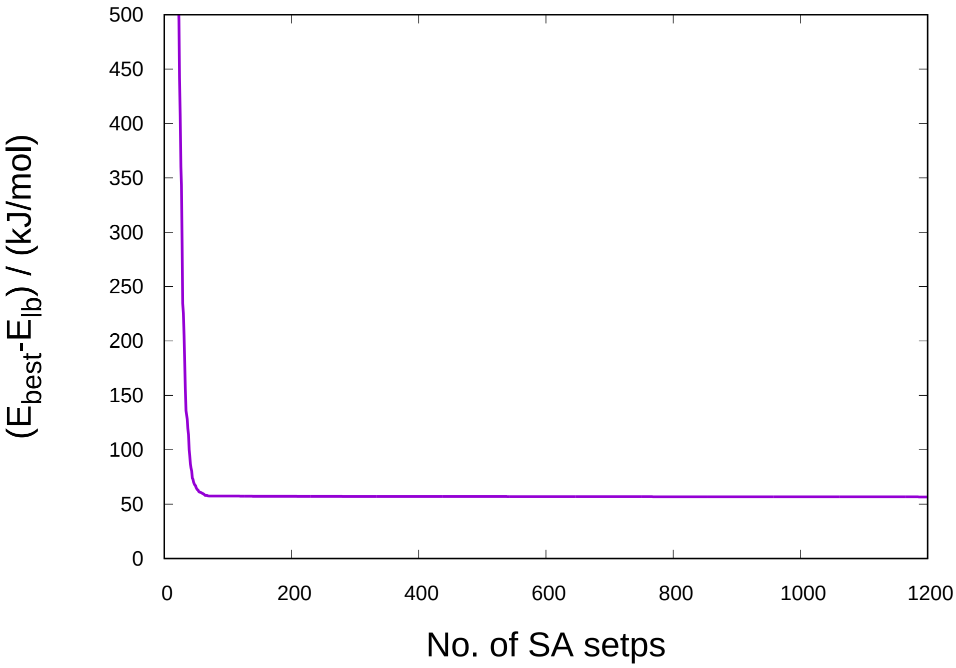
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

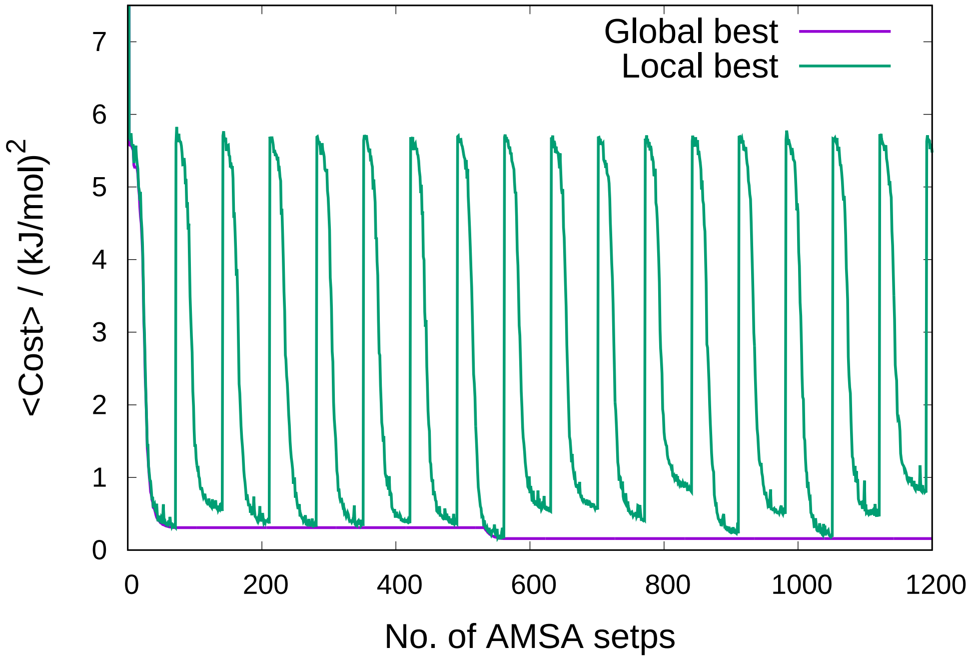


(g)Variation of Cost functional in SA

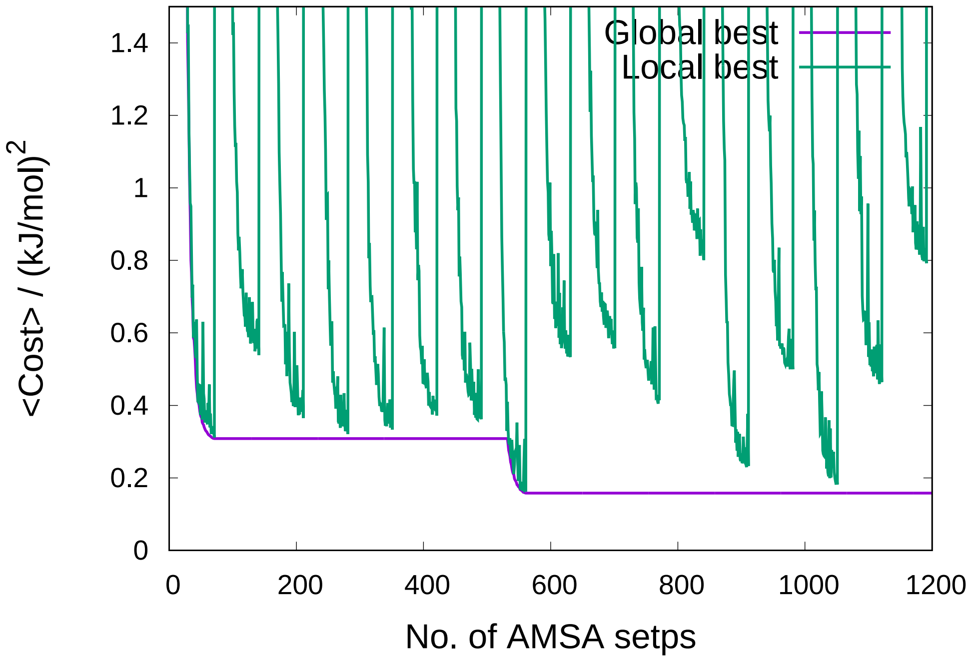


(h)Variation of energy in SA

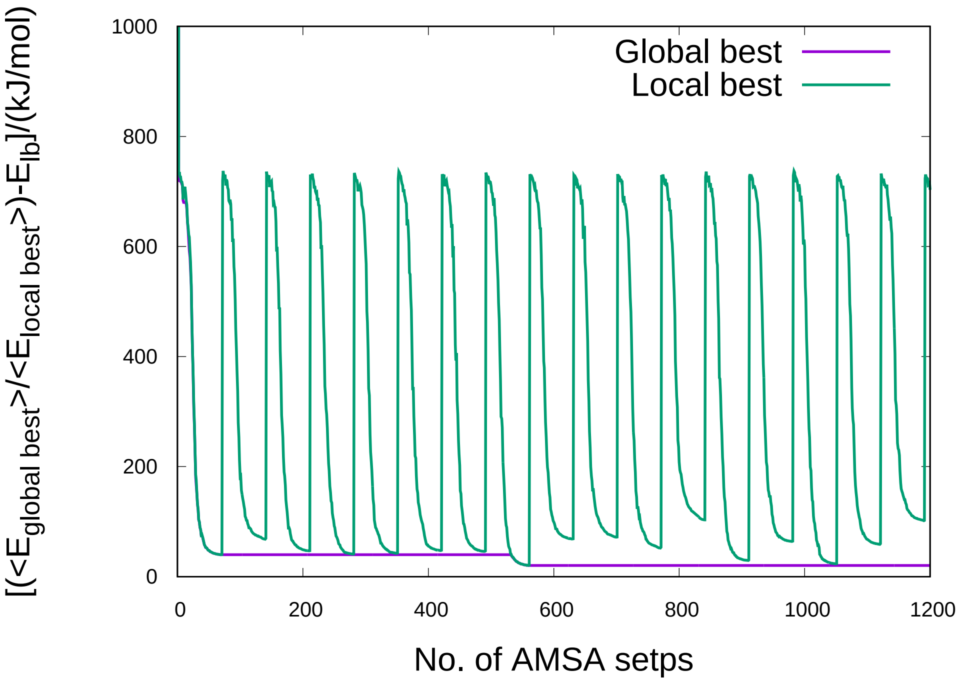
FIG. 3. Critical analysis of AMSA for $NOVER = 500$.



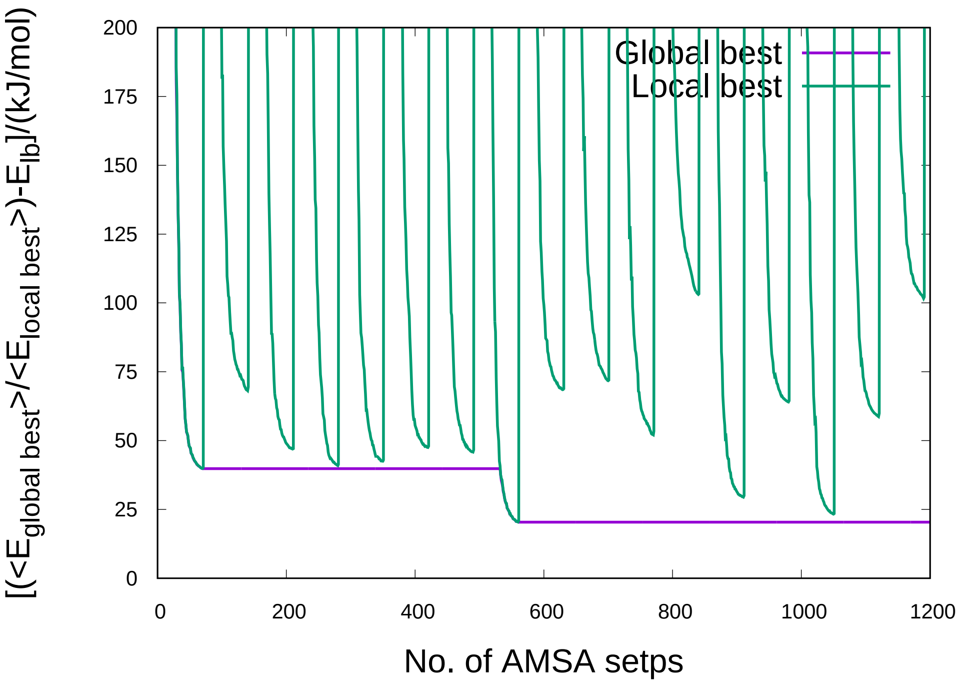
(a)Variation of Cost functional in AMSA



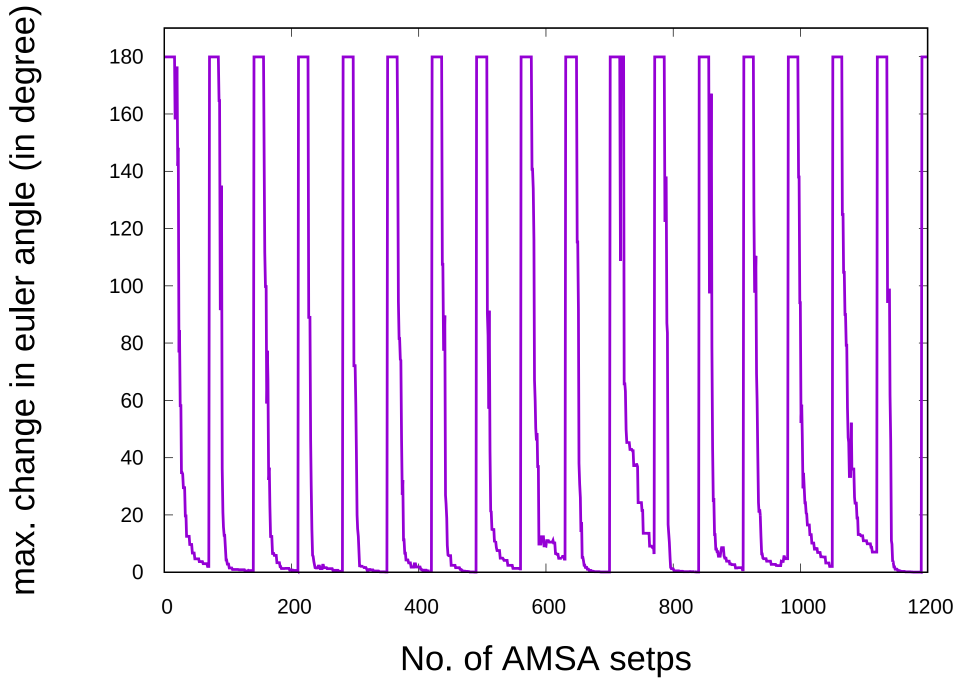
(b)Zoomed in profile of a portion of Fig. 4(a)



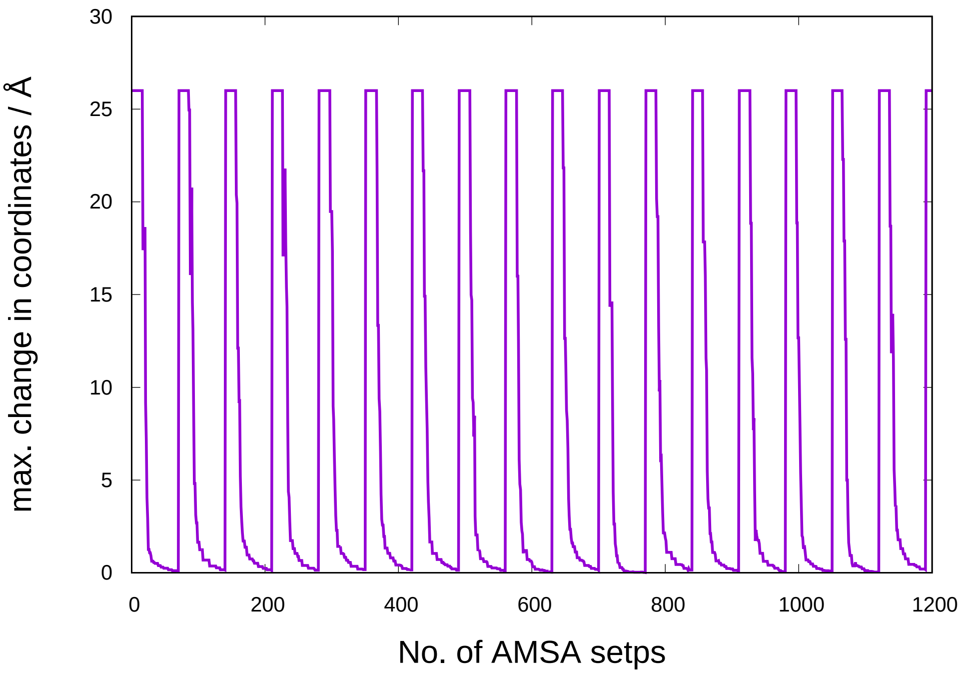
(c)Variation of energy in AMSA



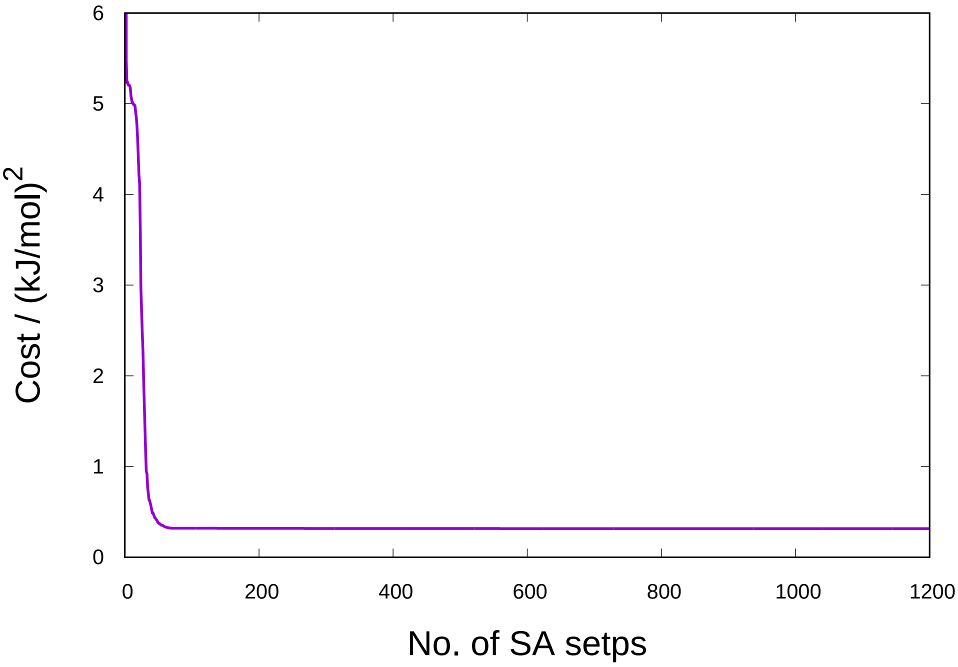
(d)Zoomed in profile of a portion of Fig. 4(c)



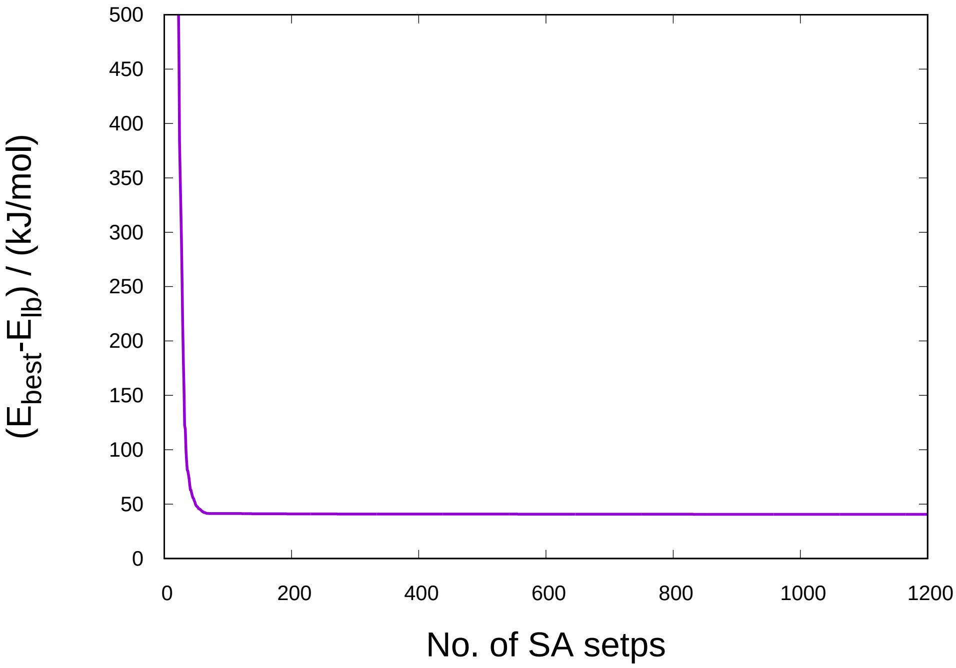
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

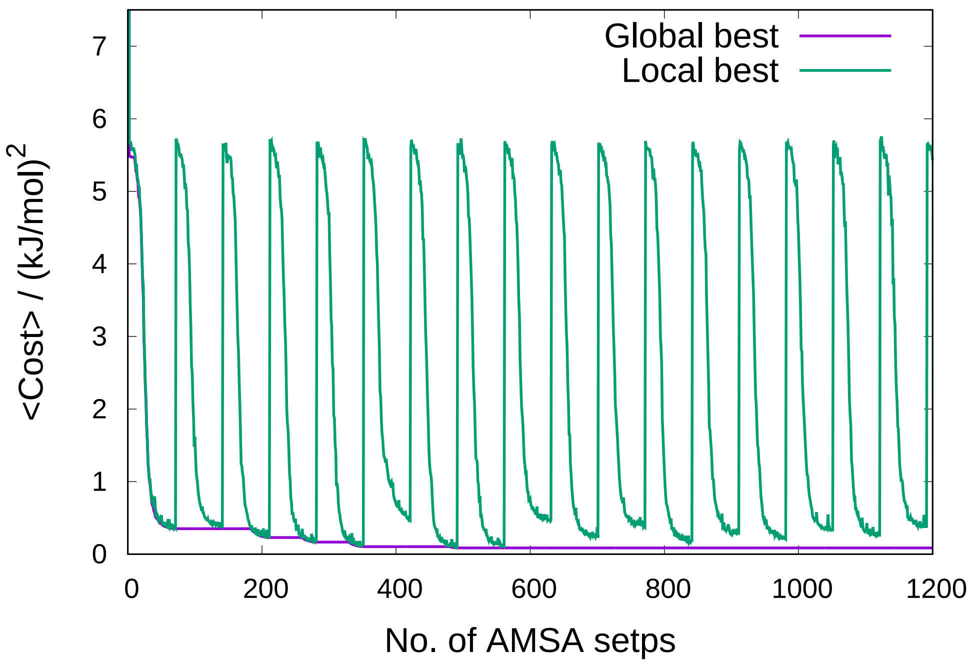


(g)Variation of Cost functional in SA

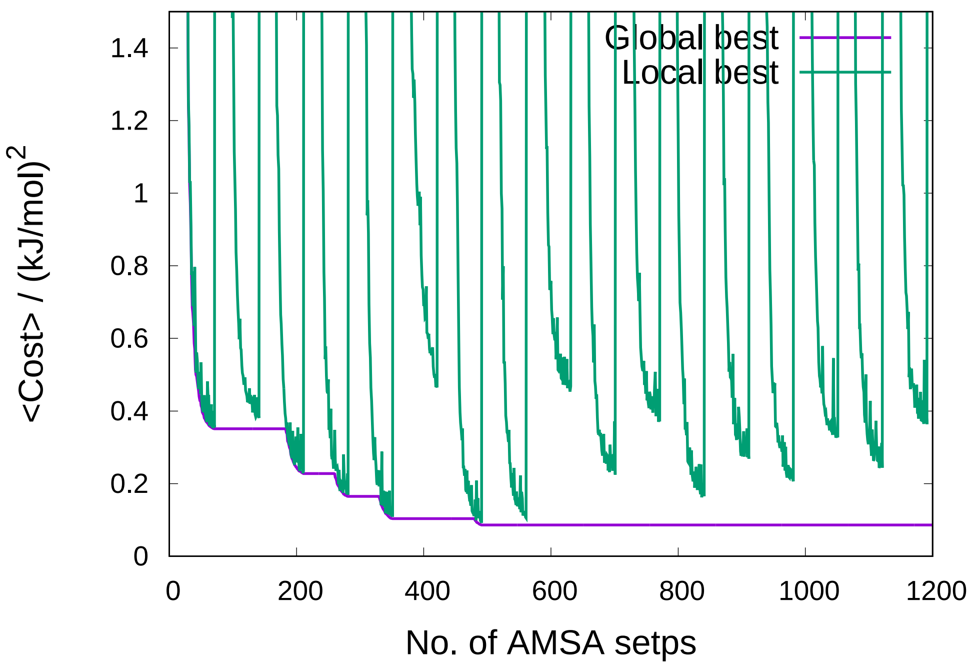


(h)Variation of energy in SA

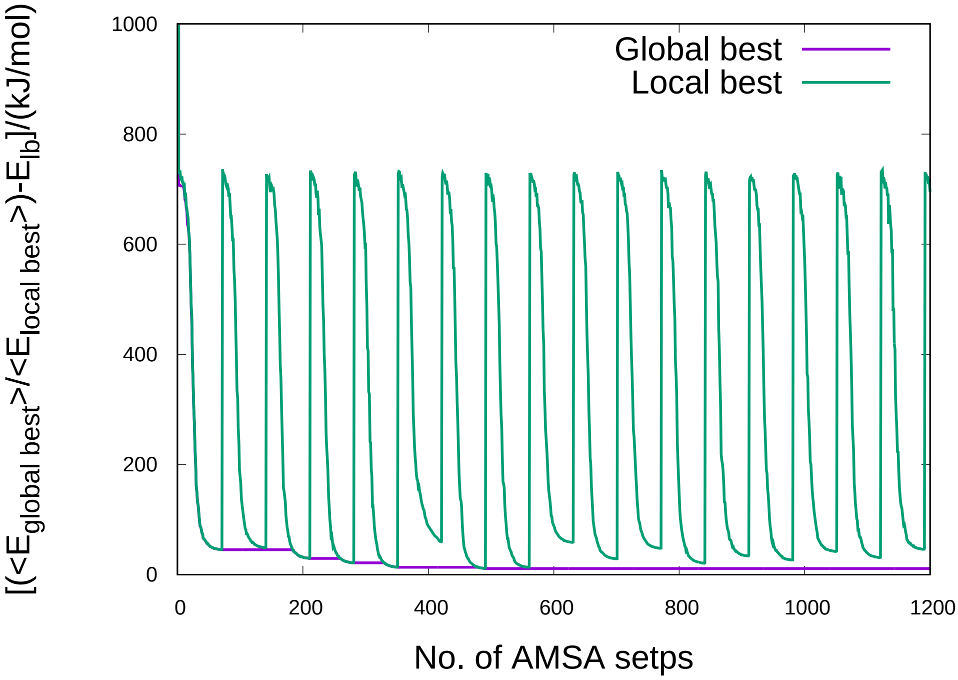
FIG. 4. Critical analysis of AMSA for $NOVER = 1000$.



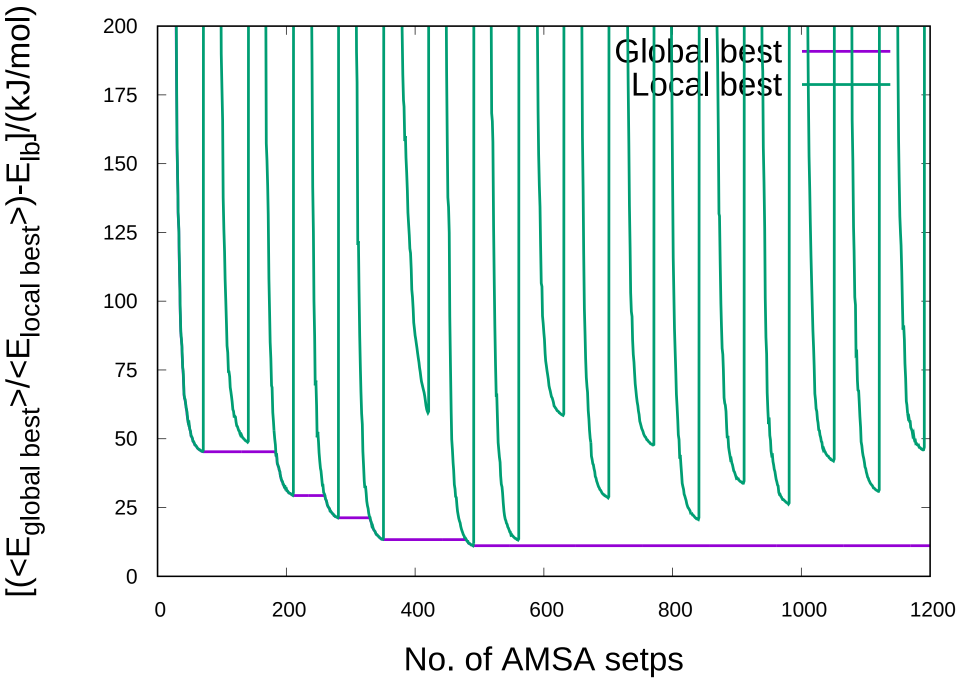
(a)Variation of Cost functional in AMSA



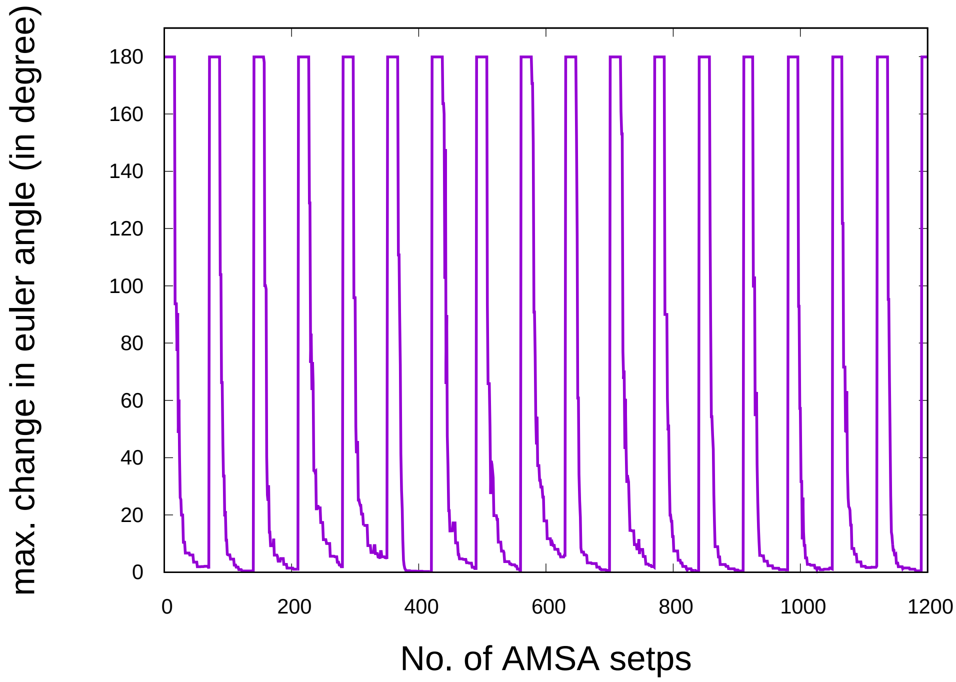
(b)Zoomed in profile of a portion of Fig. 5(a)



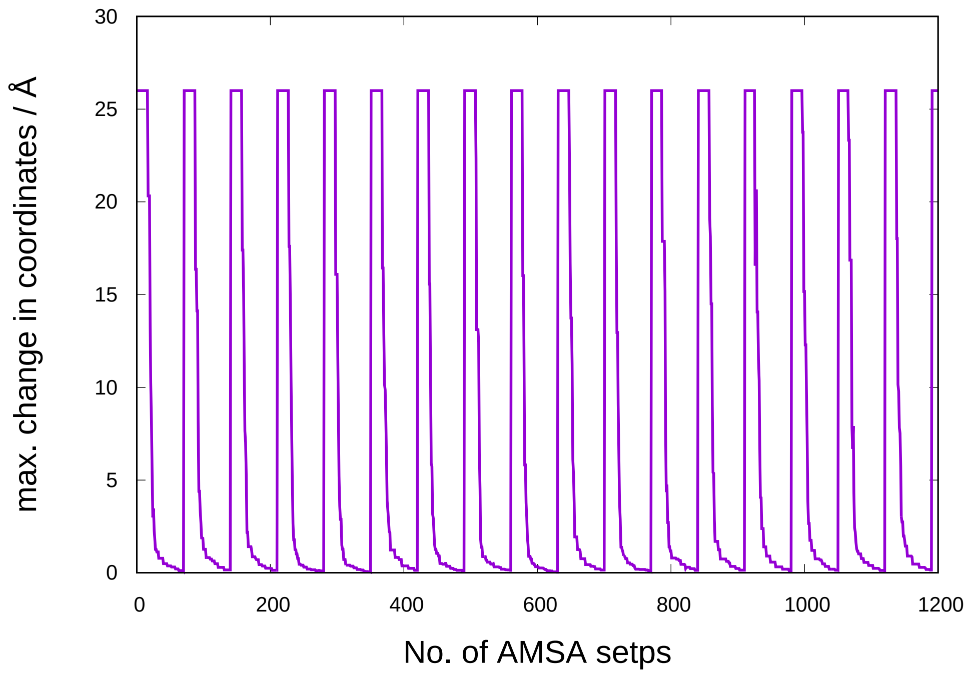
(c)Variation of energy in AMSA



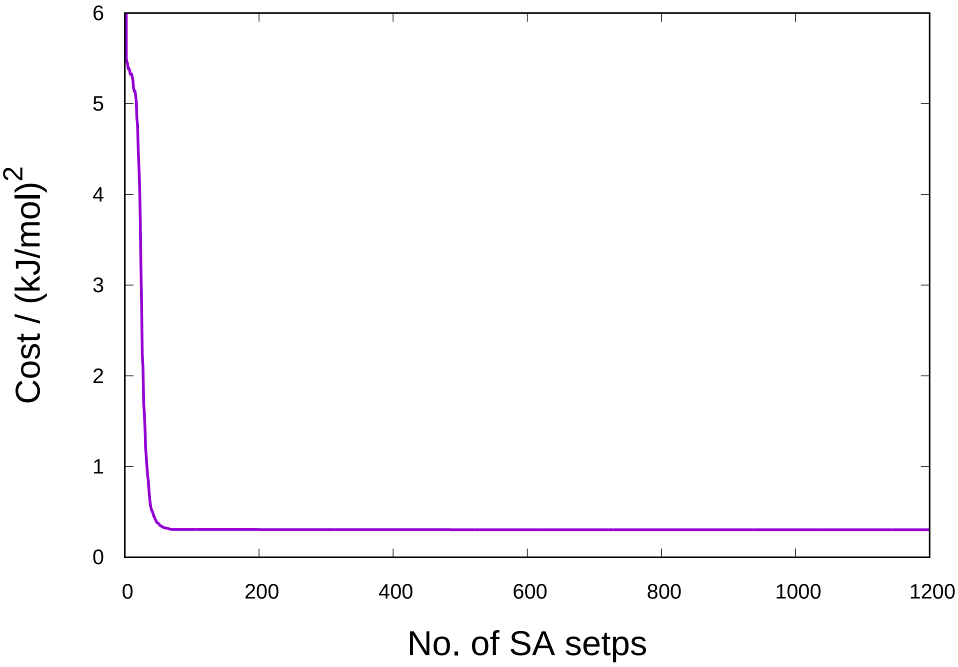
(d)Zoomed in profile of a portion of Fig. 5(c)



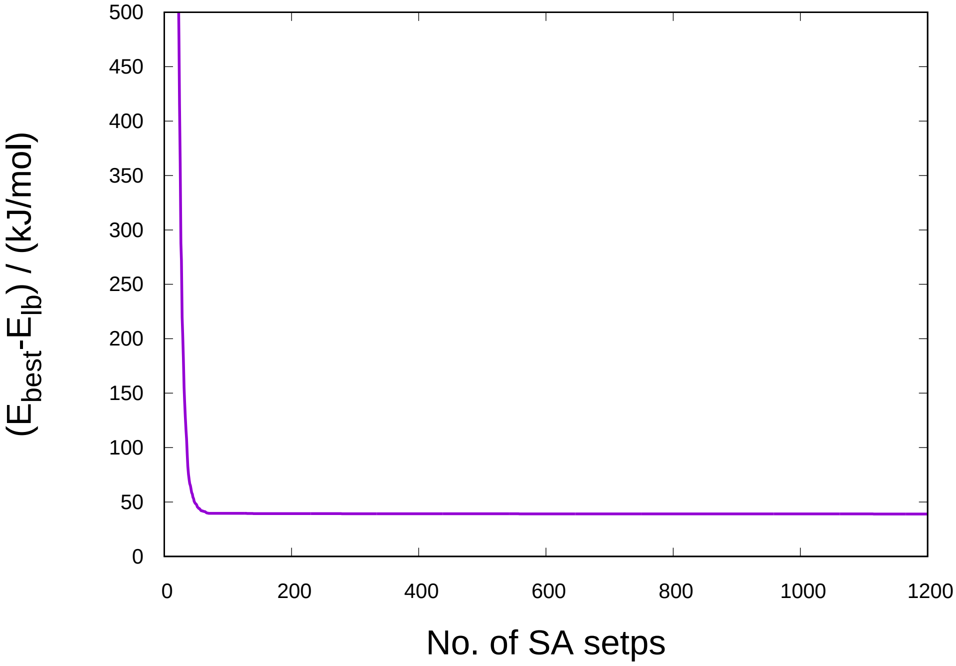
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

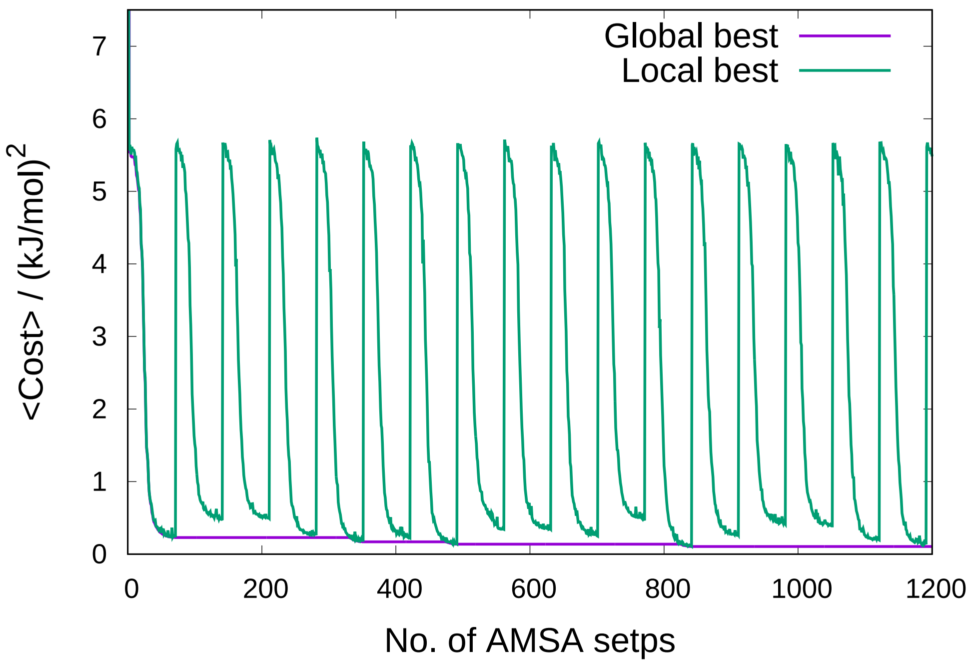


(g)Variation of Cost functional in SA

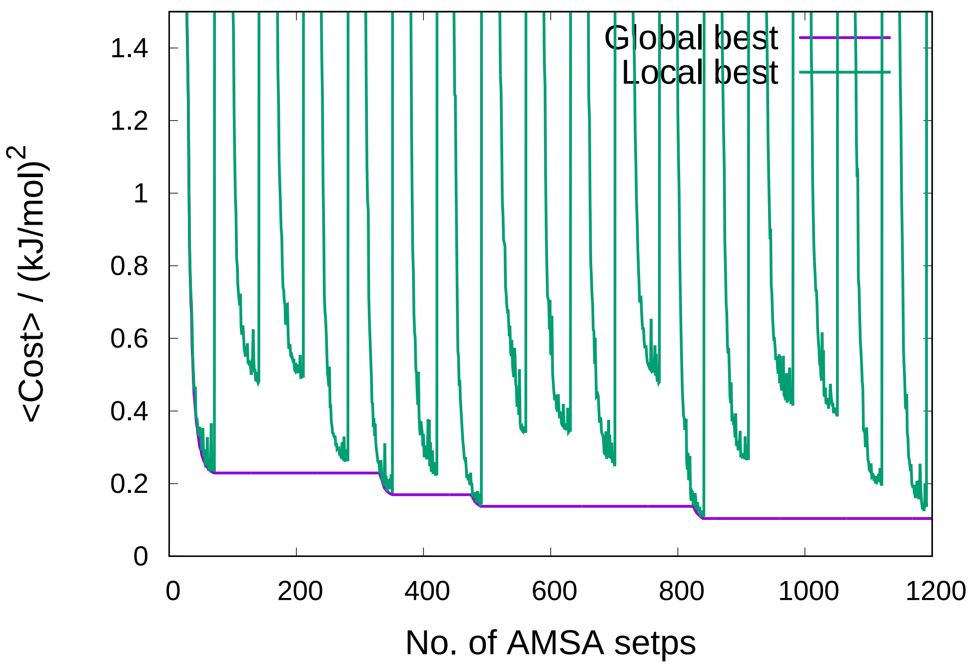


(h)Variation of energy in SA

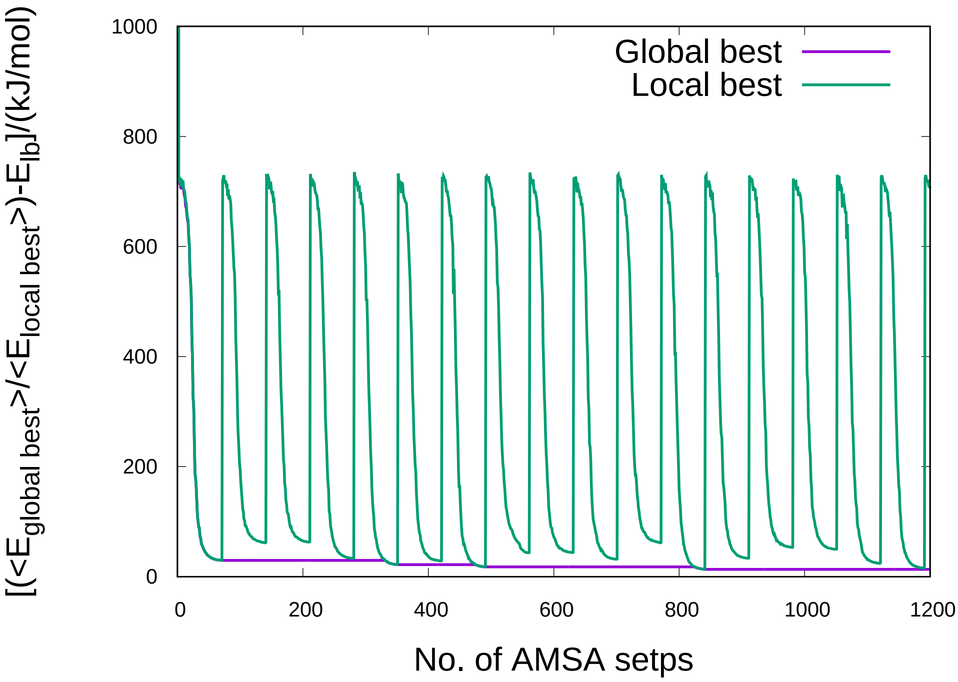
FIG. 5. Critical analysis of AMSA for $NOVER = 1500$.



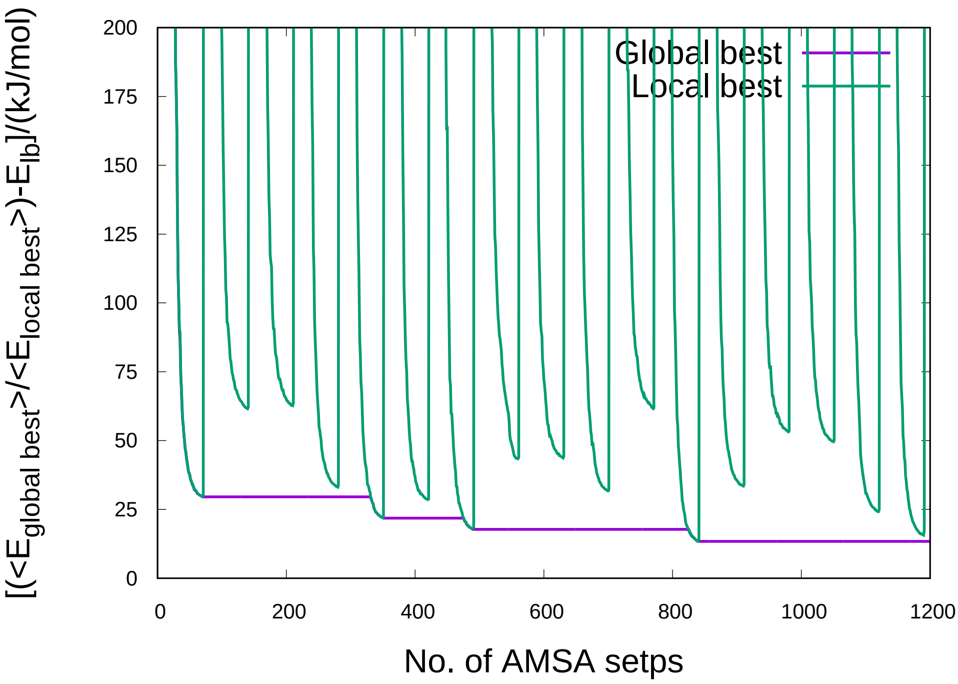
(a)Variation of Cost functional in AMSA



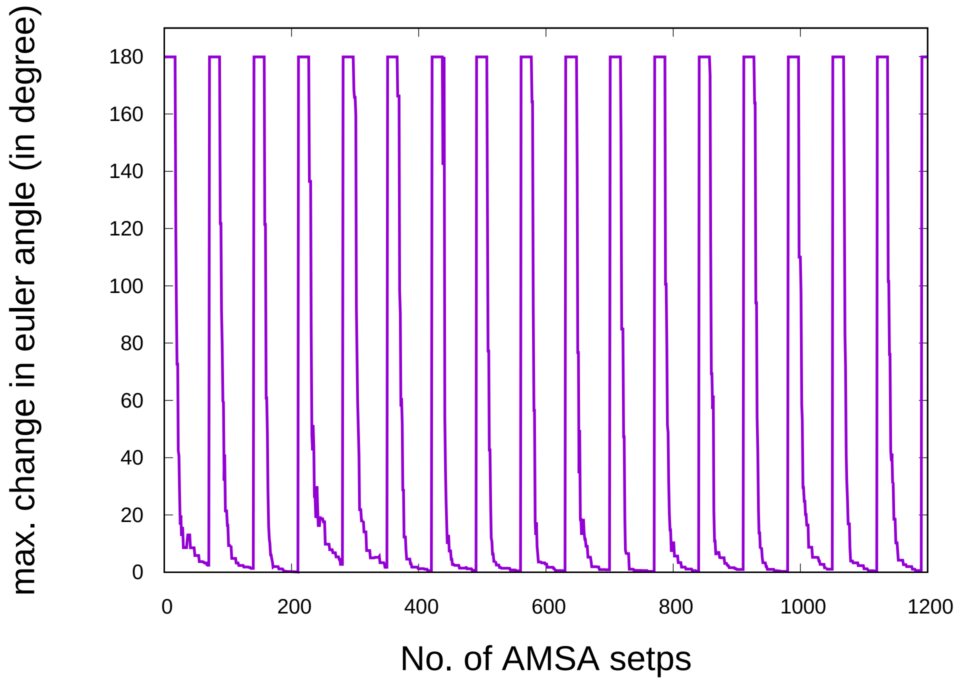
(b)Zoomed in profile of a portion of Fig. 6(a)



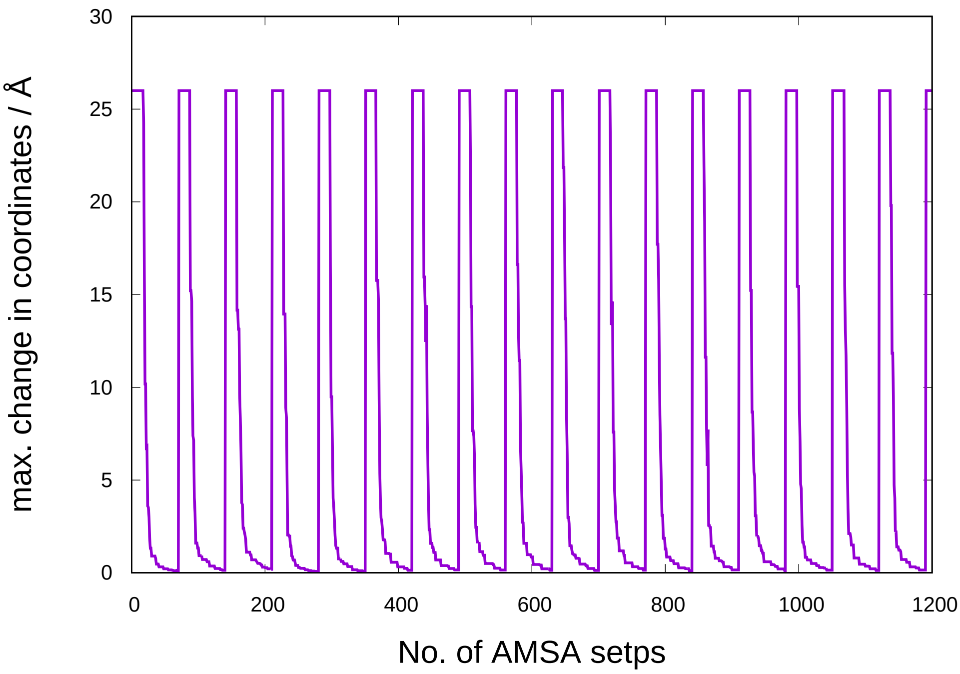
(c)Variation of energy in AMSA



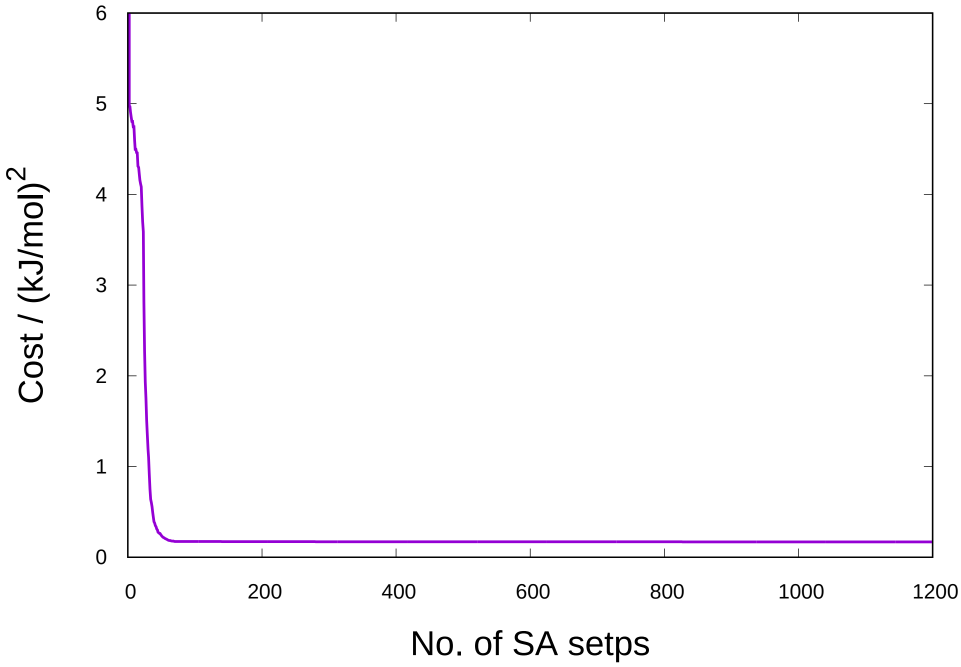
(d)Zoomed in profile of a portion of Fig. 6(c)



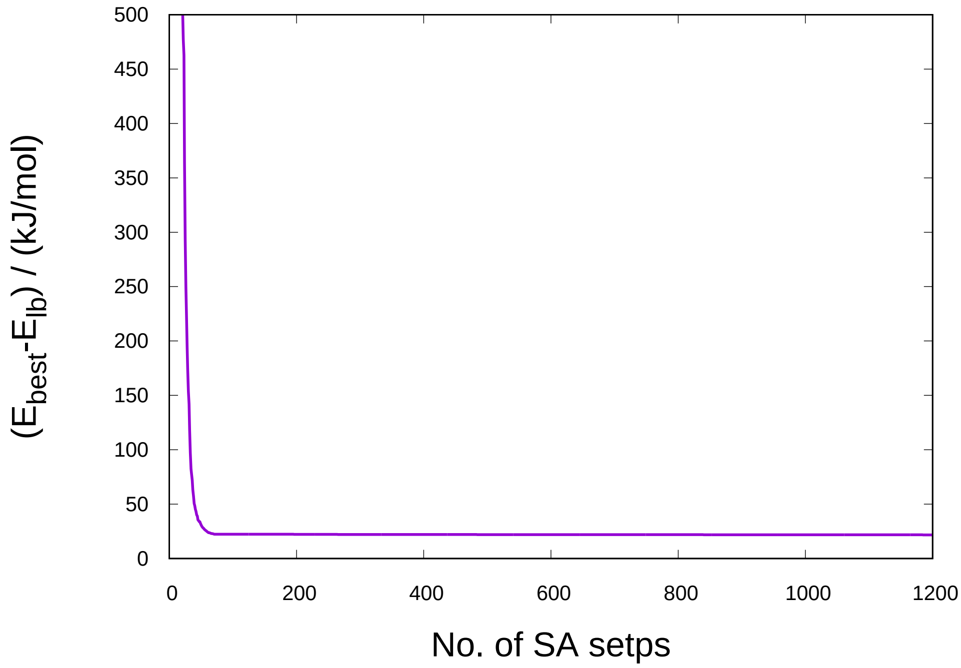
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

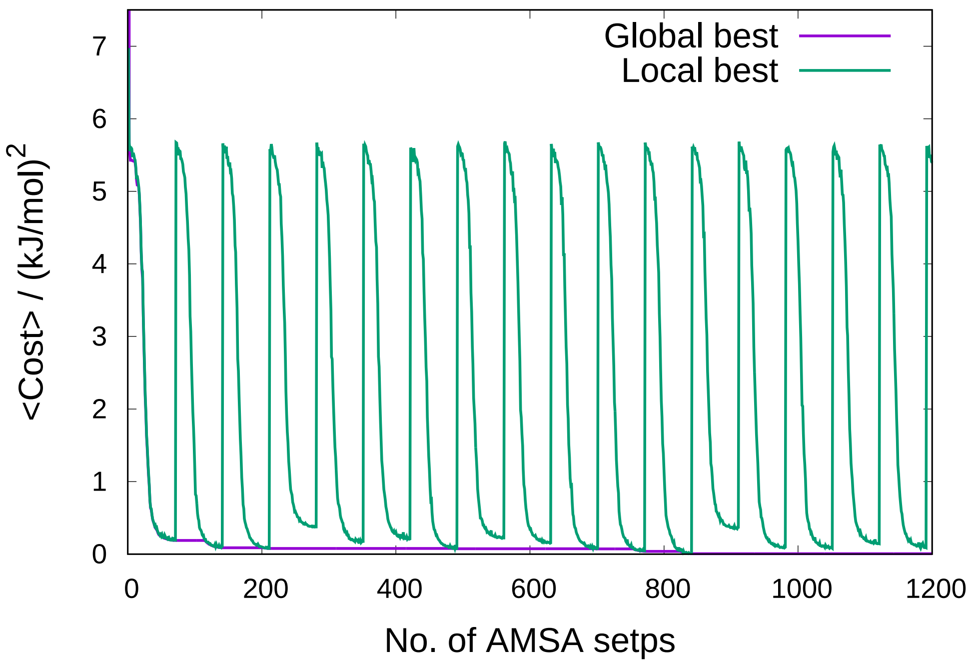


(g)Variation of Cost functional in SA

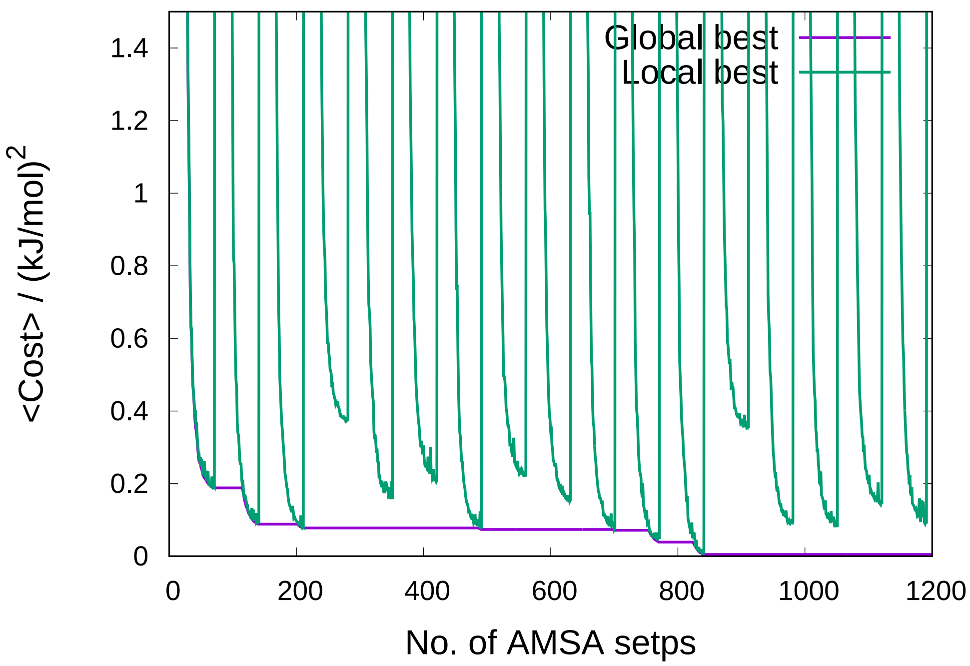


(h)Variation of energy in SA

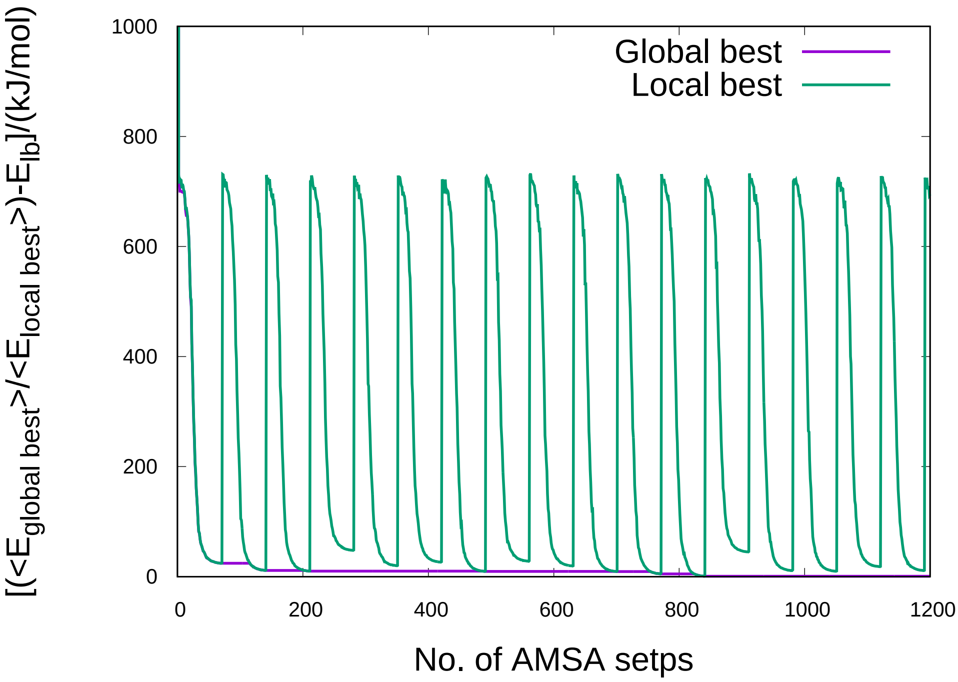
FIG. 6. Critical analysis of AMSA for $NOVER = 2000$.



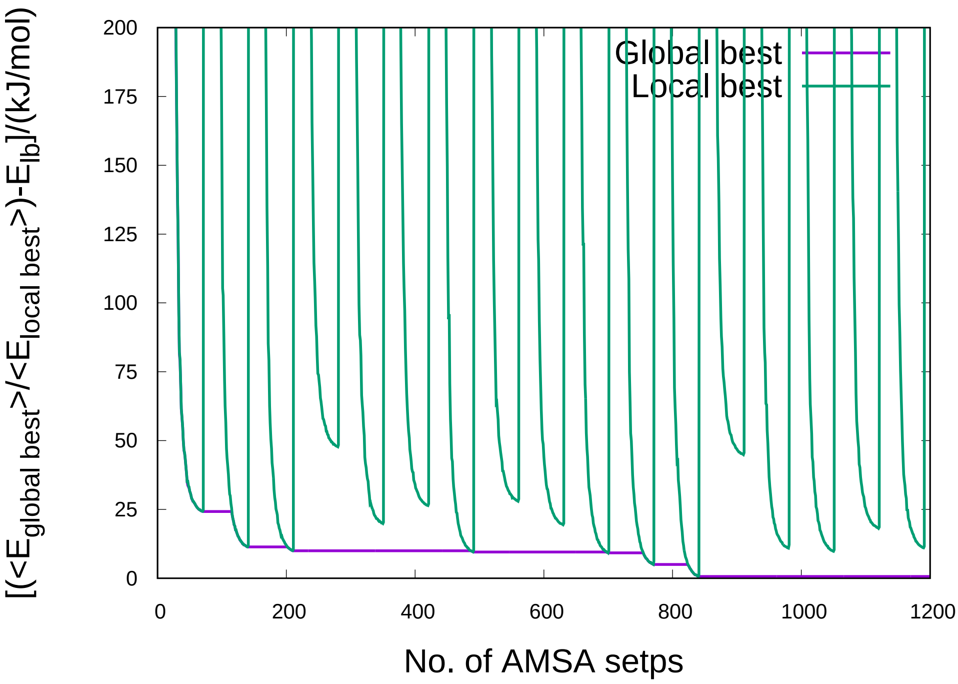
(a)Variation of Cost functional in AMSA



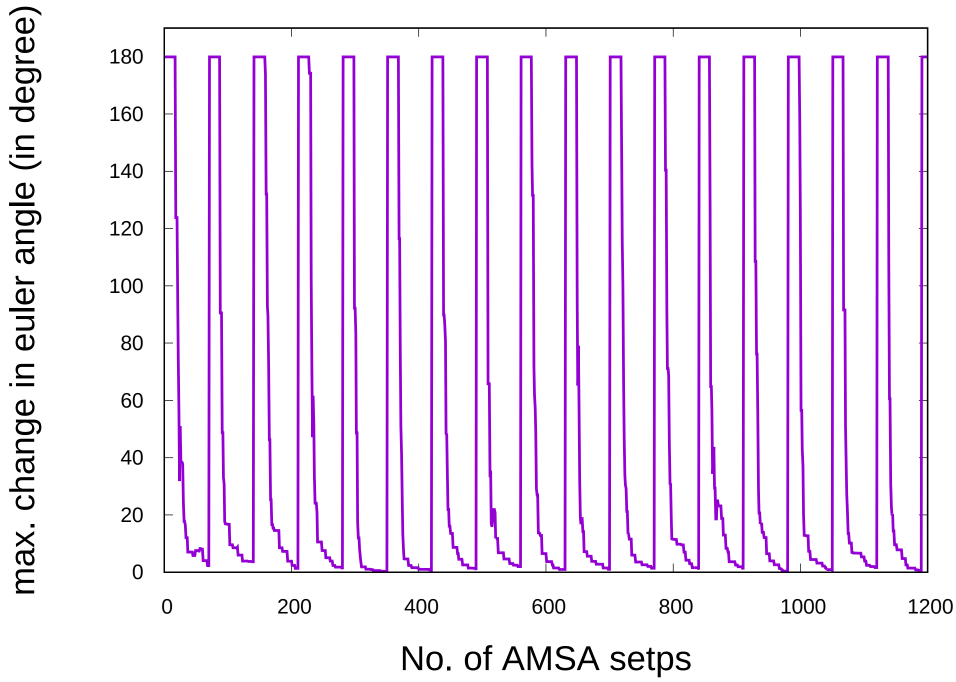
(b)Zoomed in profile of a portion of Fig. 7(a)



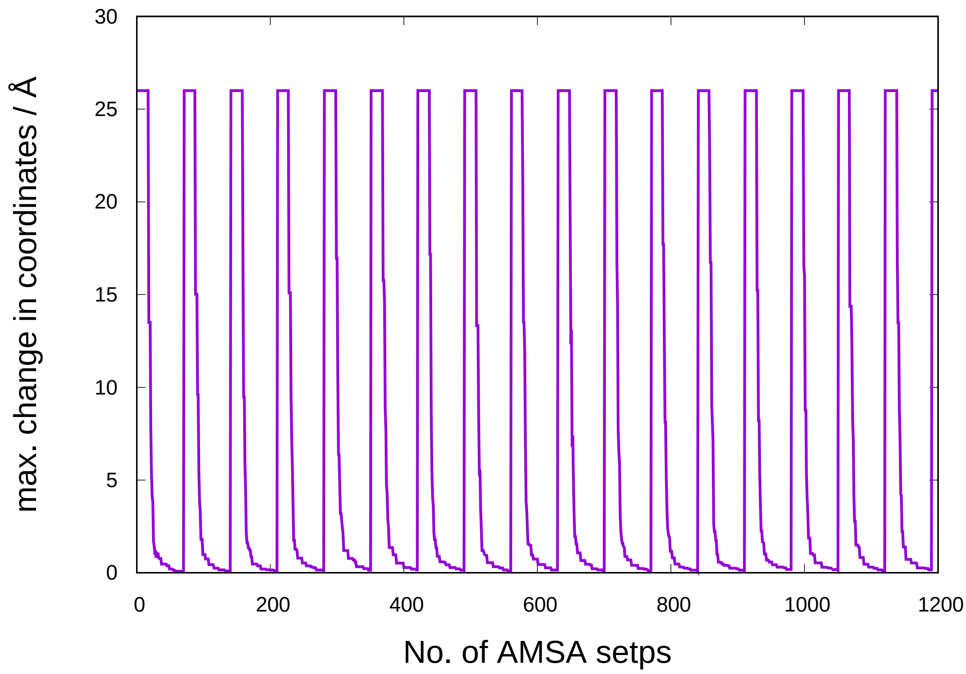
(c)Variation of energy in AMSA



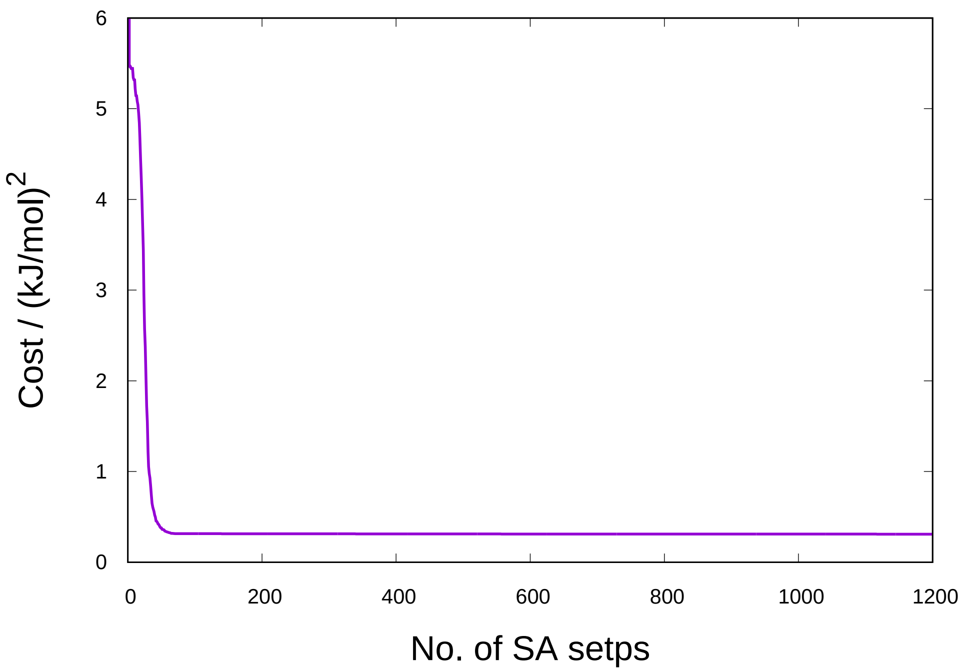
(d)Zoomed in profile of a portion of Fig. 7(c)



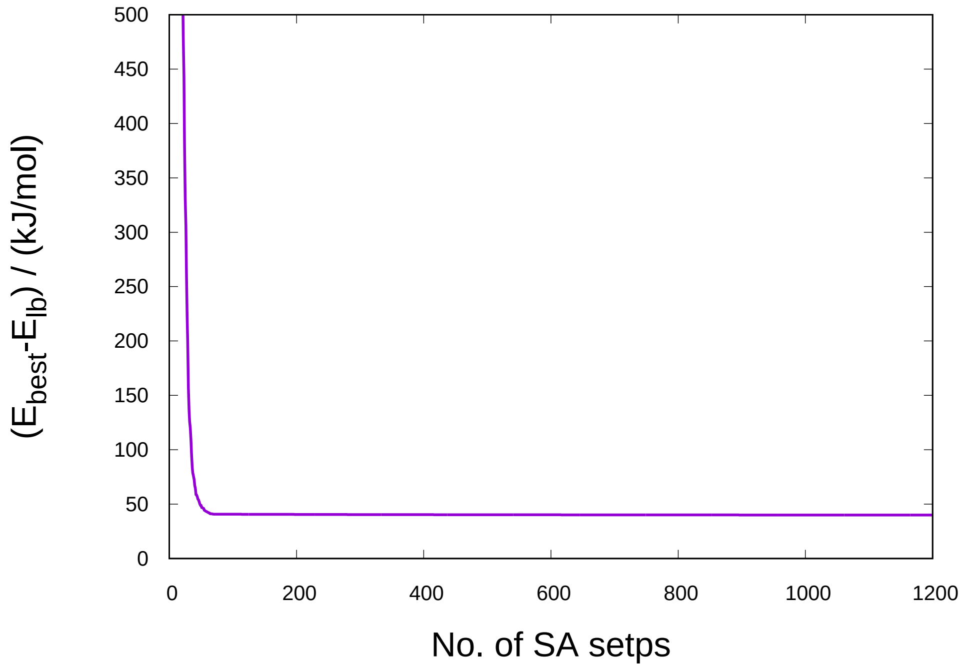
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

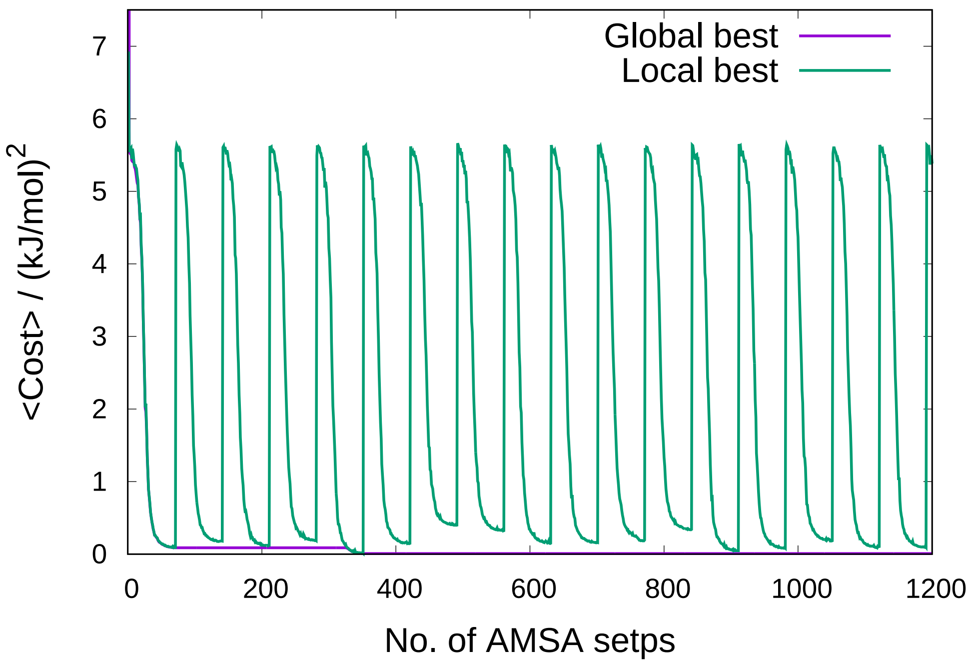


(g)Variation of Cost functional in SA

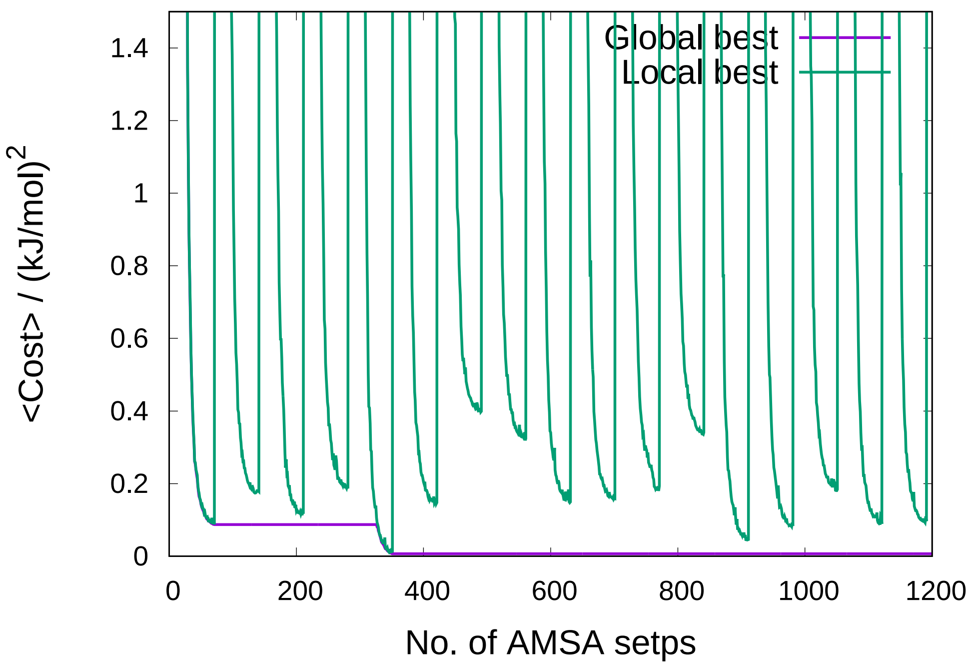


(h)Variation of energy in SA

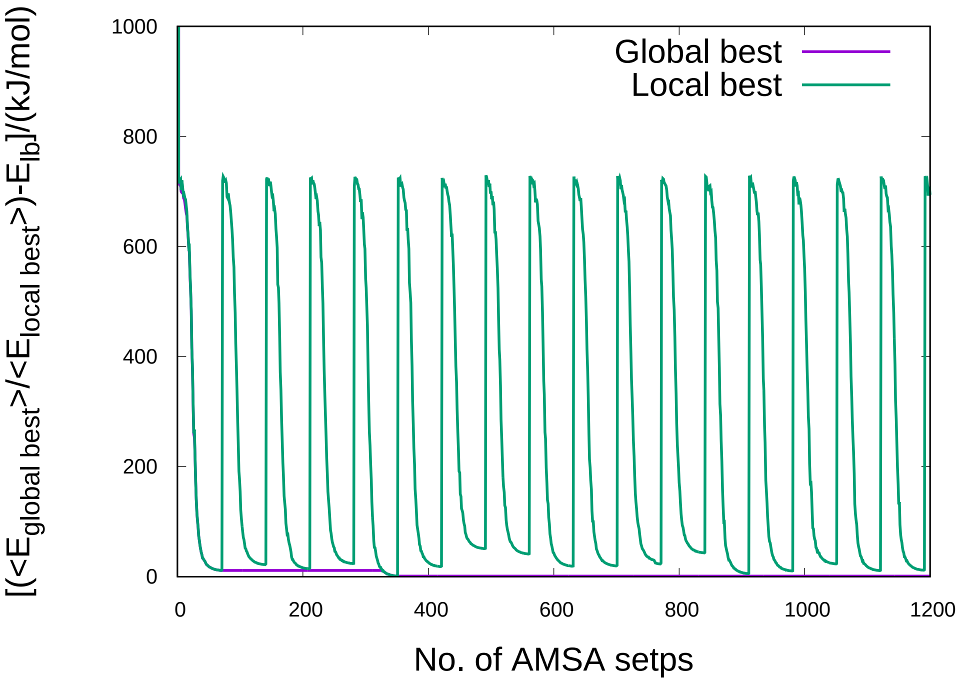
FIG. 7. Critical analysis of AMSA for $NOVER = 5000$.



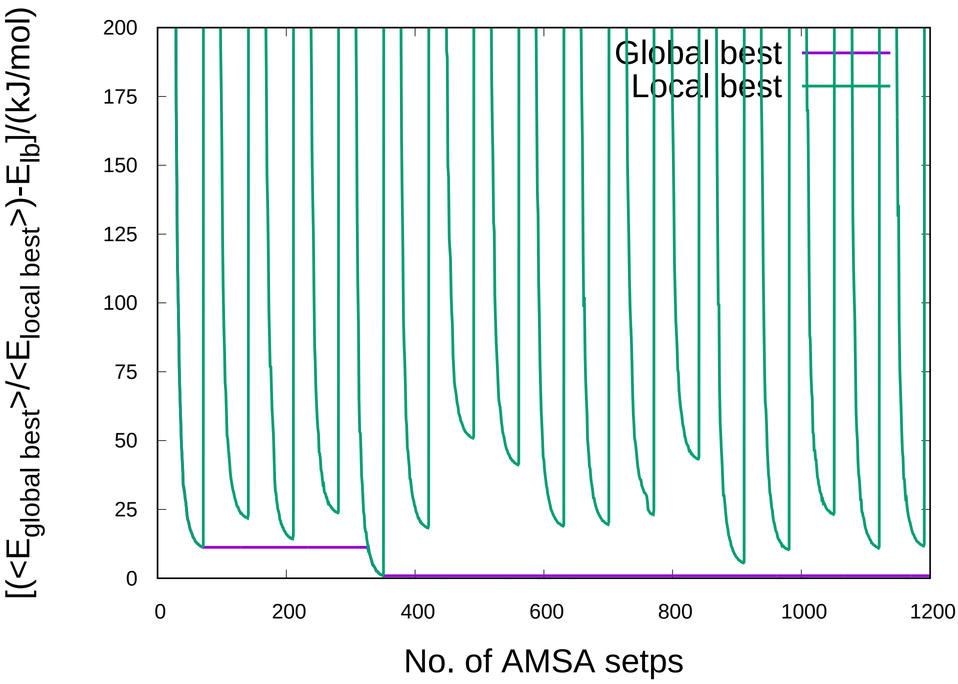
(a)Variation of Cost functional in AMSA



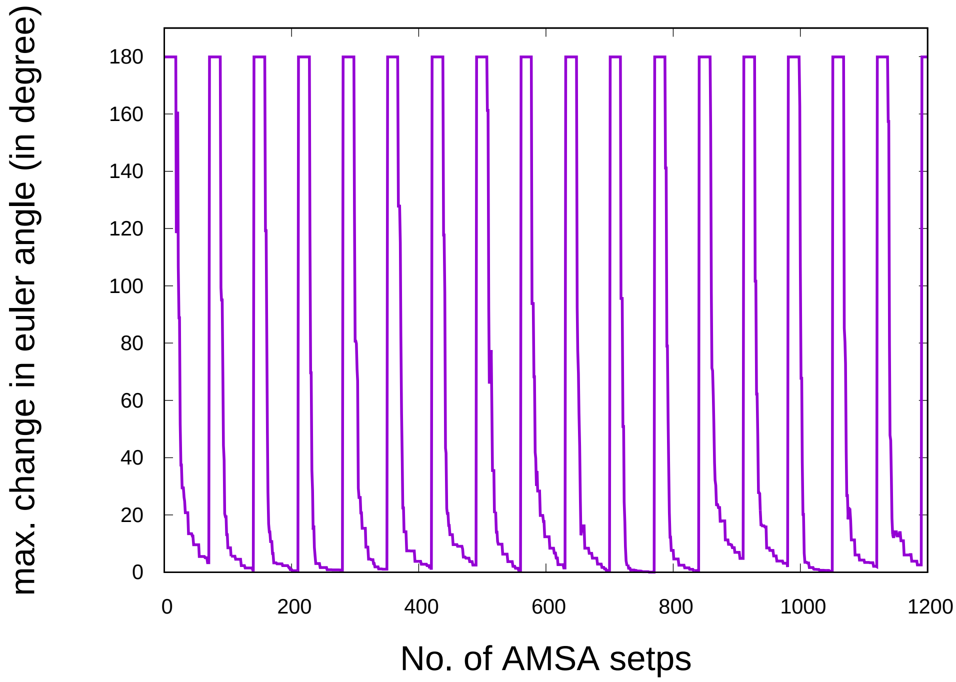
(b)Zoomed in profile of a portion of Fig. 8(a)



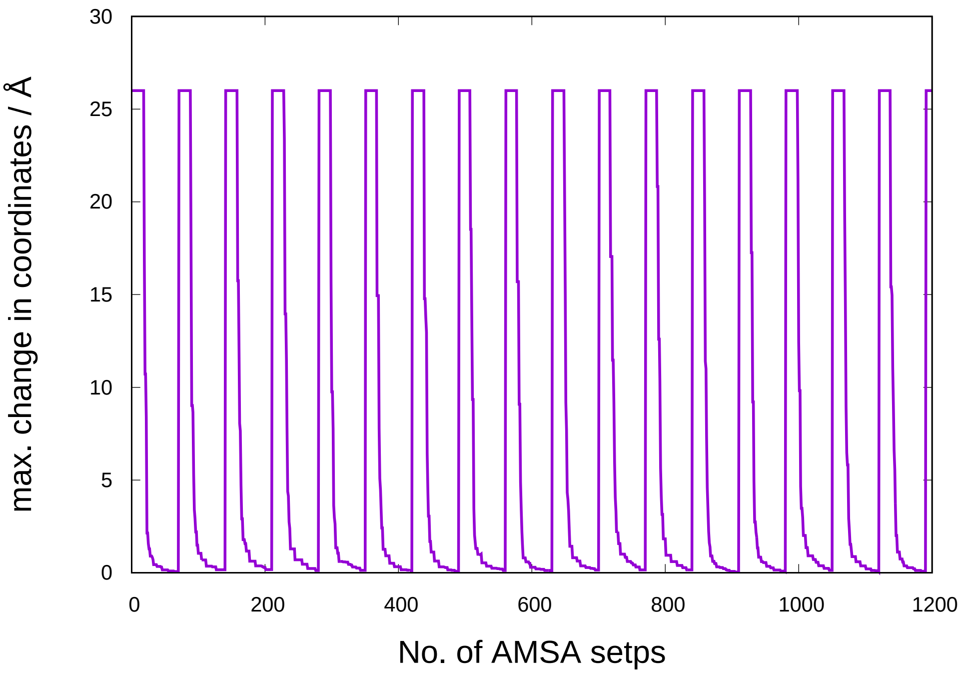
(c)Variation of energy in AMSA



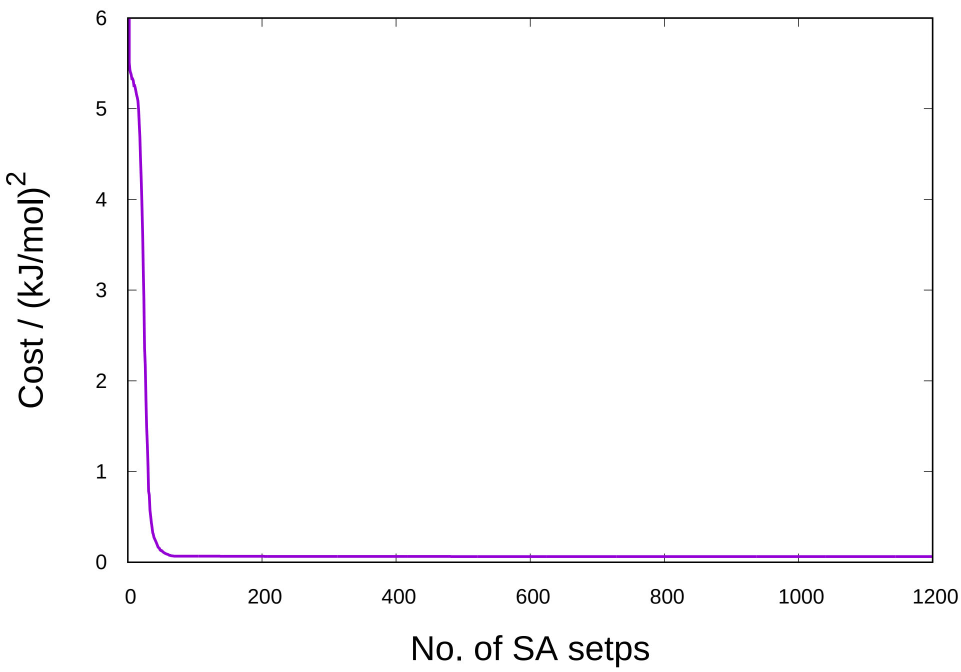
(d)Zoomed in profile of a portion of Fig. 8(c)



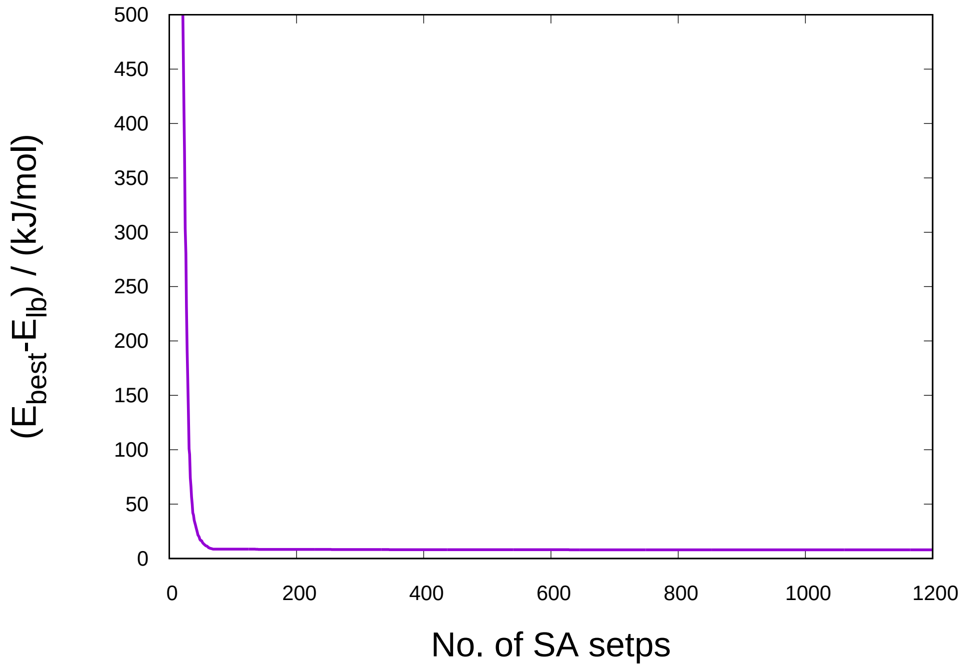
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

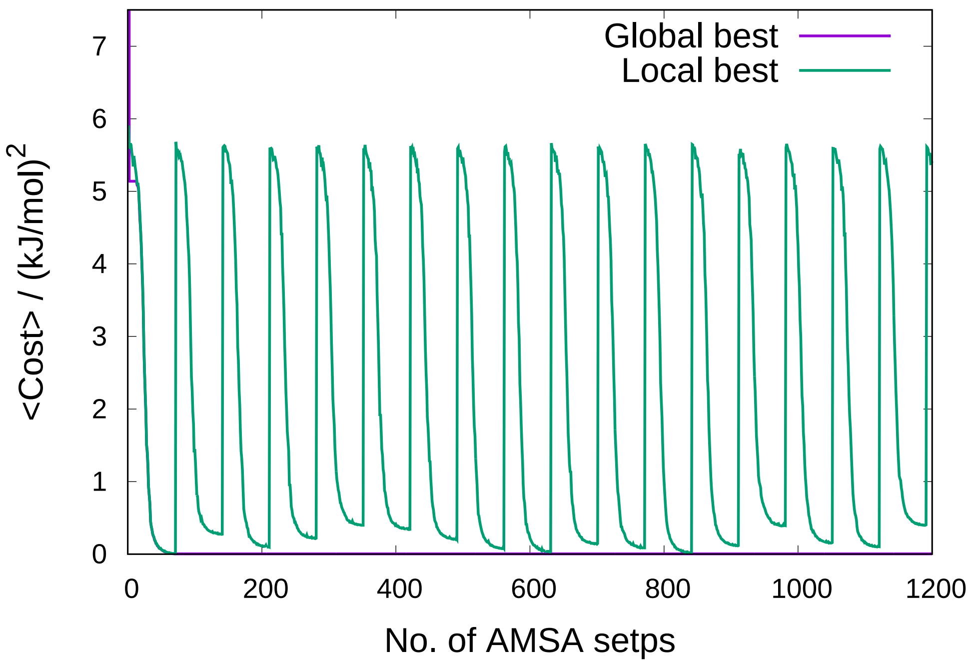


(g)Variation of Cost functional in SA

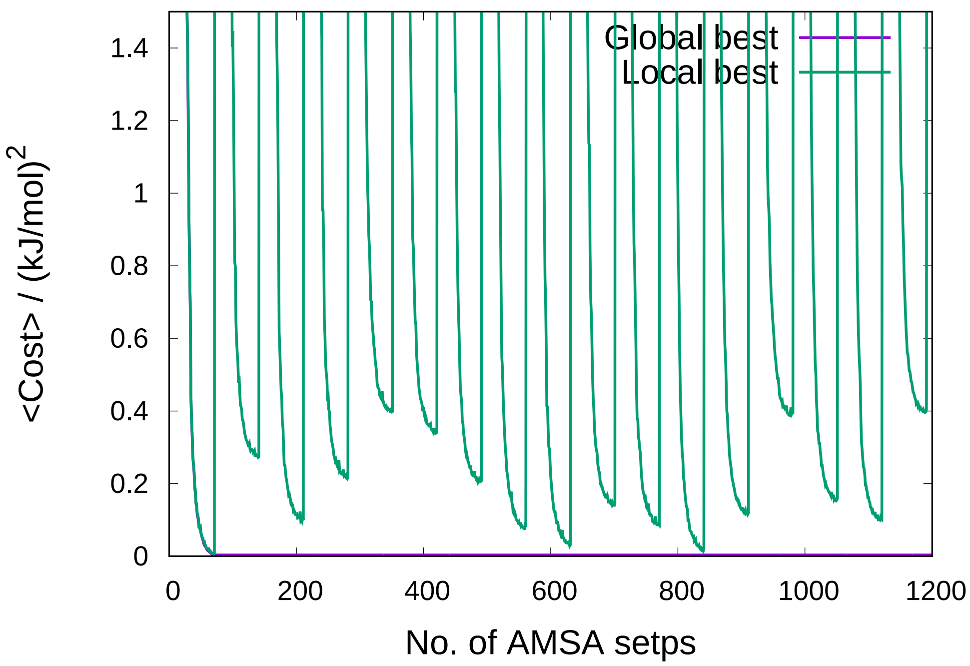


(h)Variation of energy in SA

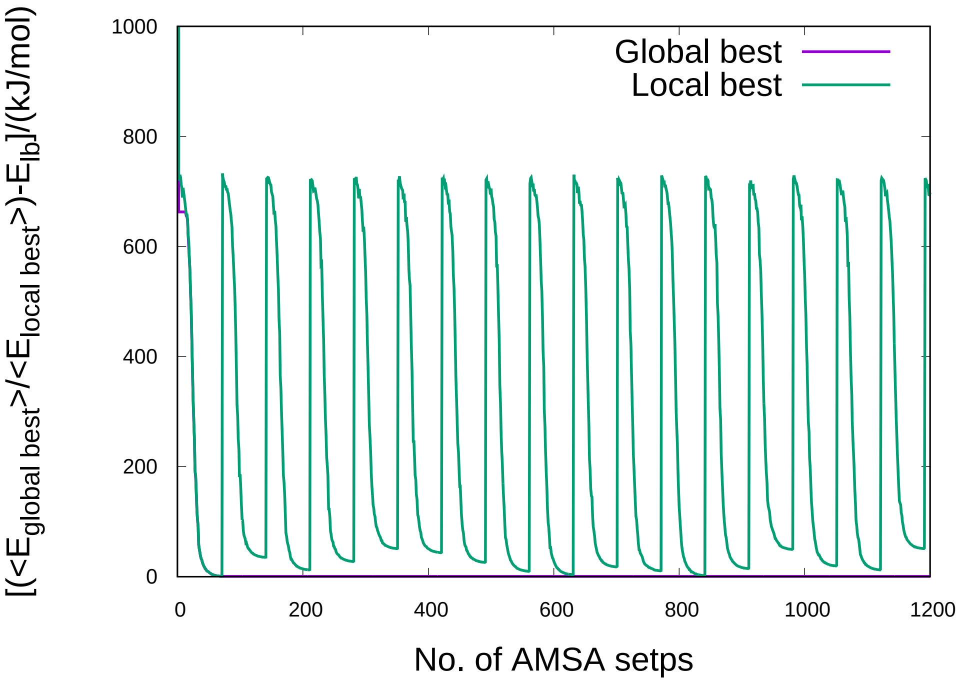
FIG. 8. Critical analysis of AMSA for $NOVER = 7000$.



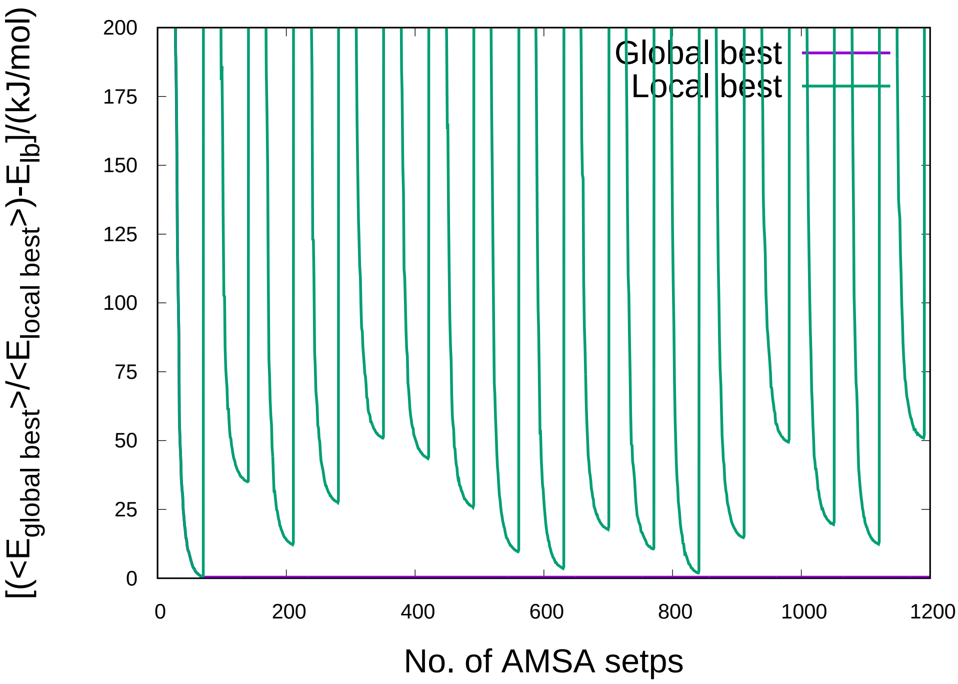
(a)Variation of Cost functional in AMSA



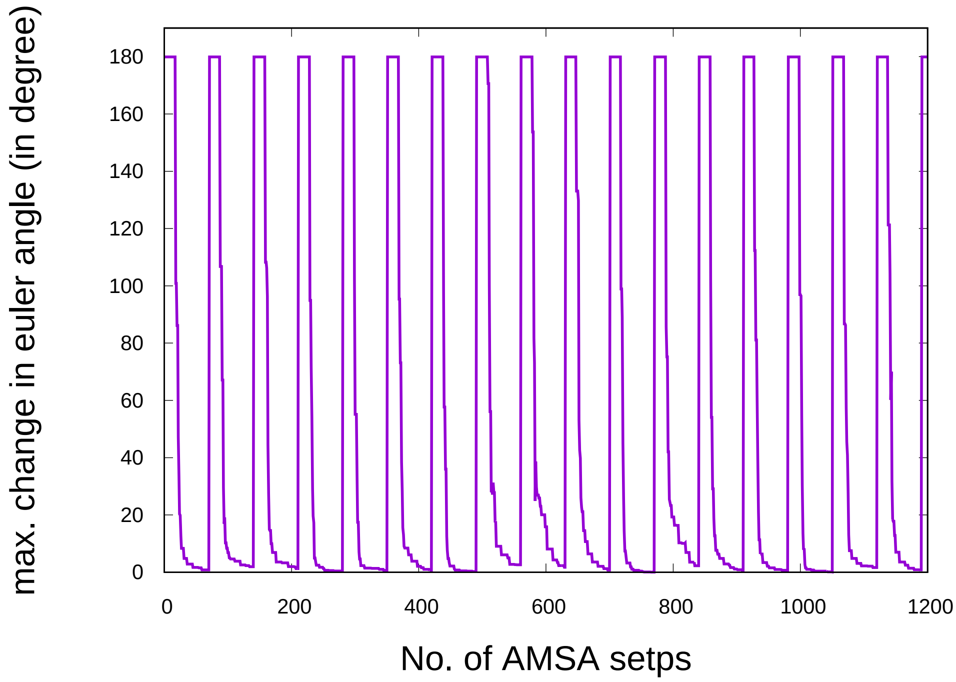
(b)Zoomed in profile of a portion of Fig. 9(a)



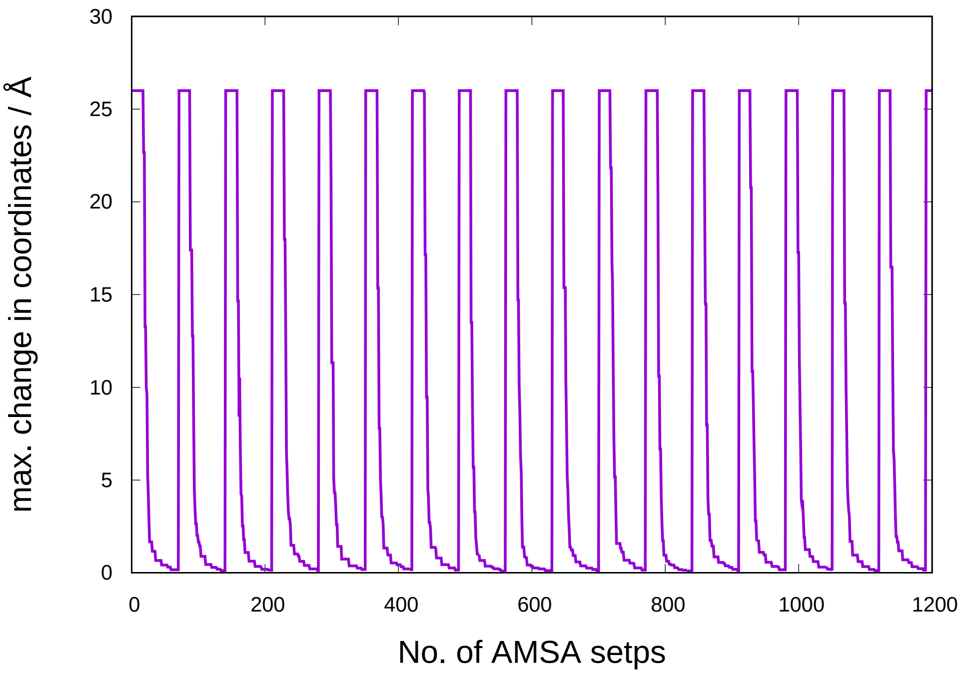
(c)Variation of energy in AMSA



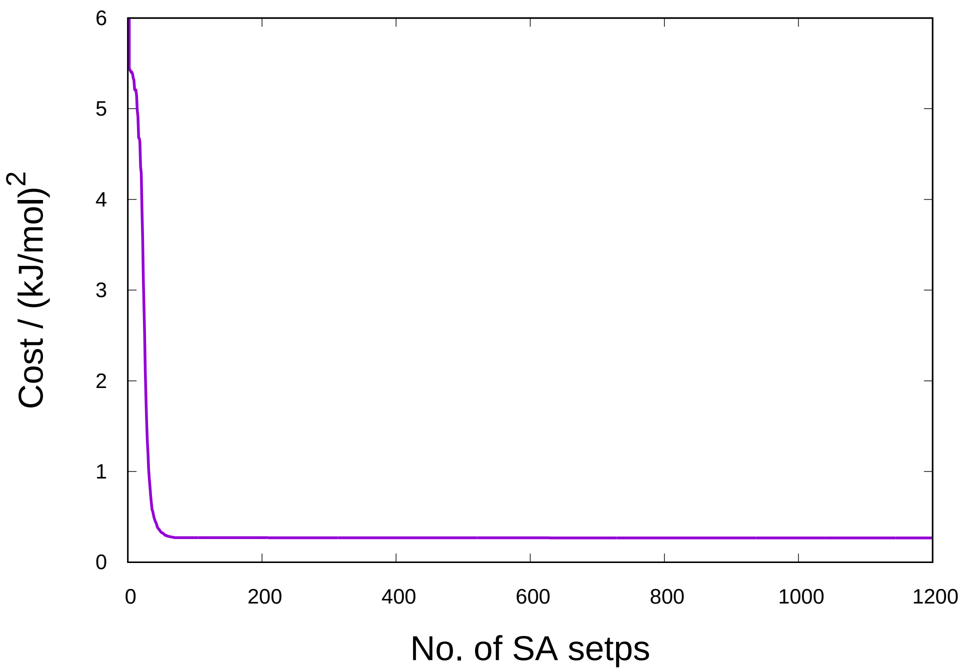
(d)Zoomed in profile of a portion of Fig. 9(c)



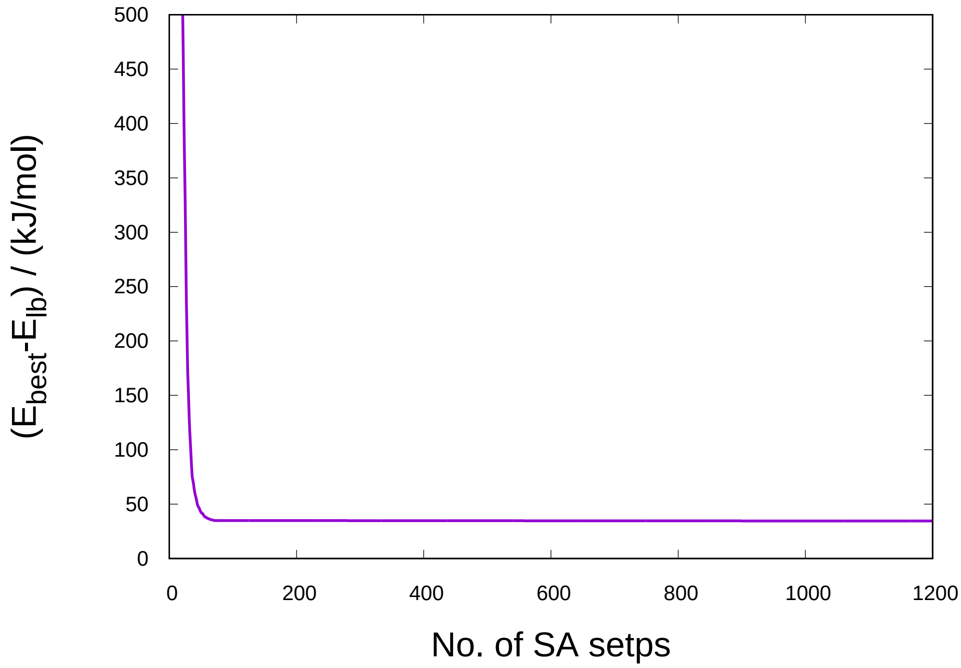
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

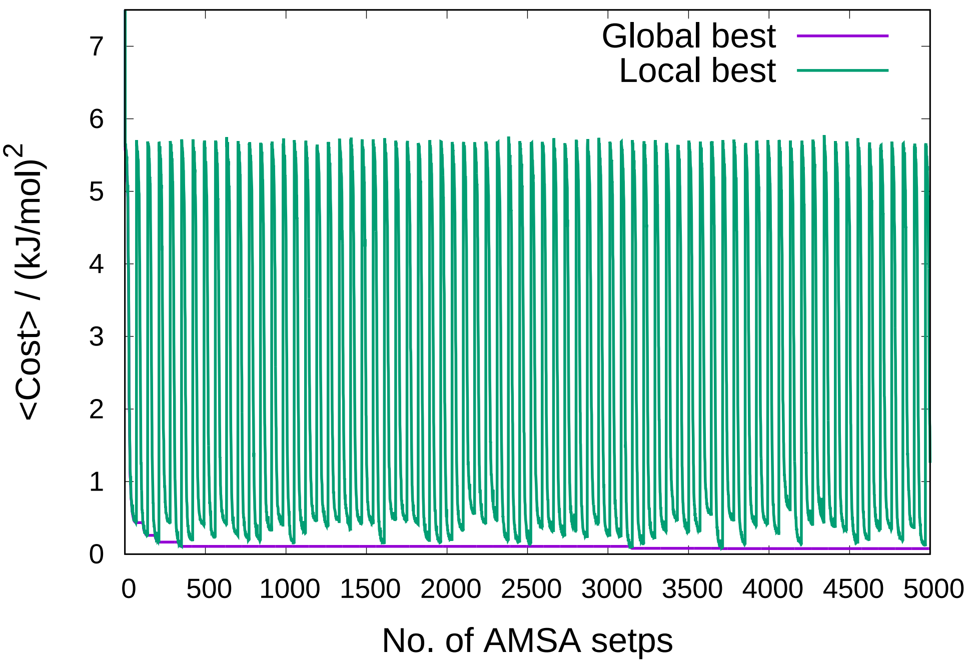


(g)Variation of Cost functional in SA

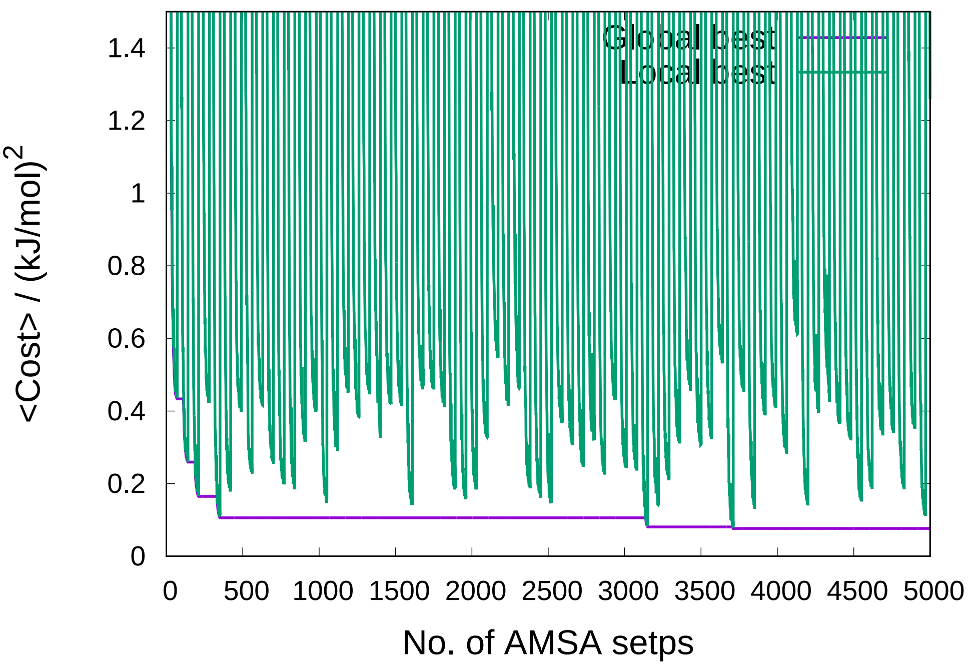


(h)Variation of energy in SA

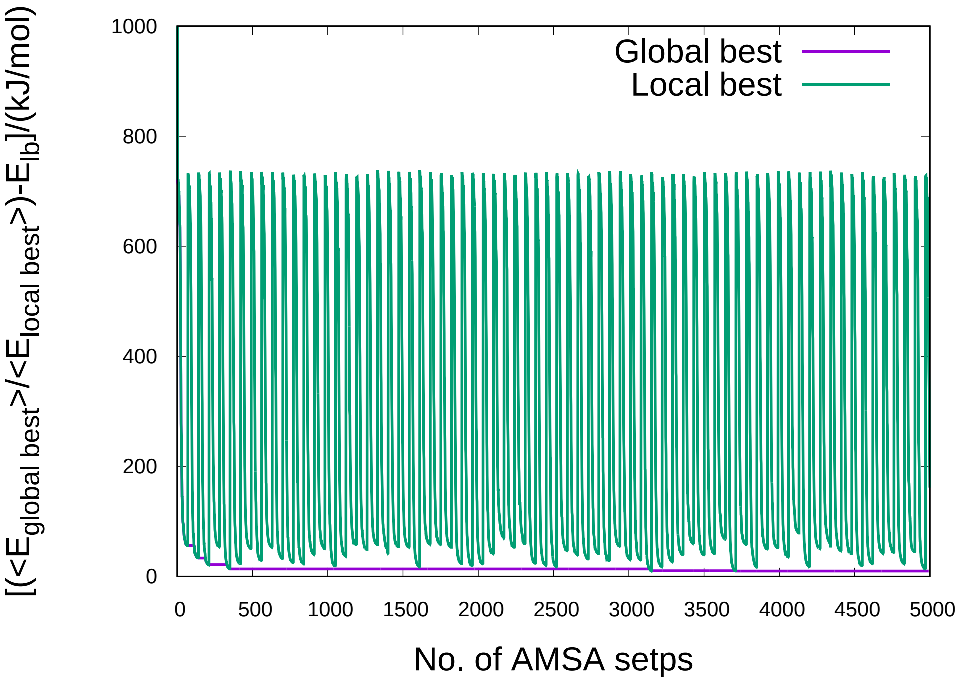
FIG. 9. Critical analysis of AMSA for $NOVER = 10000$.



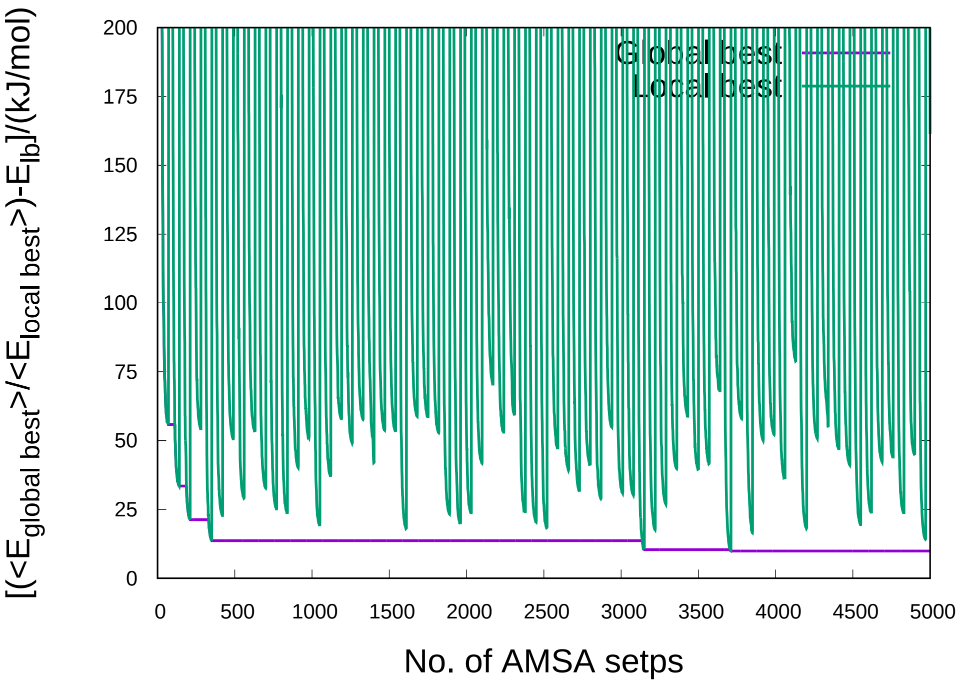
(a)Variation of Cost functional in AMSA



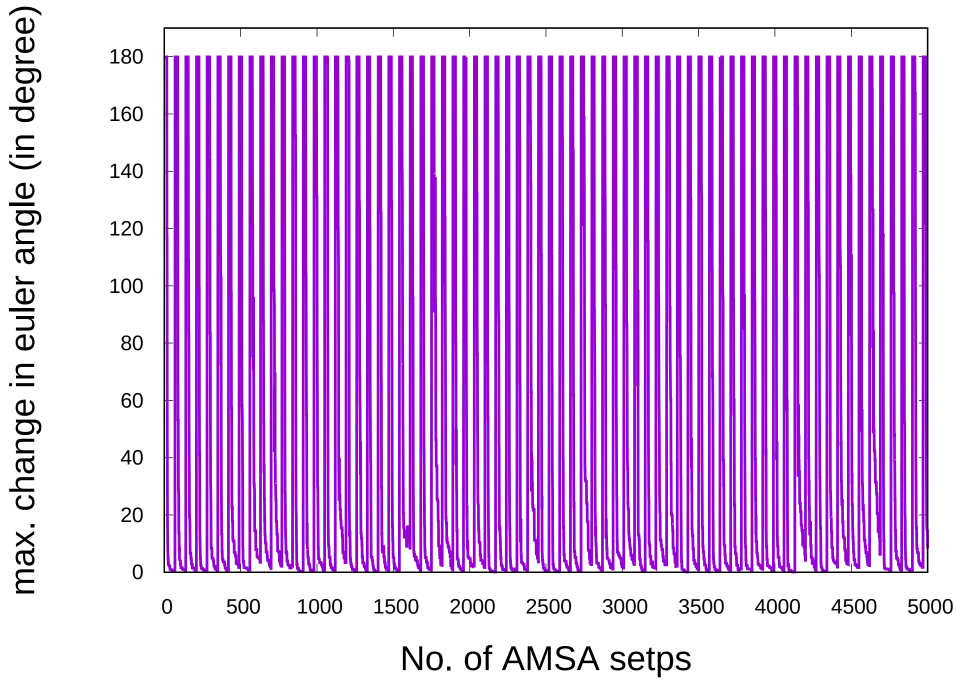
(b)Zoomed in profile of Fig. 10(a)



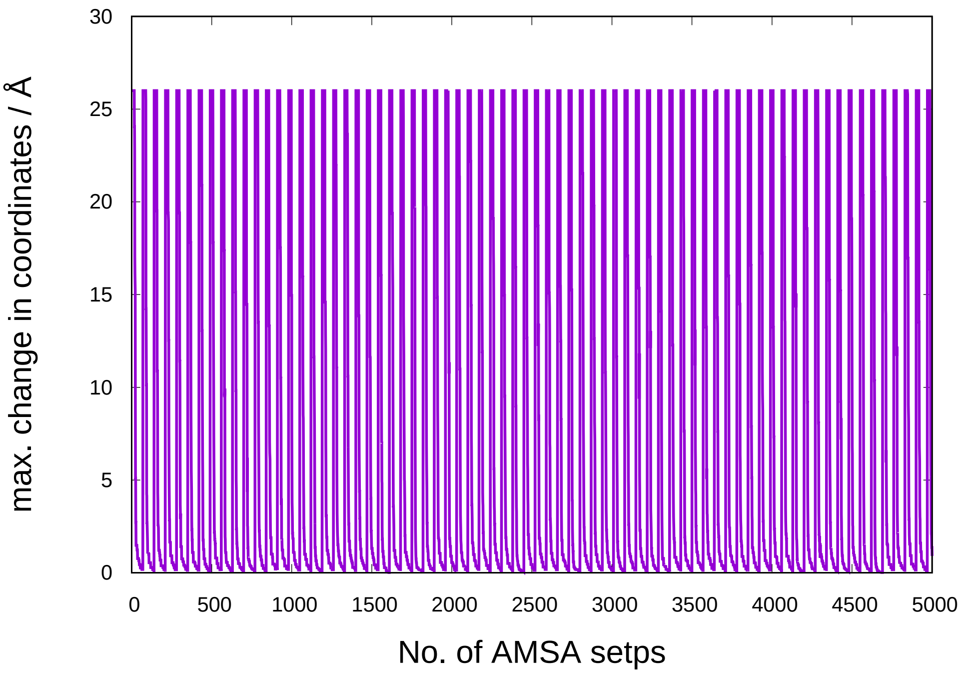
(c)Variation of energy in AMSA



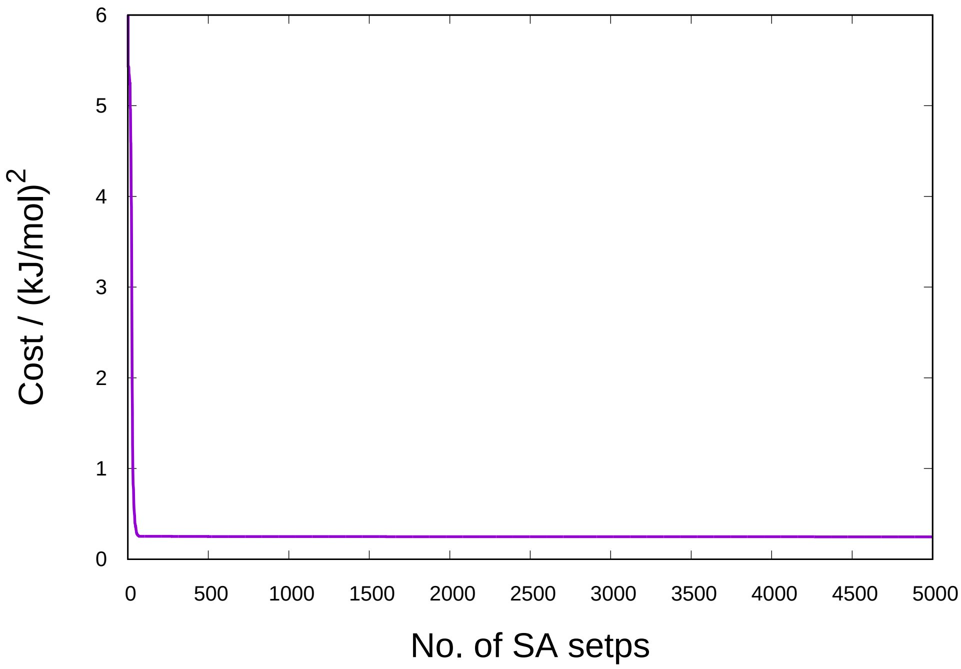
(d)Zoomed in profile of a portion of Fig. 10(c)



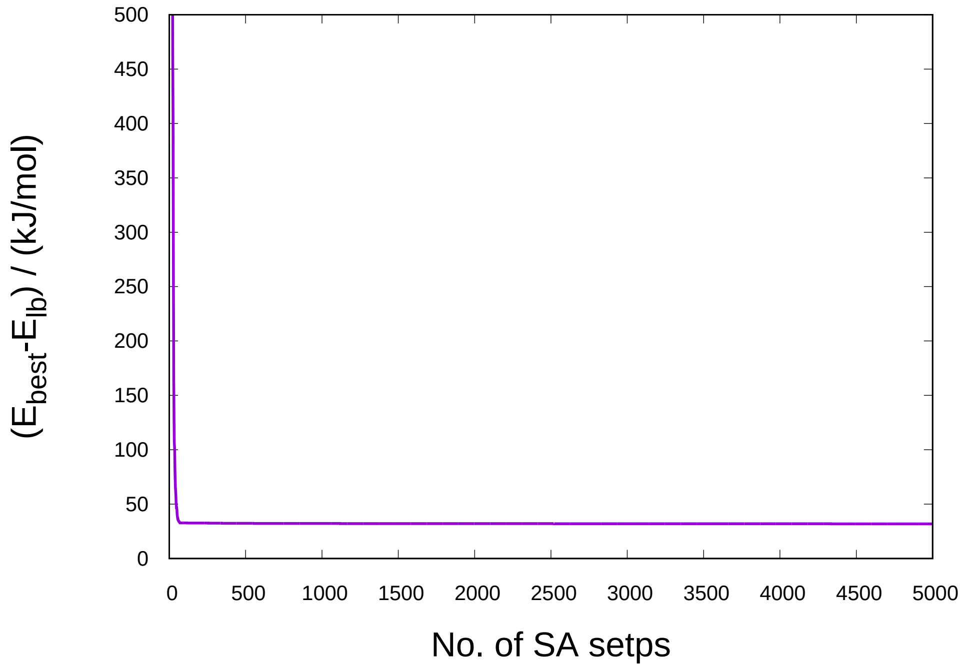
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

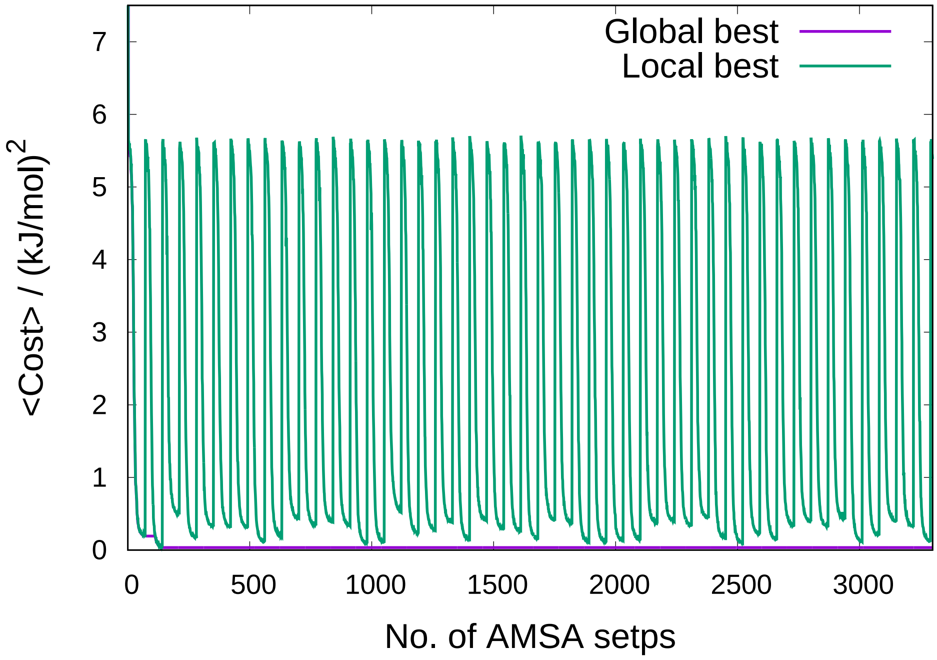


(g)Variation of Cost functional in SA

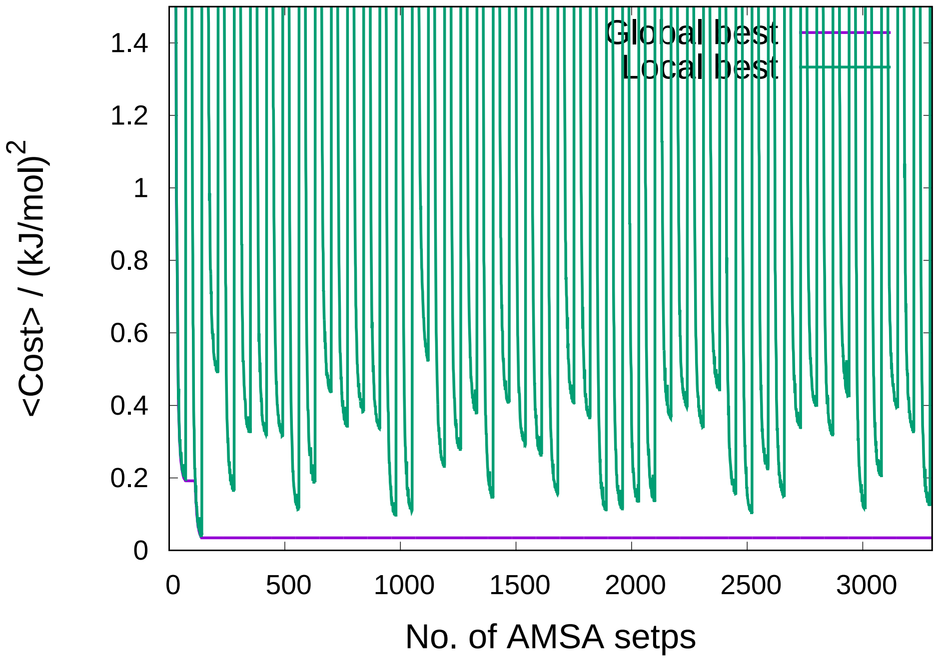


(h)Variation of energy in SA

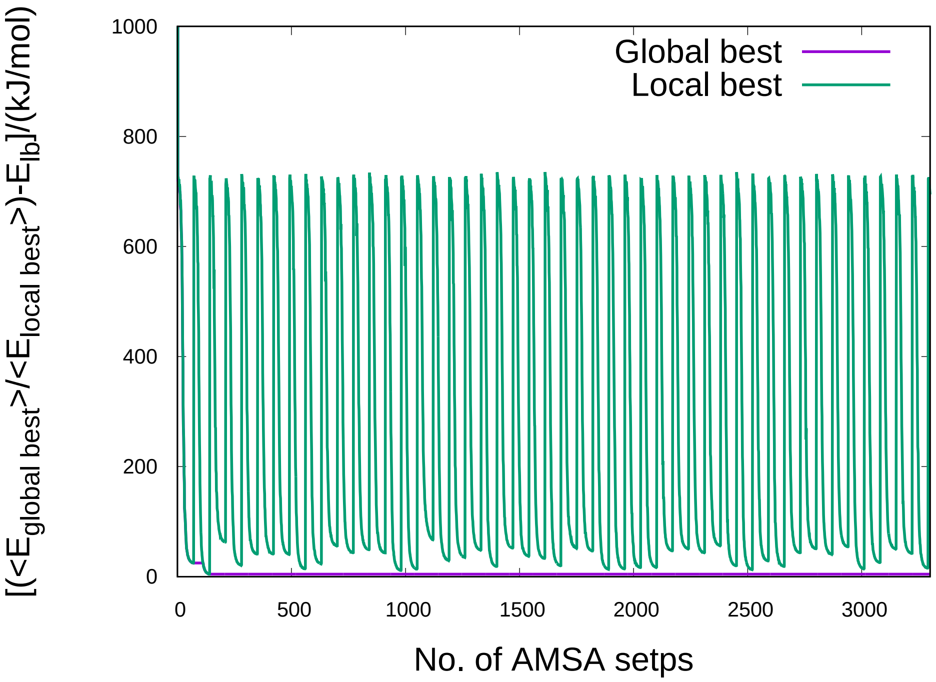
FIG. 10. Critical analysis of AMSA for $NOVER = 2000$.



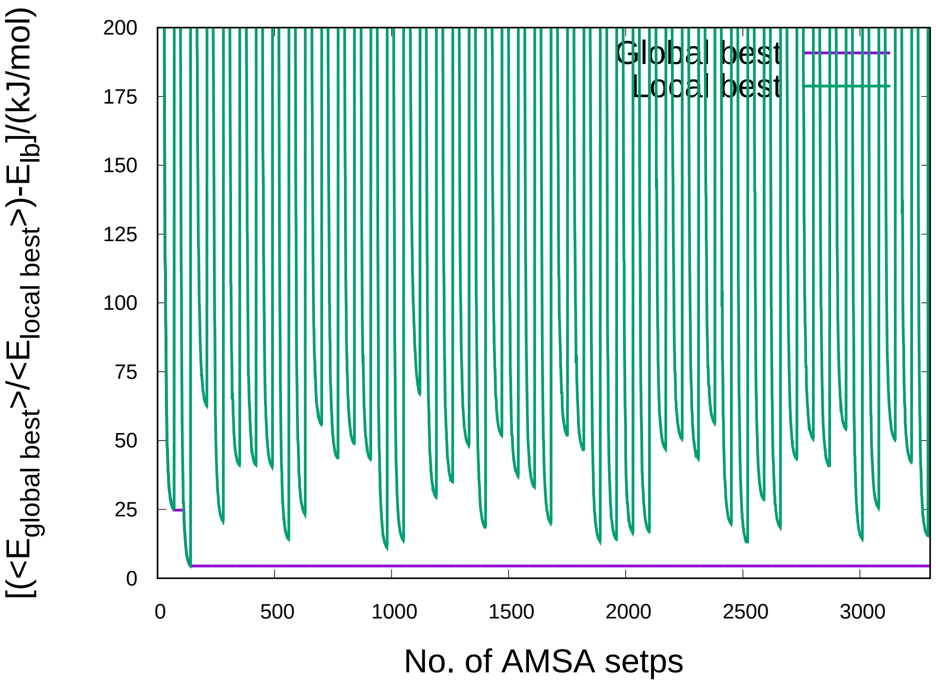
(a)Variation of Cost functional in AMSA



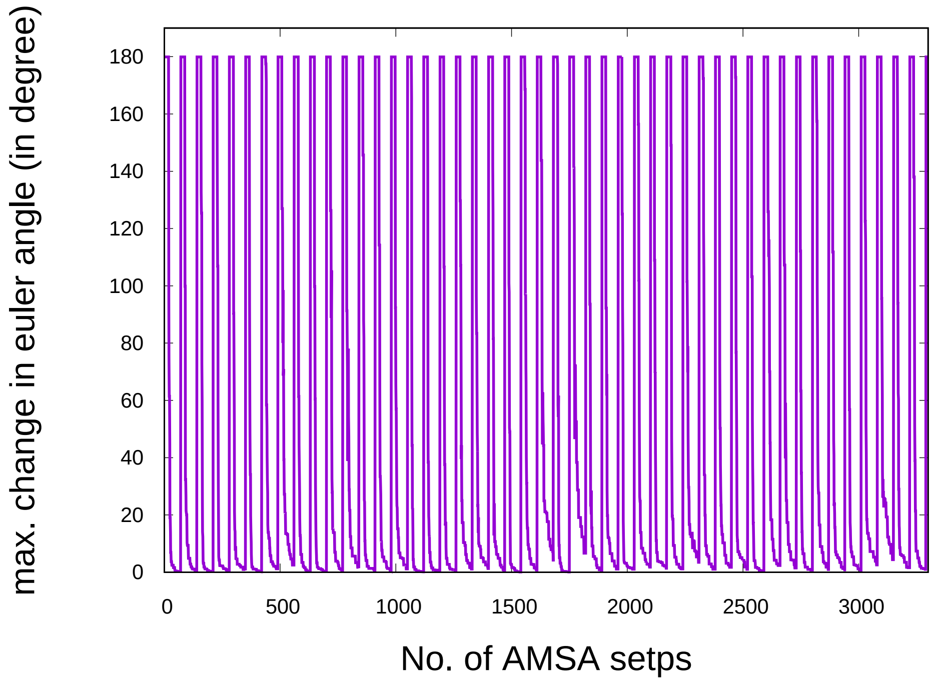
(b)Zoomed in profile of a portion of Fig. 11(a)



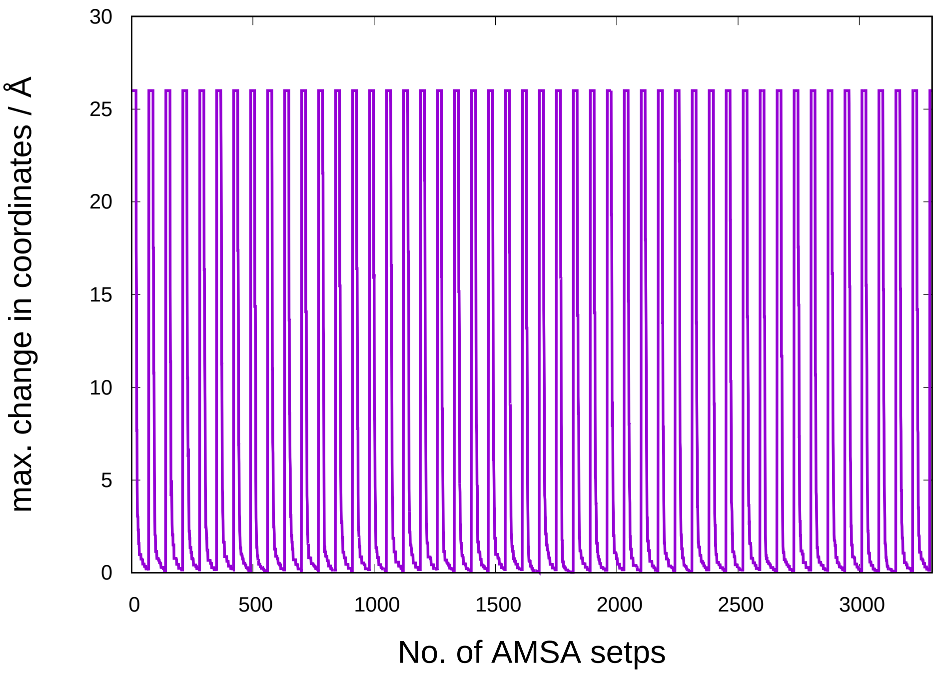
(c)Variation of energy in AMSA



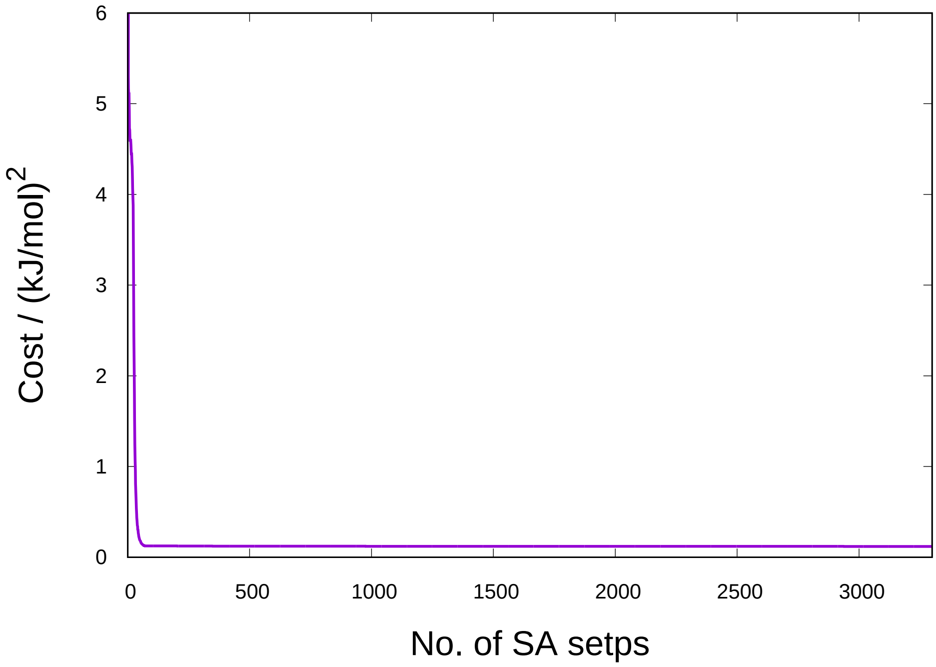
(d)Zoomed in profile of a portion of Fig. 11(c)



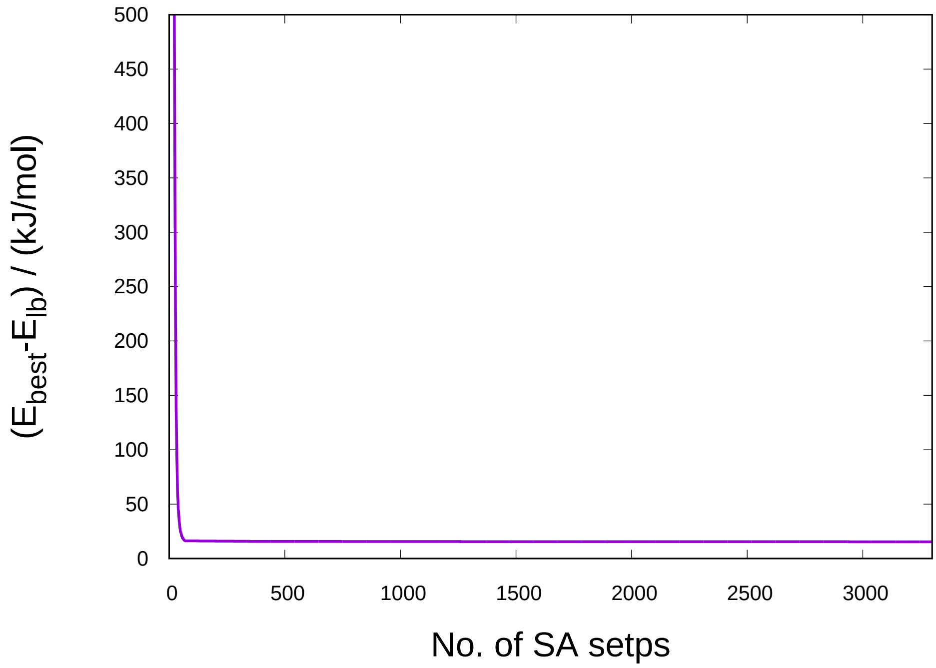
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

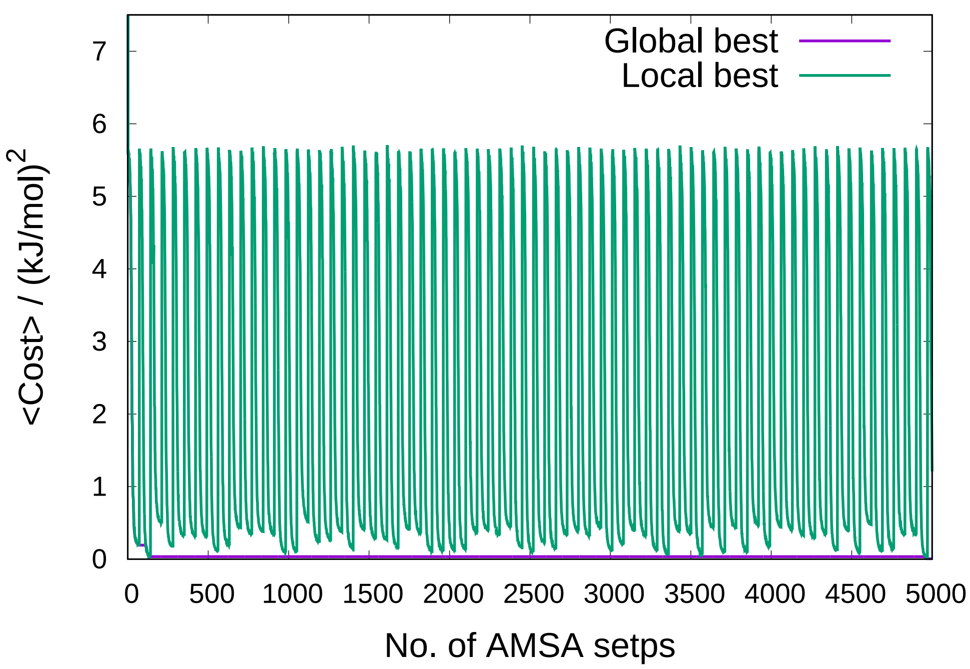


(g)Variation of Cost functional in SA

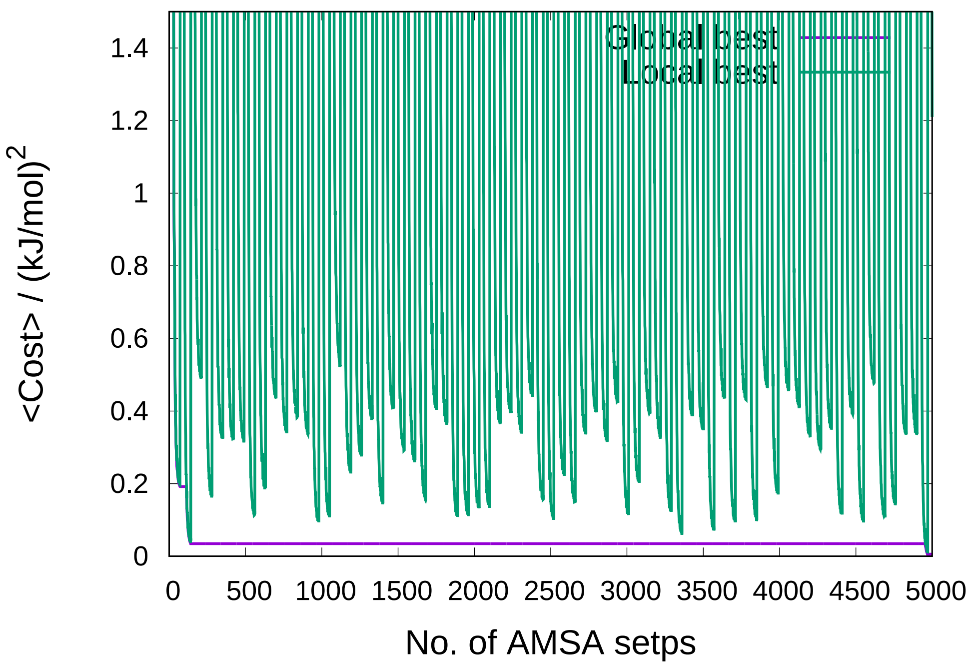


(h)Variation of energy in SA

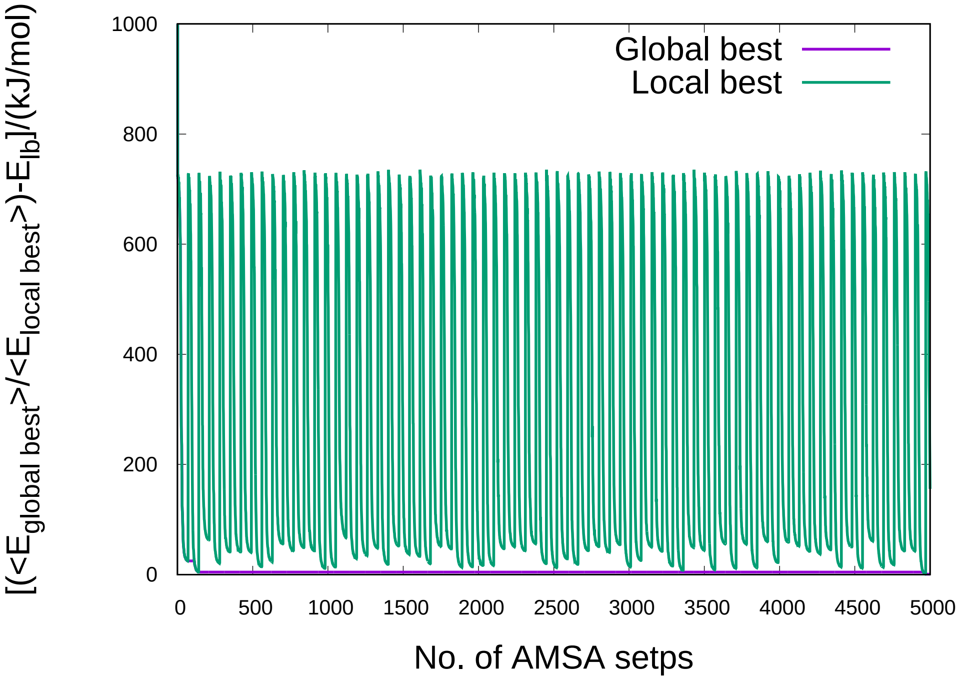
FIG. 11. Critical analysis of AMSA for $NOVER = 5000$.



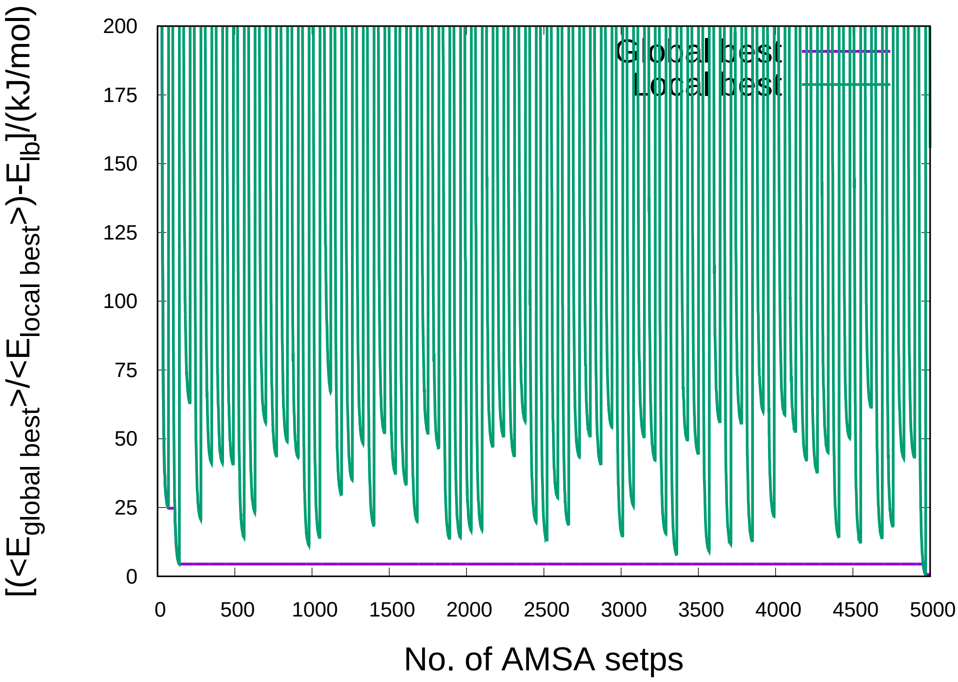
(a)Variation of Cost functional in AMSA



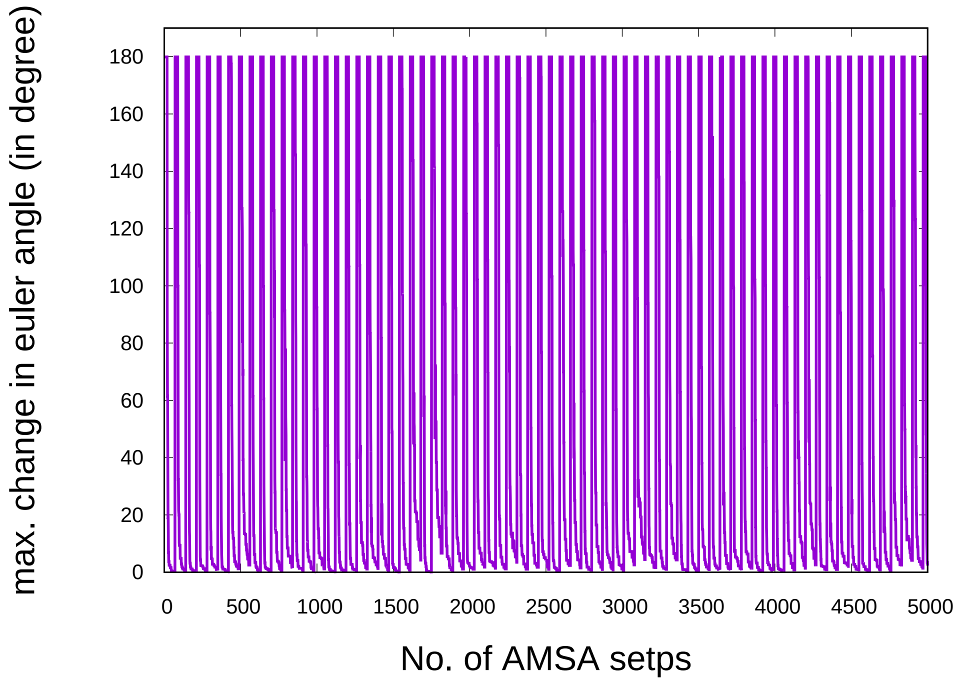
(b)Zoomed in profile of a portion of Fig. 12(a)



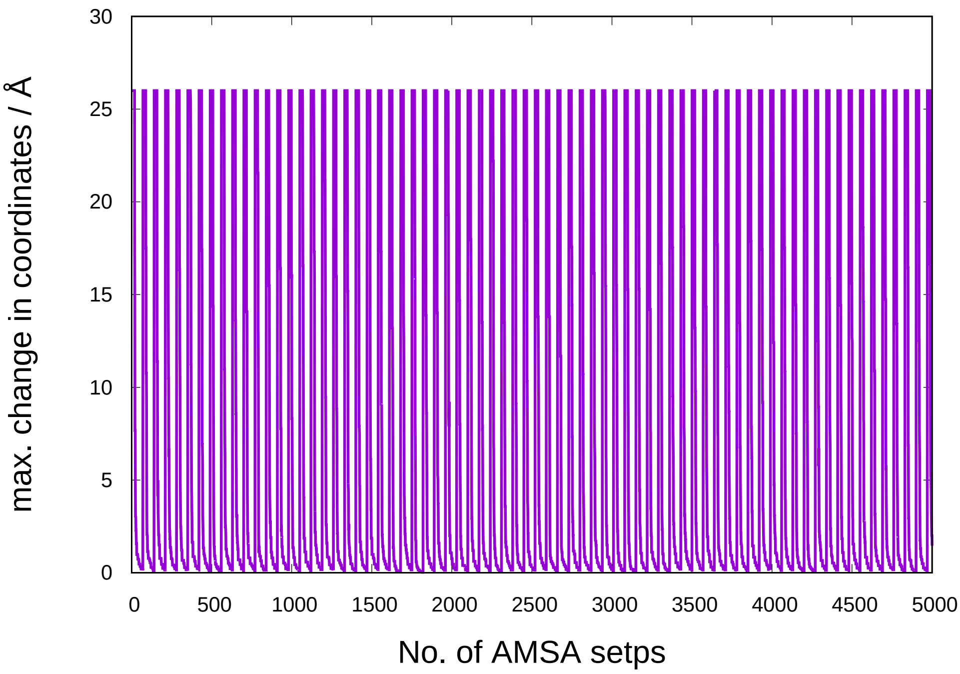
(c)Variation of energy in AMSA



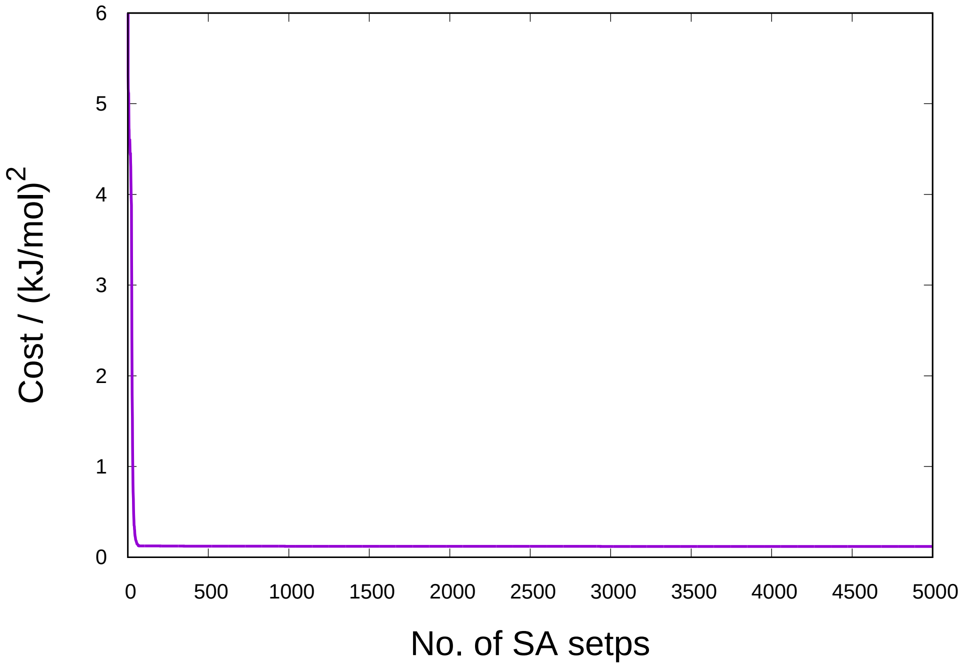
(d)Zoomed in profile of a portion of Fig. 12(c)



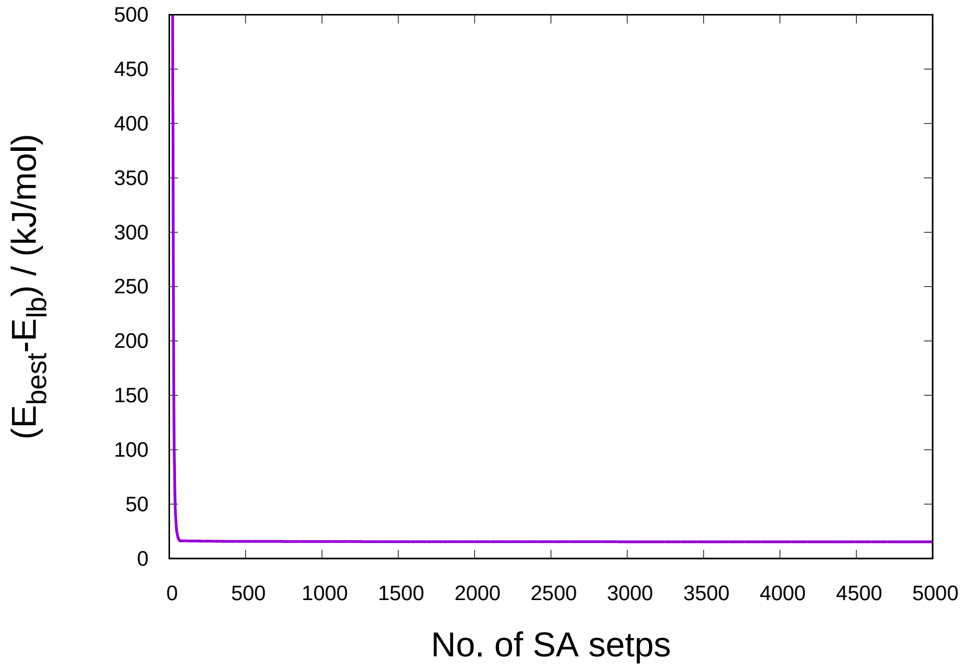
(e)Variation of max. change in coordinates in AMSA



(f)Variation of max. change in Euler angles in AMSA

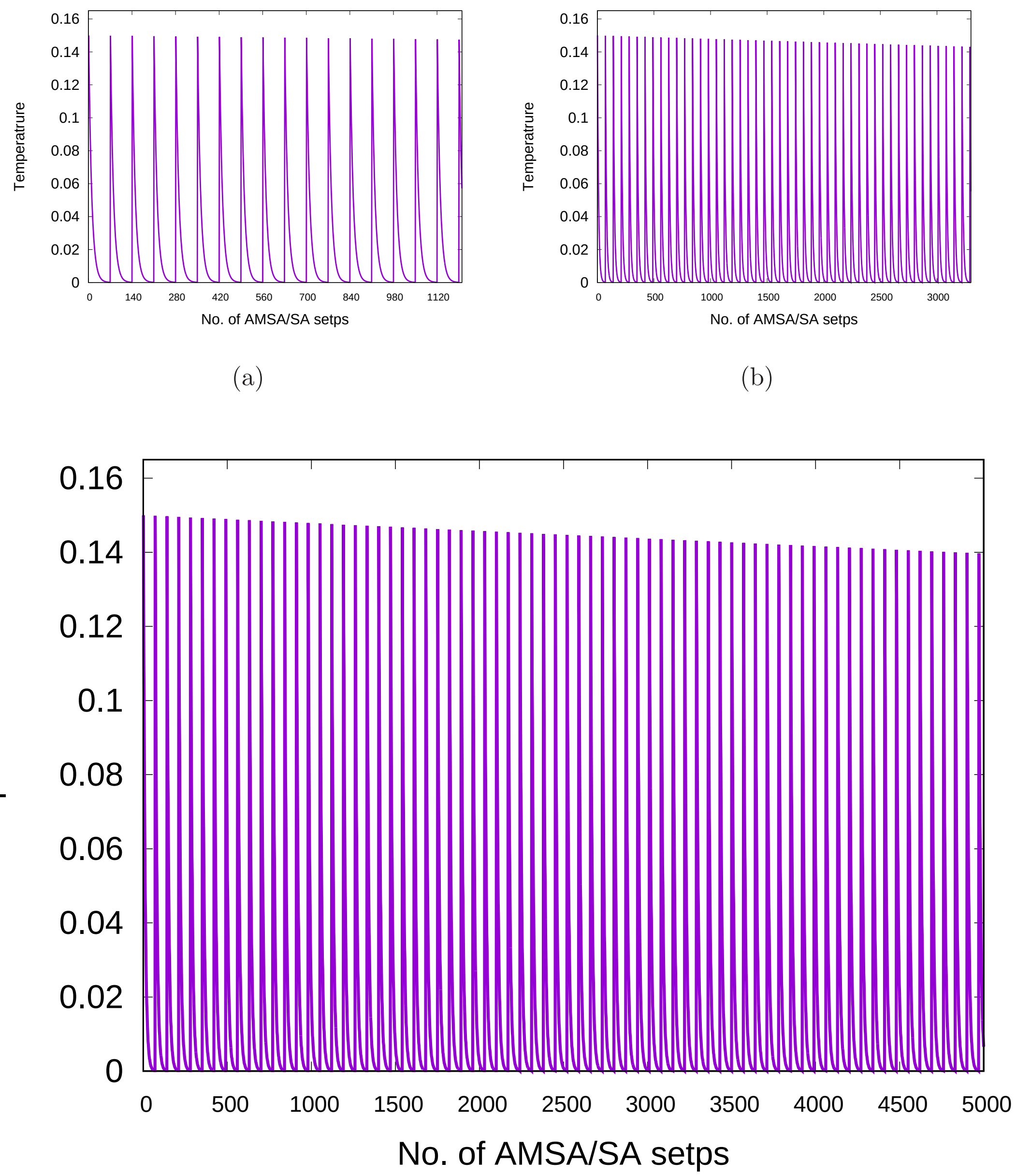


(g)Variation of Cost functional in SA



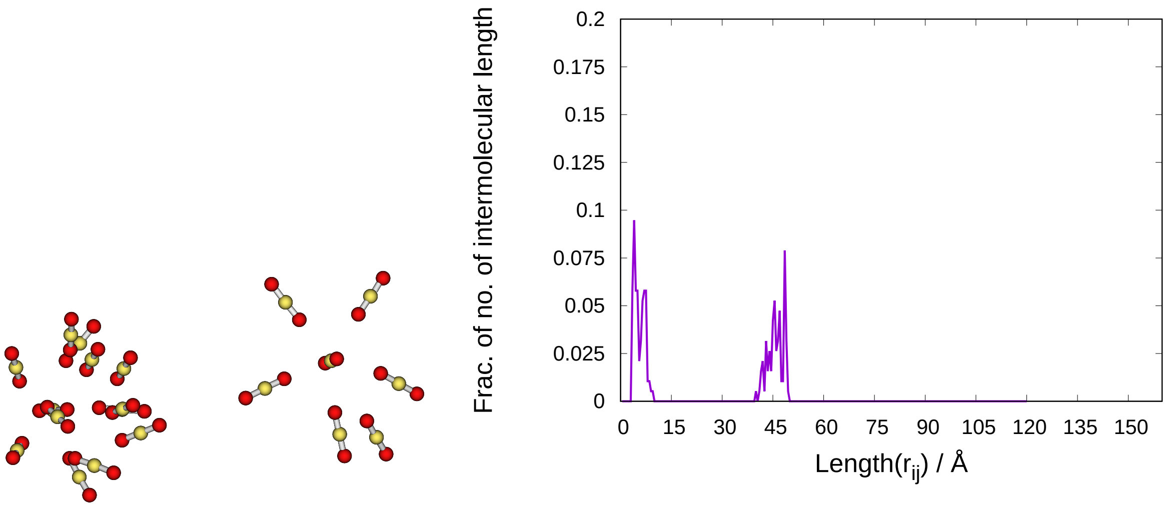
(h)Variation of energy in SA

FIG. 12. Critical analysis of AMSA for $NOVER = 5000$.

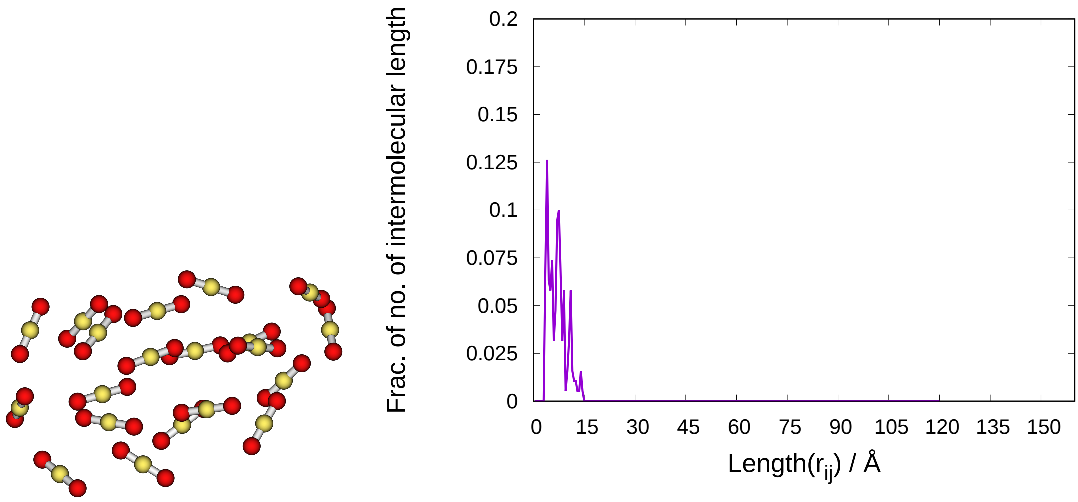


(a) (b) (c)

FIG. 13. Variation of temperature in AMSA.



(a) (b)



(c) (d)

FIG. 14. Structures and fragment patterns for $n = 20$.

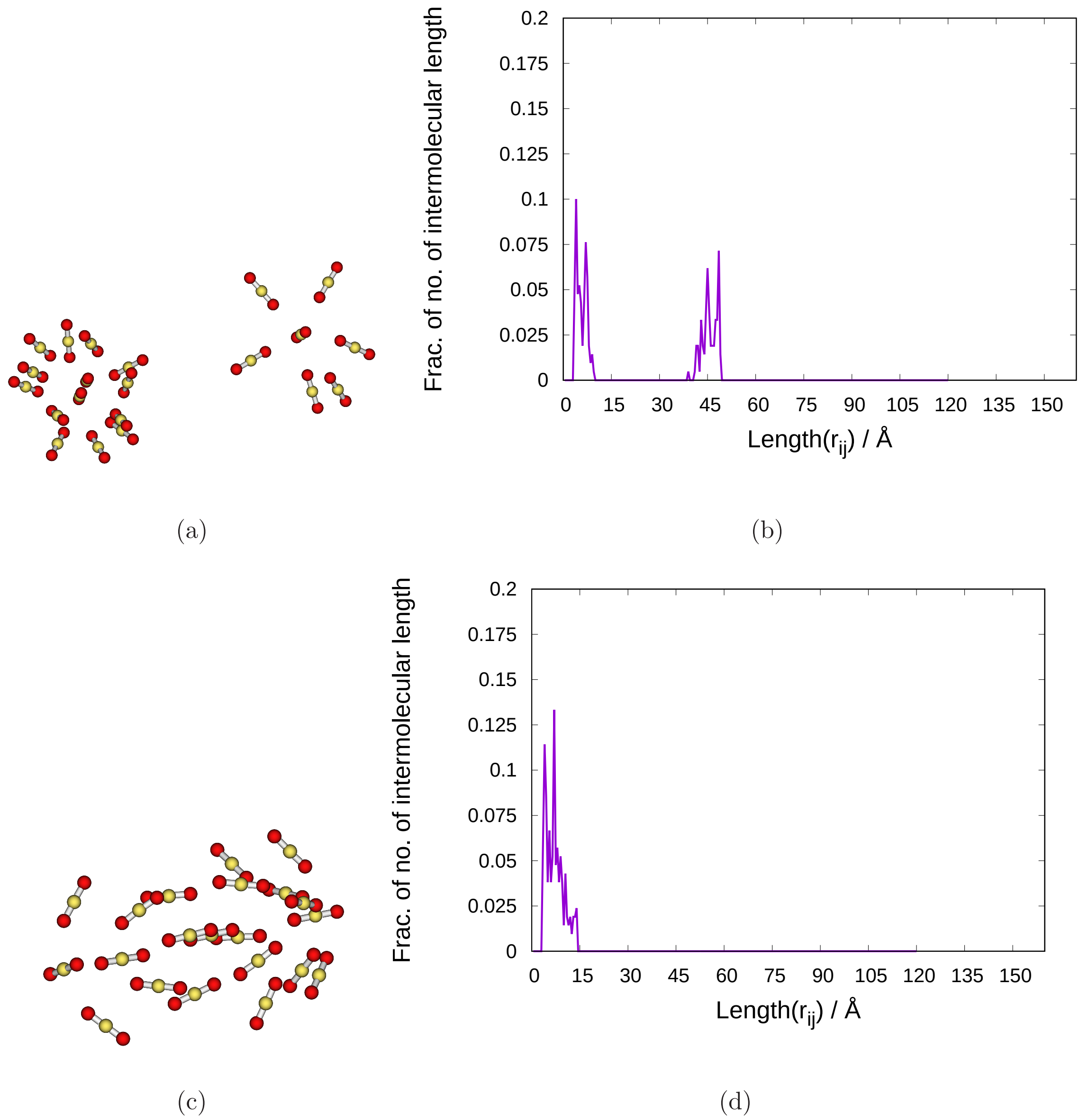


FIG. 15. Structures and fragment patterns for $n = 21$.

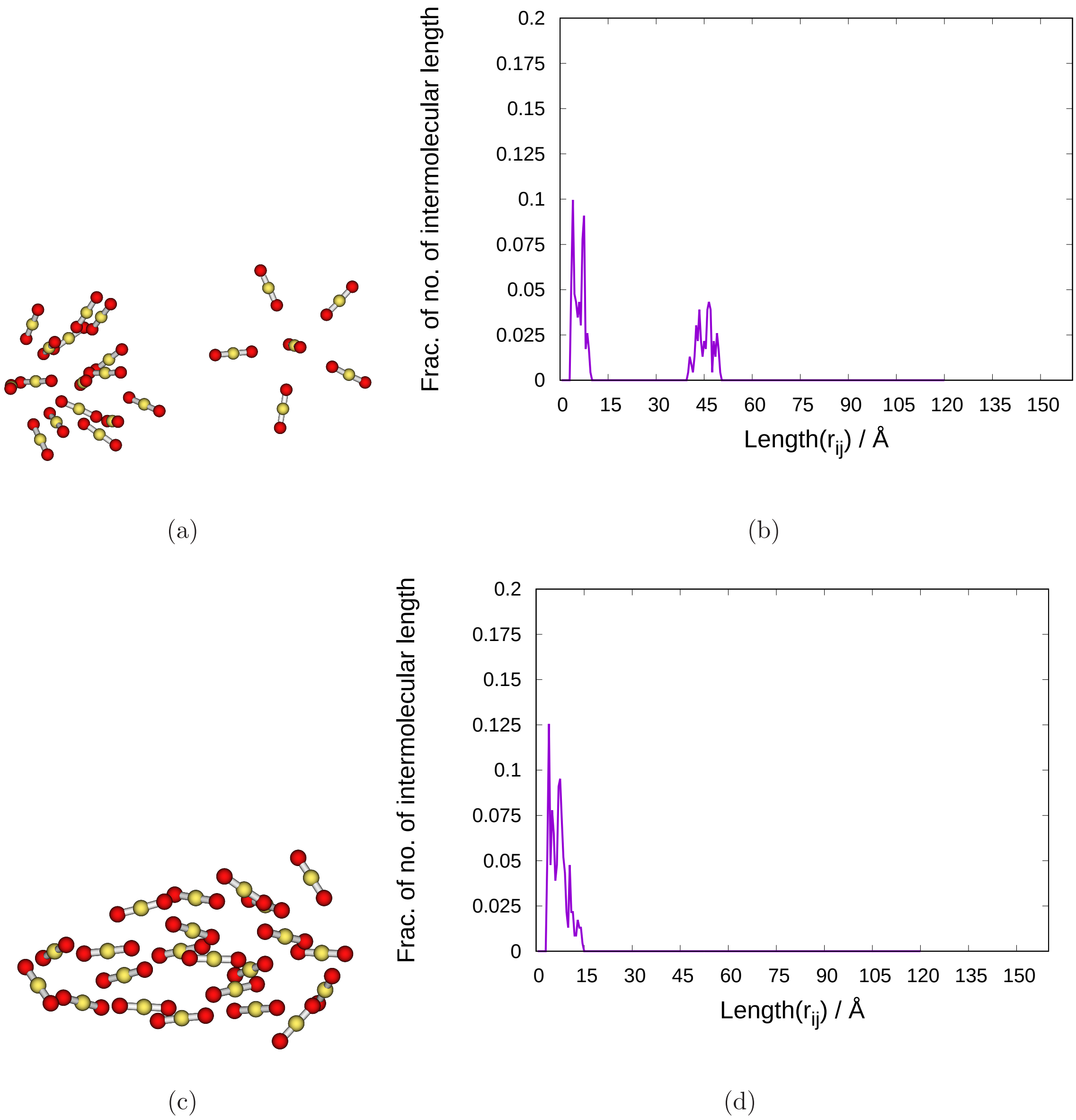
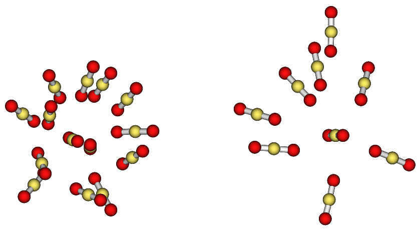
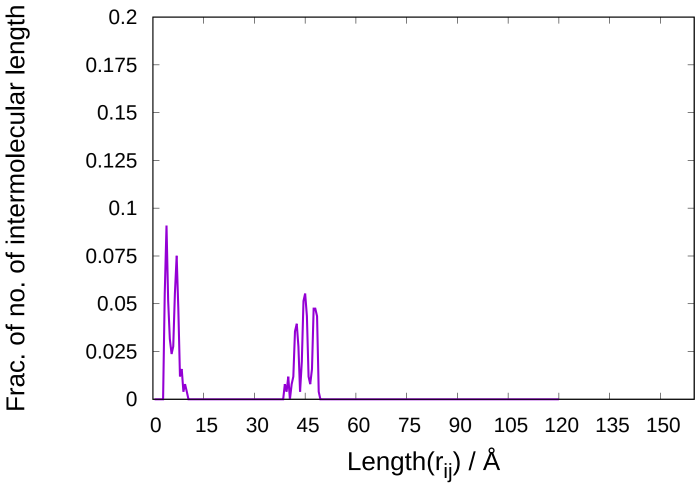


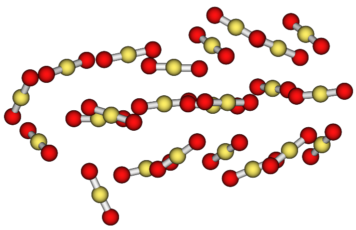
FIG. 16. Structures and fragment patterns for $n = 22$.



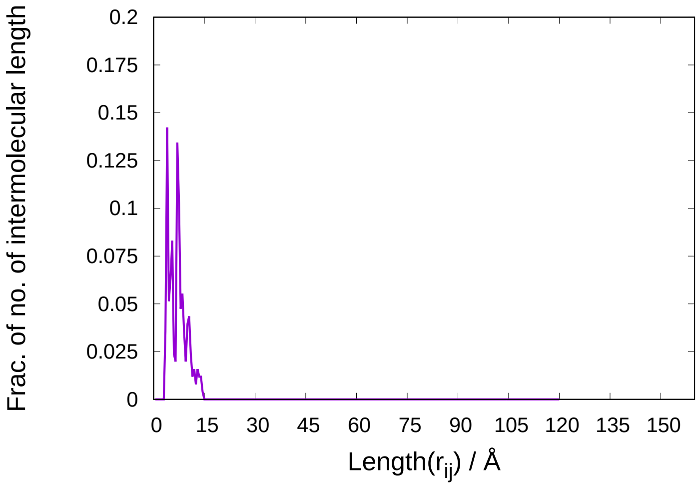
(a)



(b)

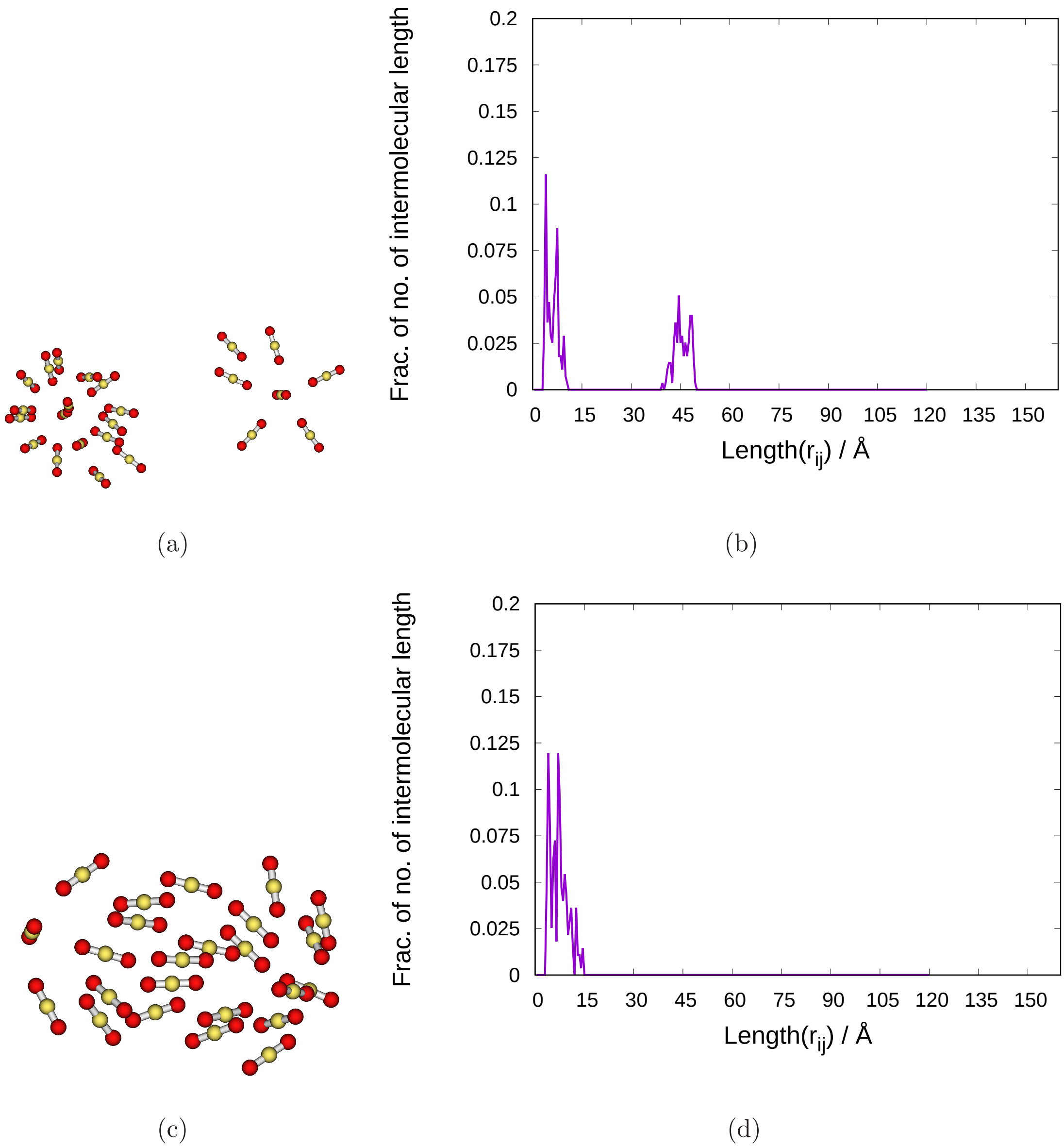


(c)



(d)

FIG. 17. Structures and fragment patterns for $n = 23$.



(a) (b)

(c) (d)

FIG. 18. Structures and fragment patterns for $n = 24$.

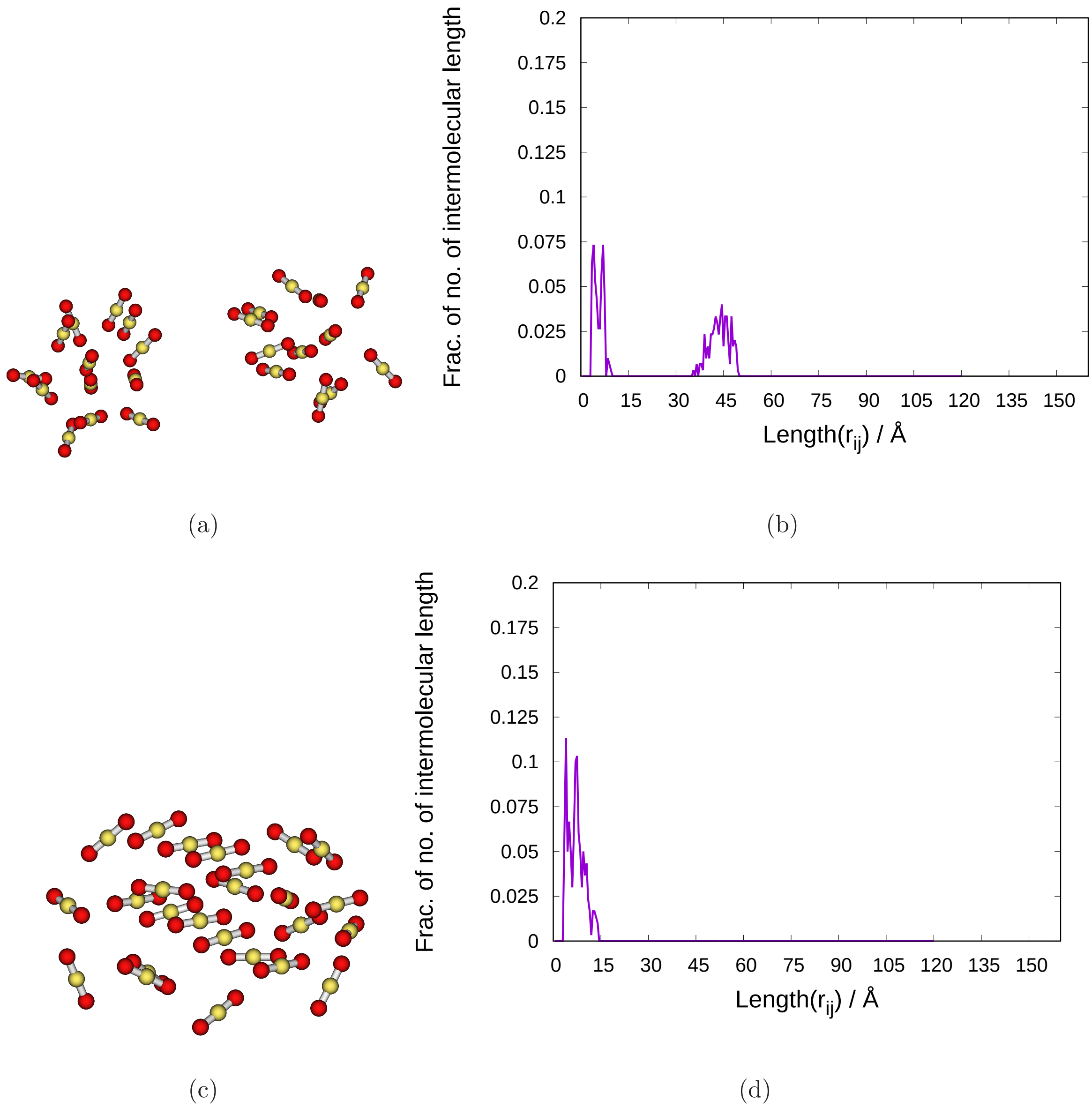
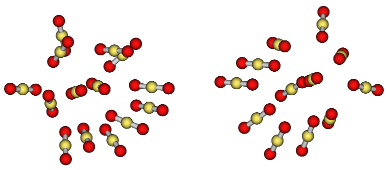
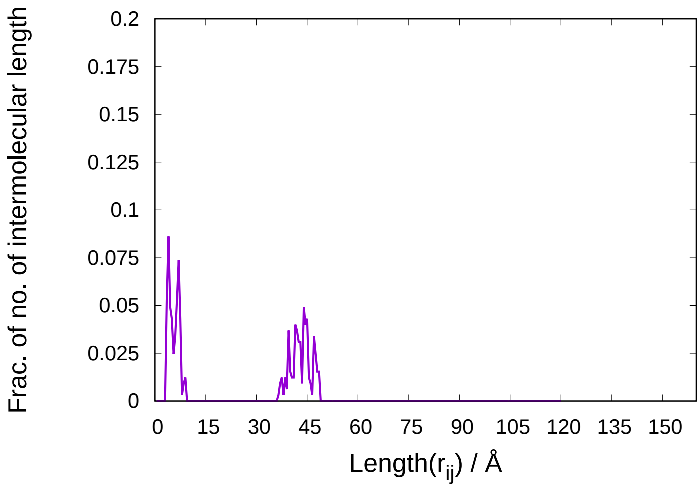


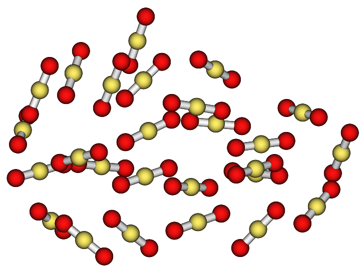
FIG. 19. Structures and fragment patterns for $n = 25$.

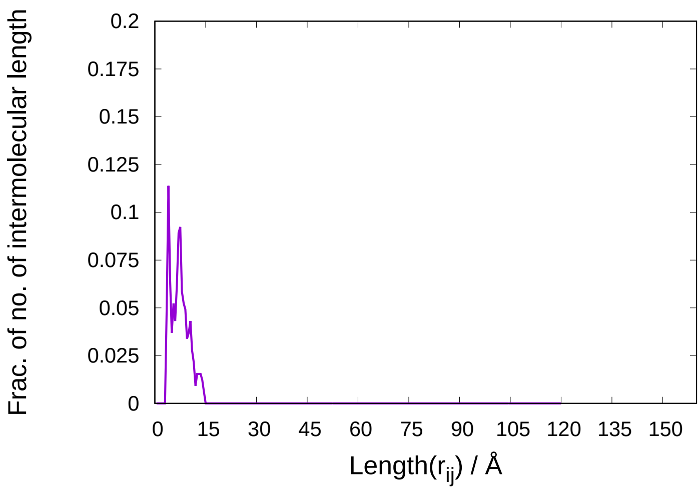




(a)

(b)





(c)

(d)

FIG. 20. Structures and fragment patterns for $n = 26$.

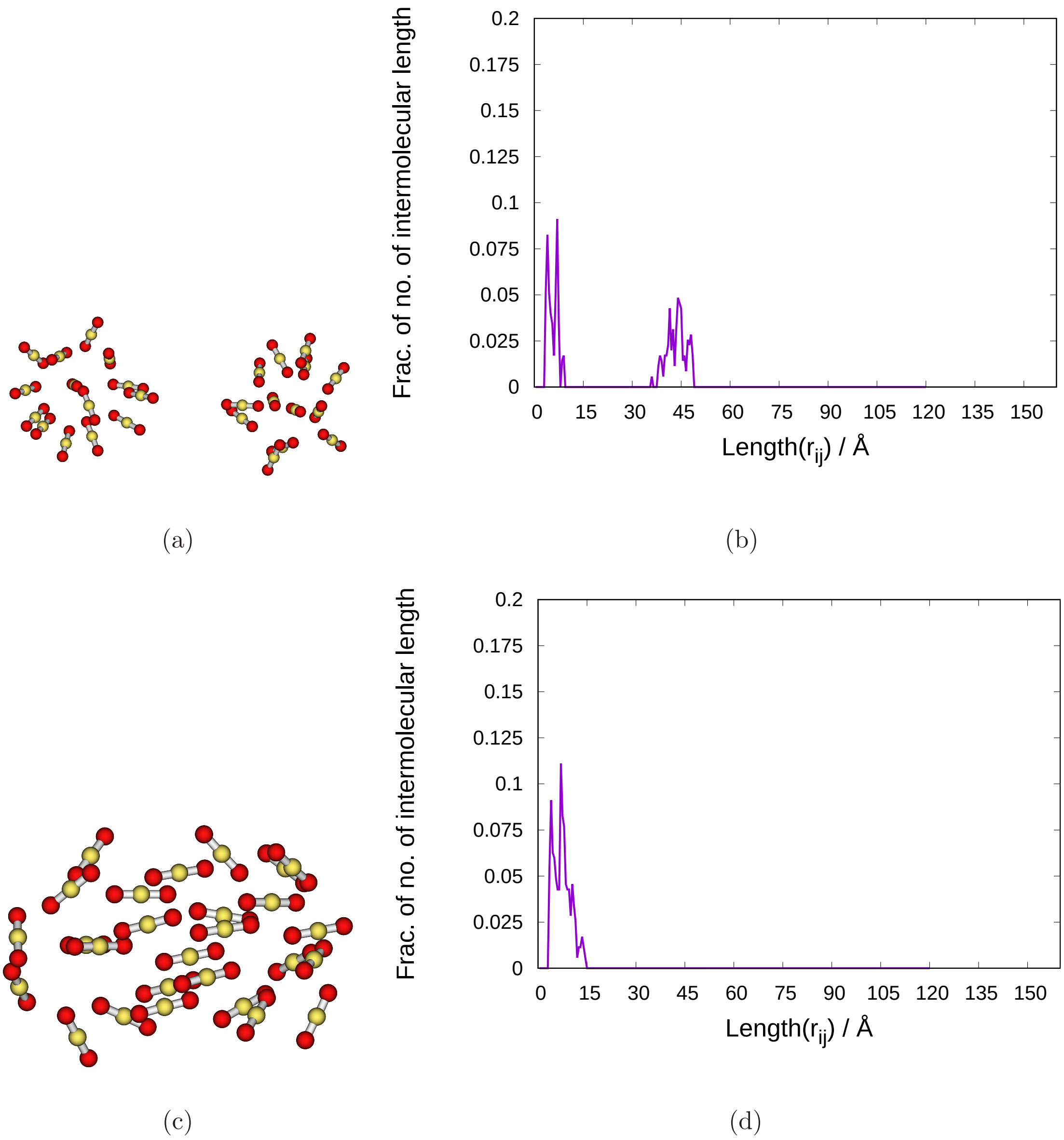


FIG. 21. Structures and fragment patterns for $n = 27$.

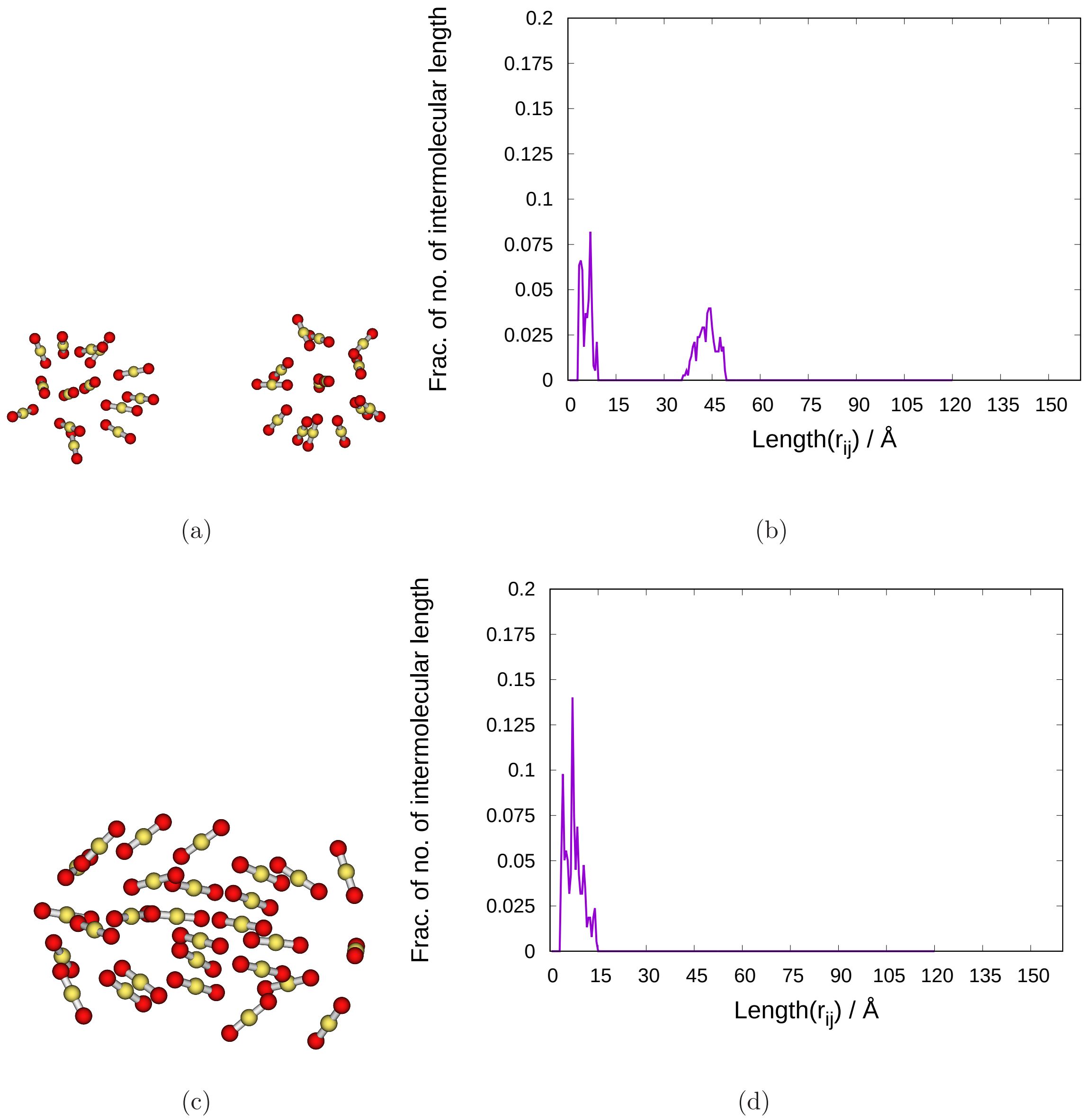


FIG. 22. Structures and fragment patterns for $n = 28$.

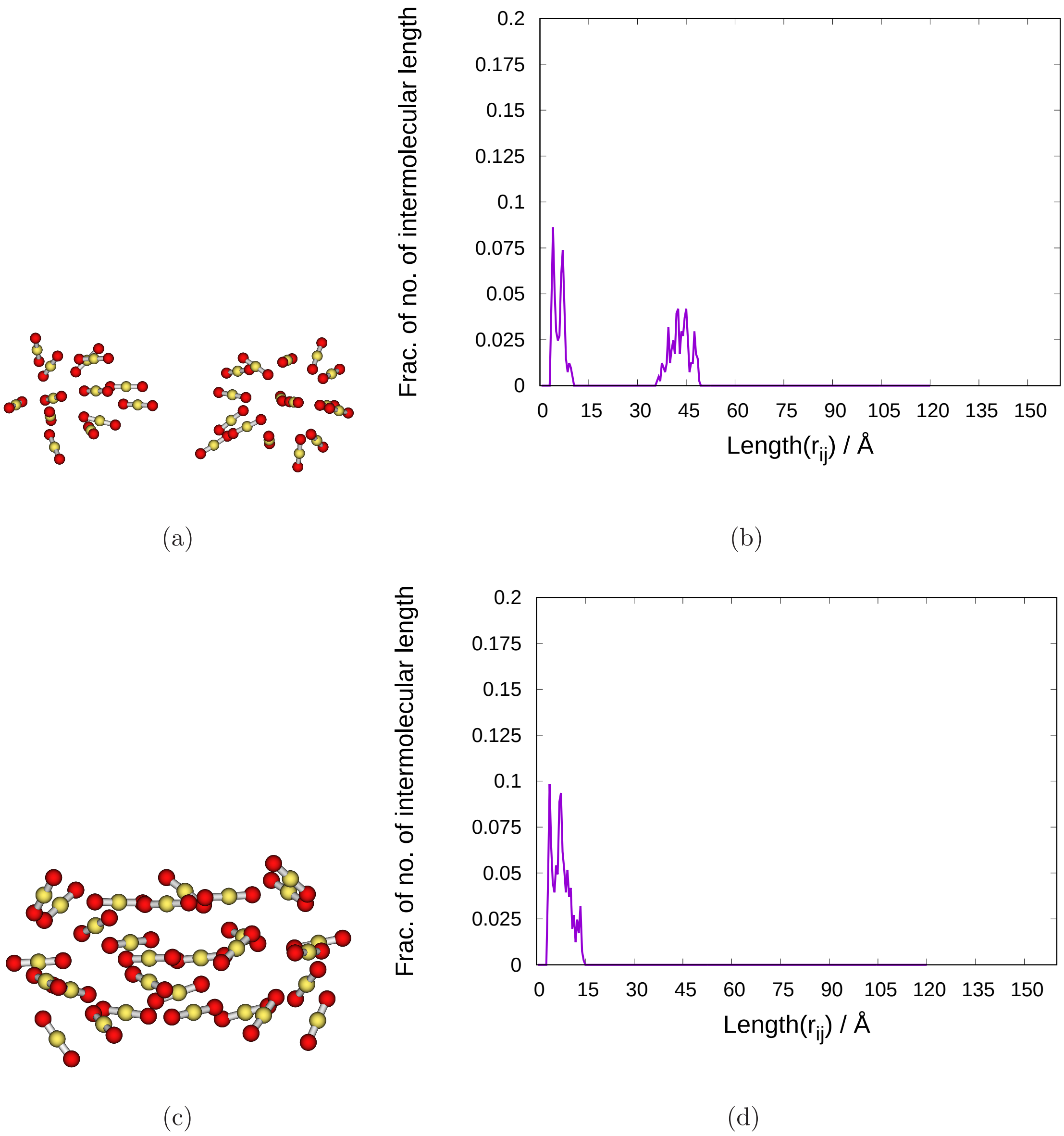
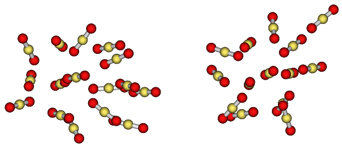
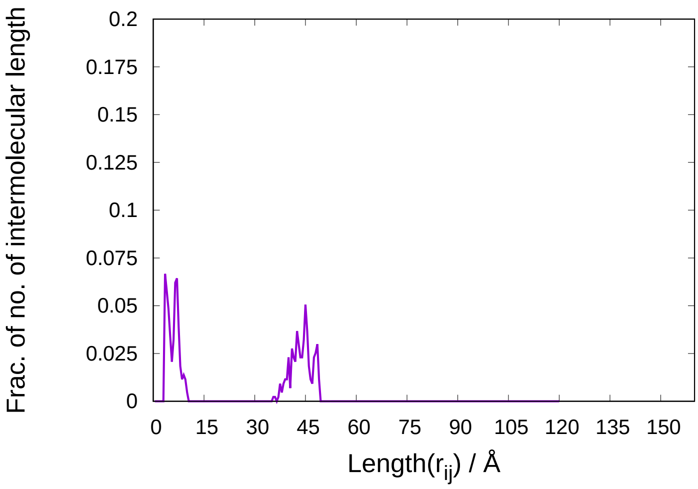


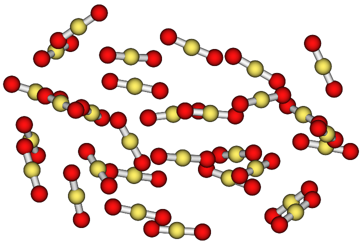
FIG. 23. Structures and fragment patterns for $n = 29$.



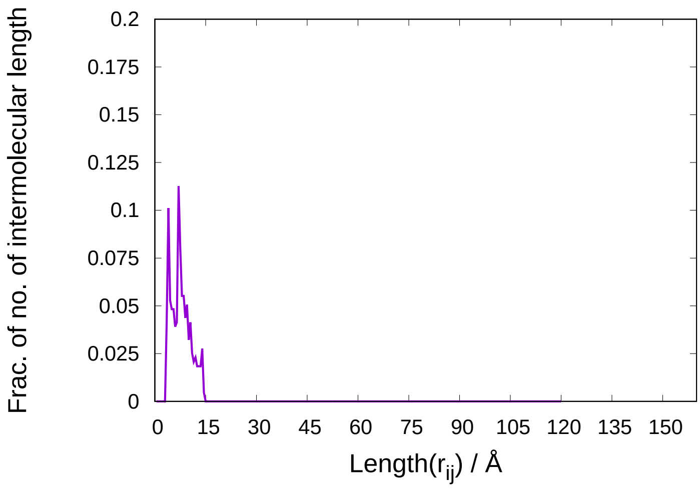
(a)



(b)

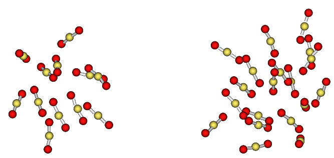


(c)

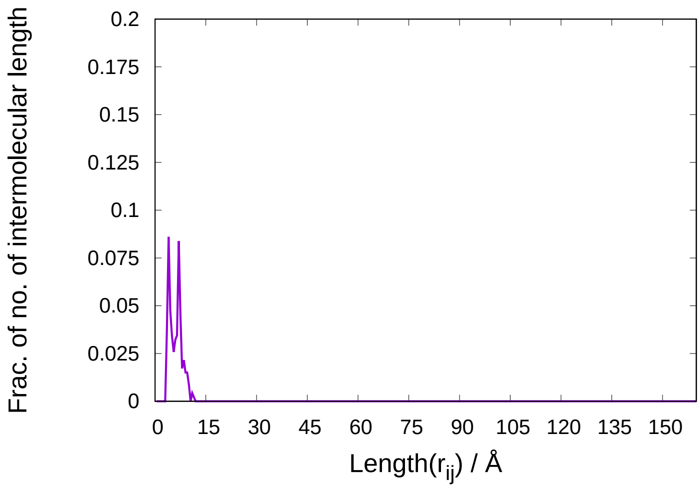


(d)

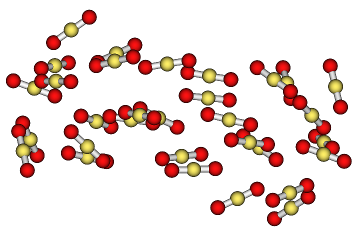
FIG. 24. Structures and fragment patterns for $n = 30$.



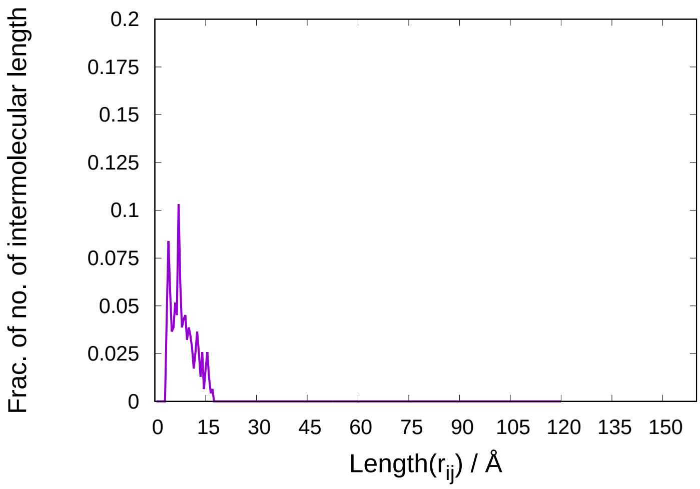
(a)



(b)

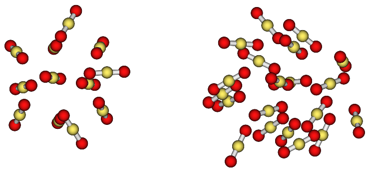


(c)

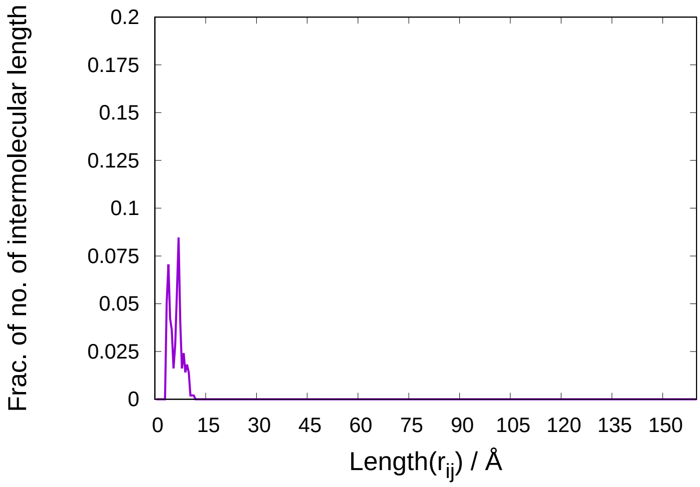


(d)

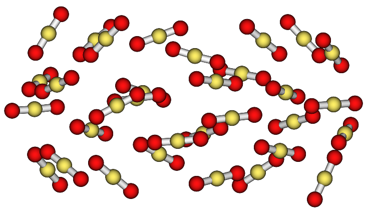
FIG. 25. Structures and fragment patterns for $n = 31$.



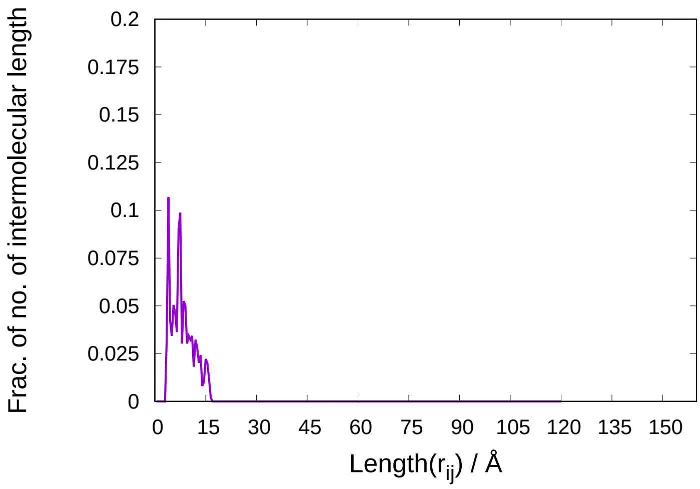
(a)



(b)

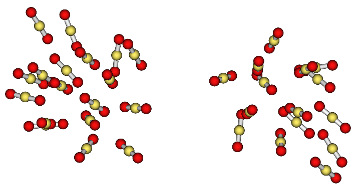


(c)

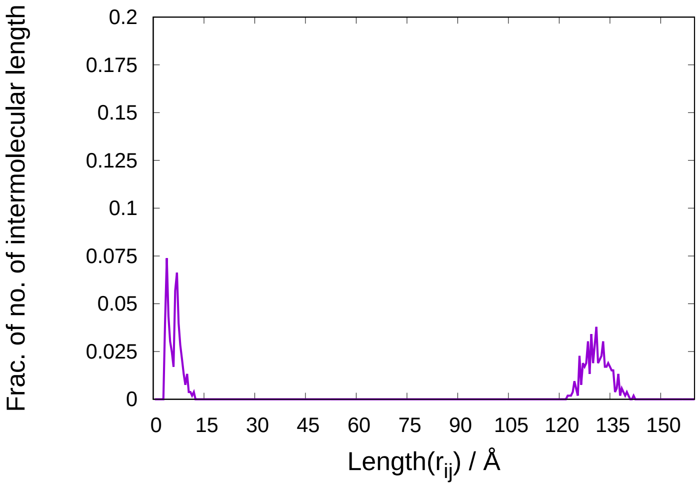


(d)

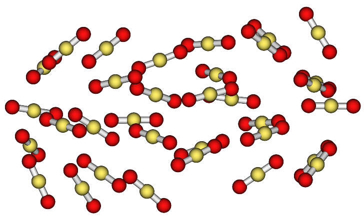
FIG. 26. Structures and fragment patterns for $n = 32$.



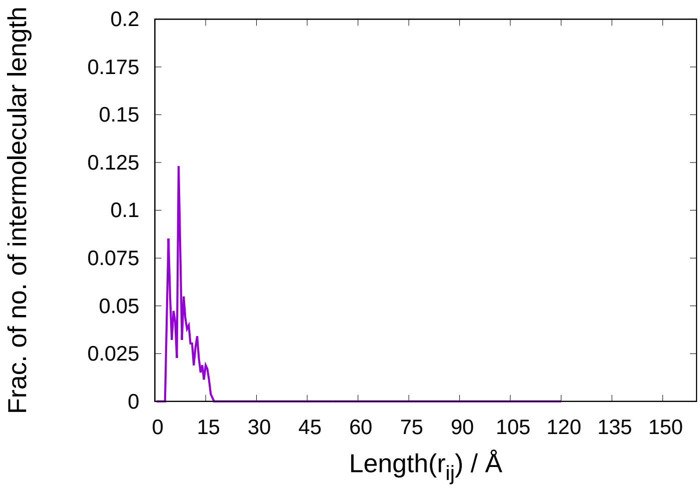
(a)



(b)



(c)



(d)

FIG. 27. Structures and fragment patterns for $n = 33$.

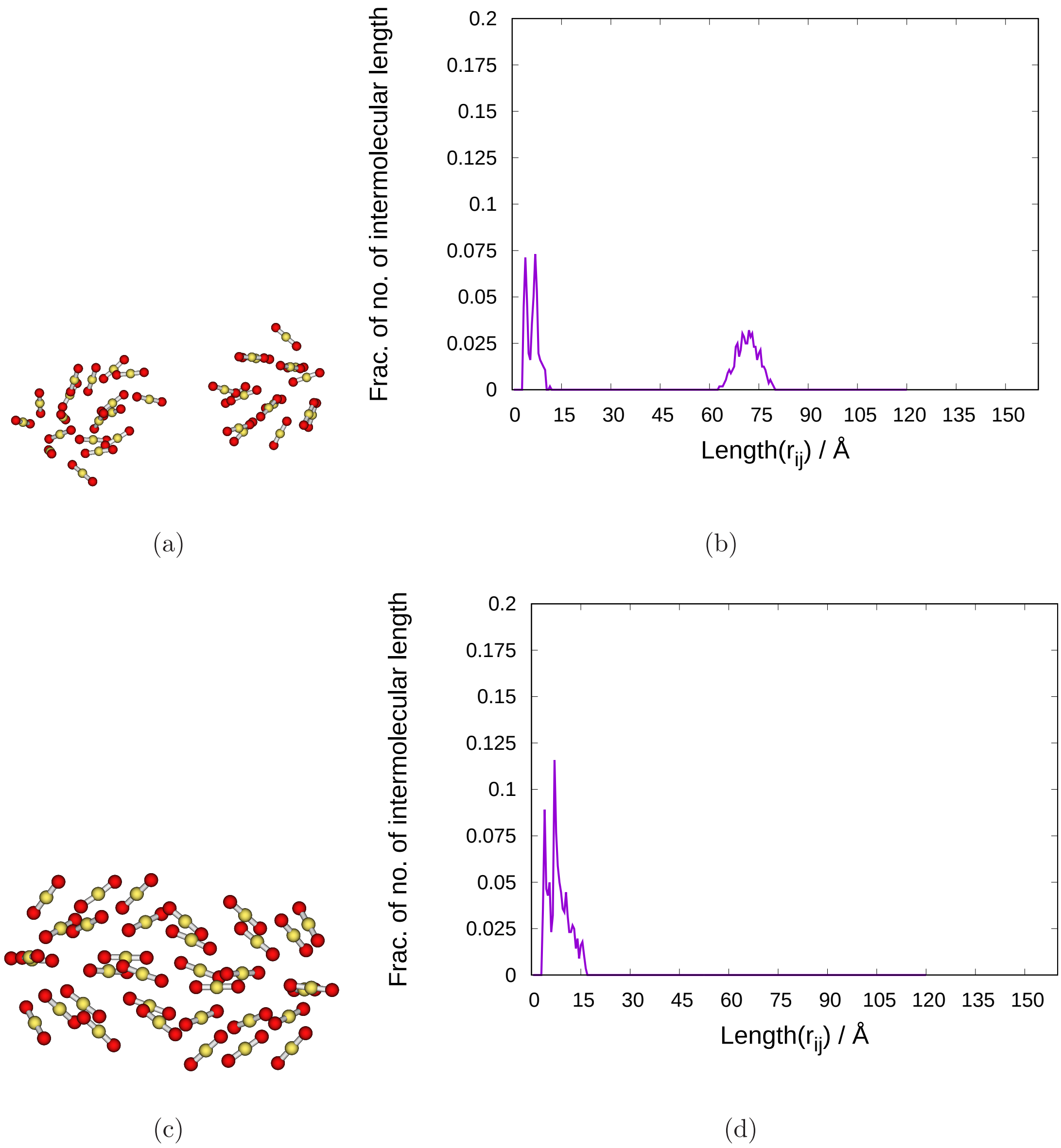
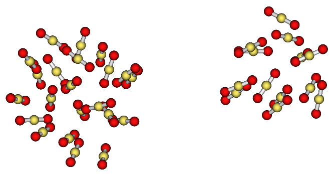
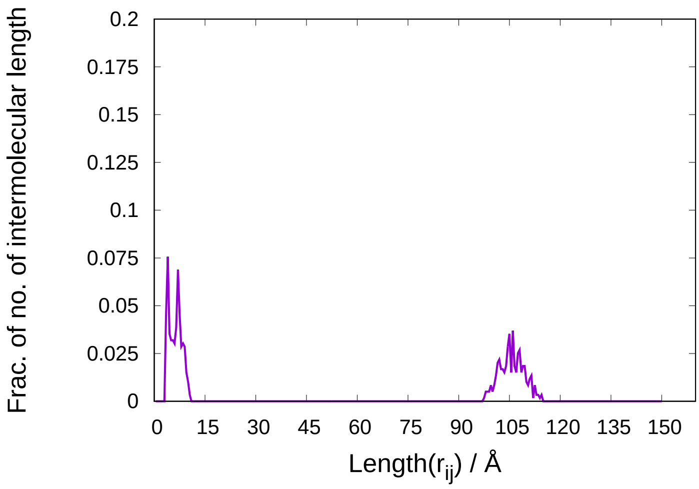


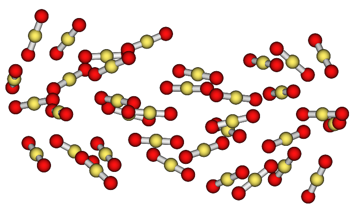
FIG. 28. Structures and fragment patterns for $n = 34$.

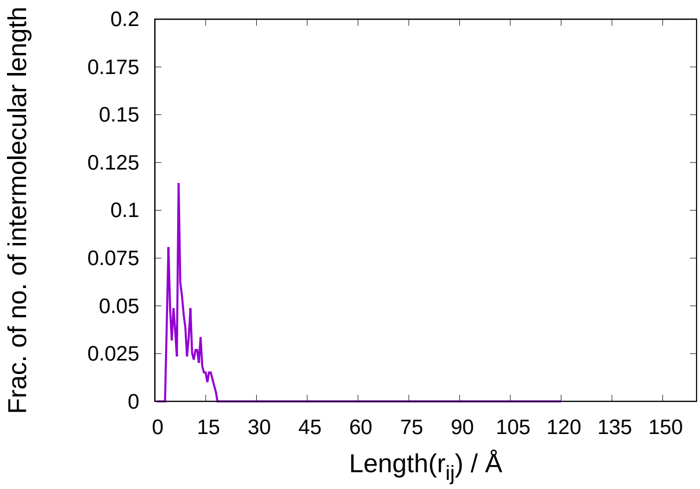




(a)

(b)





(c)

(d)

FIG. 29. Structures and fragment patterns for $n = 35$.

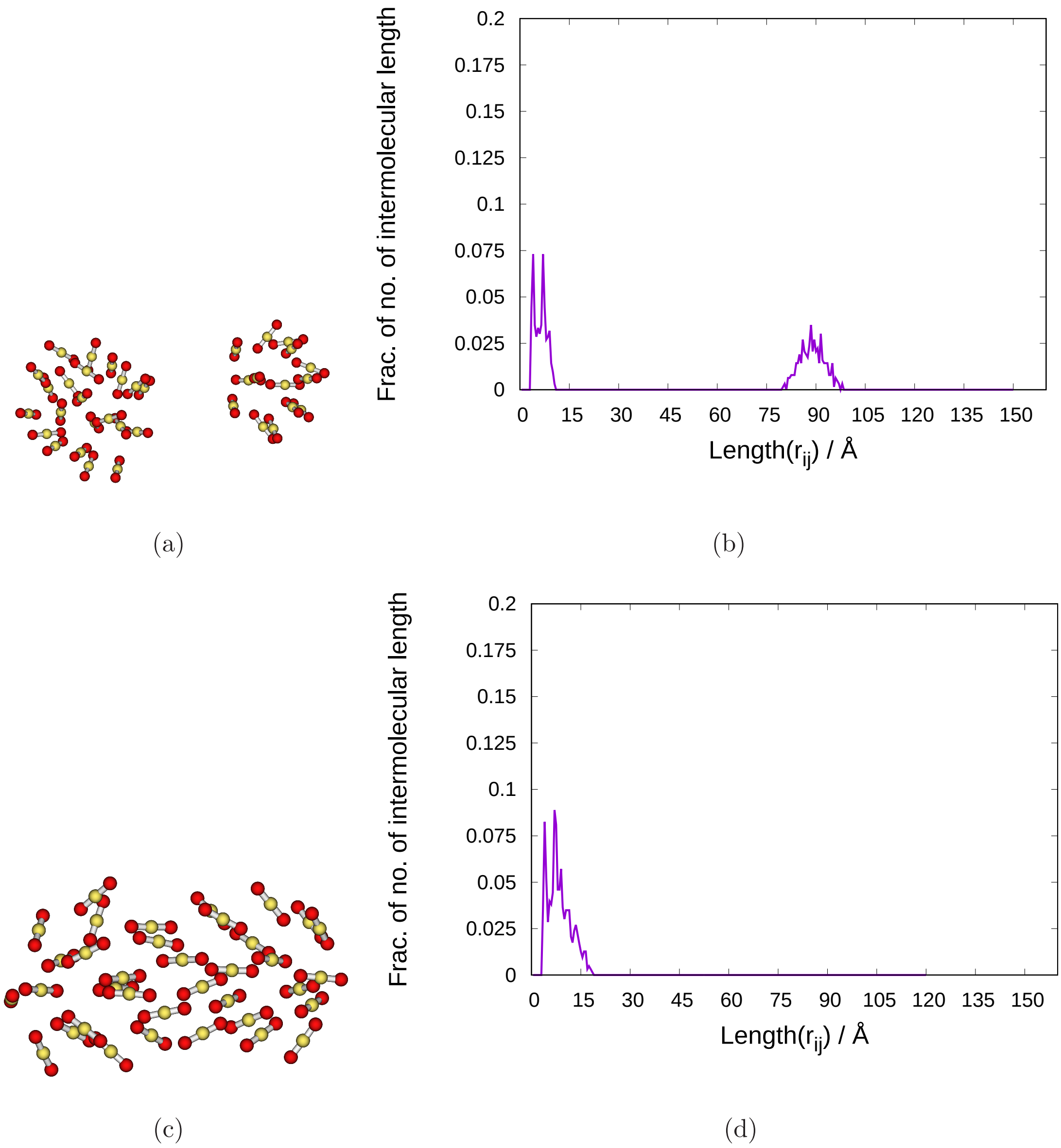


FIG. 30. Structures and fragment patterns for $n = 36$.

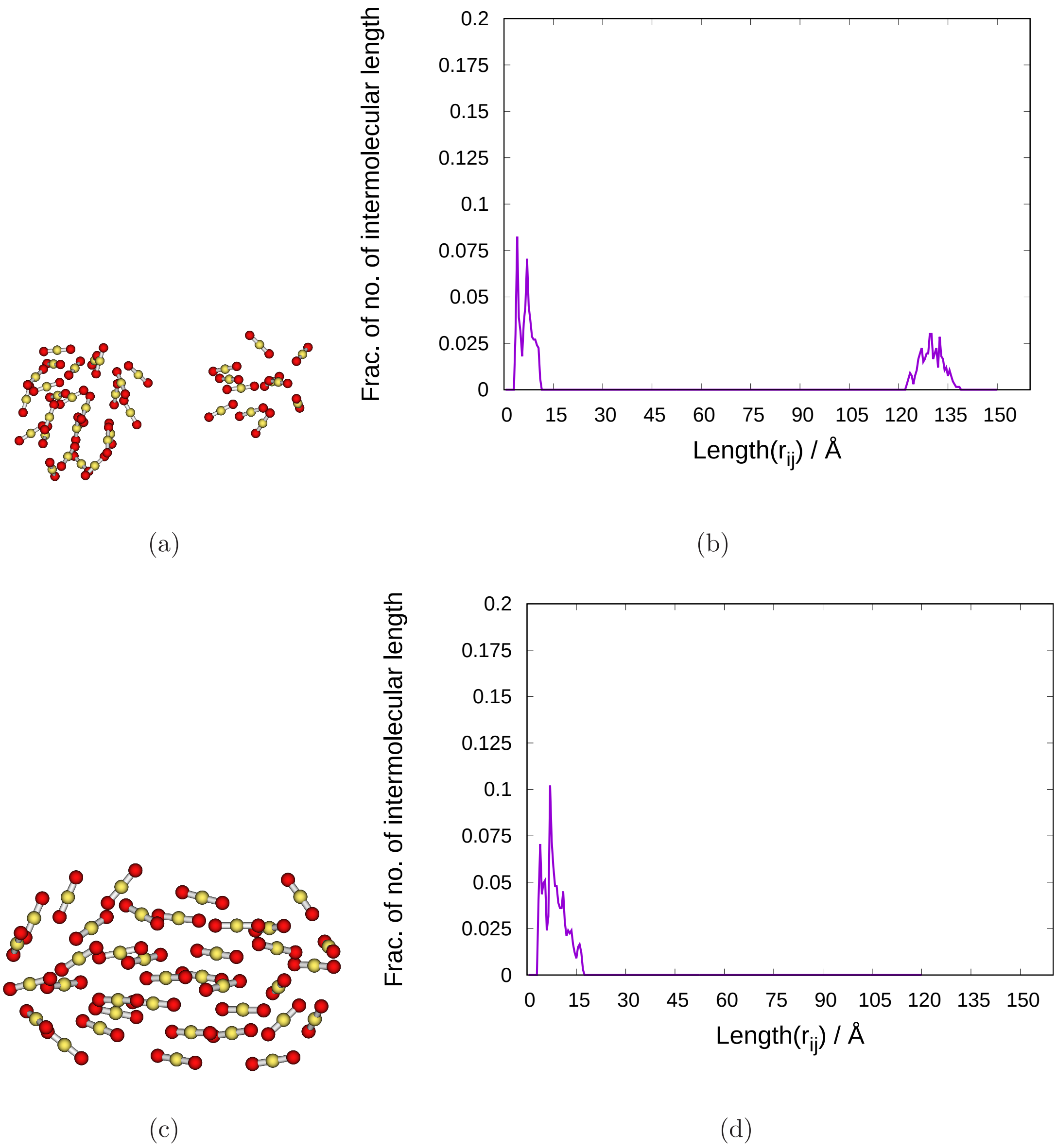


FIG. 31. Structures and fragment patterns for $n = 37$.

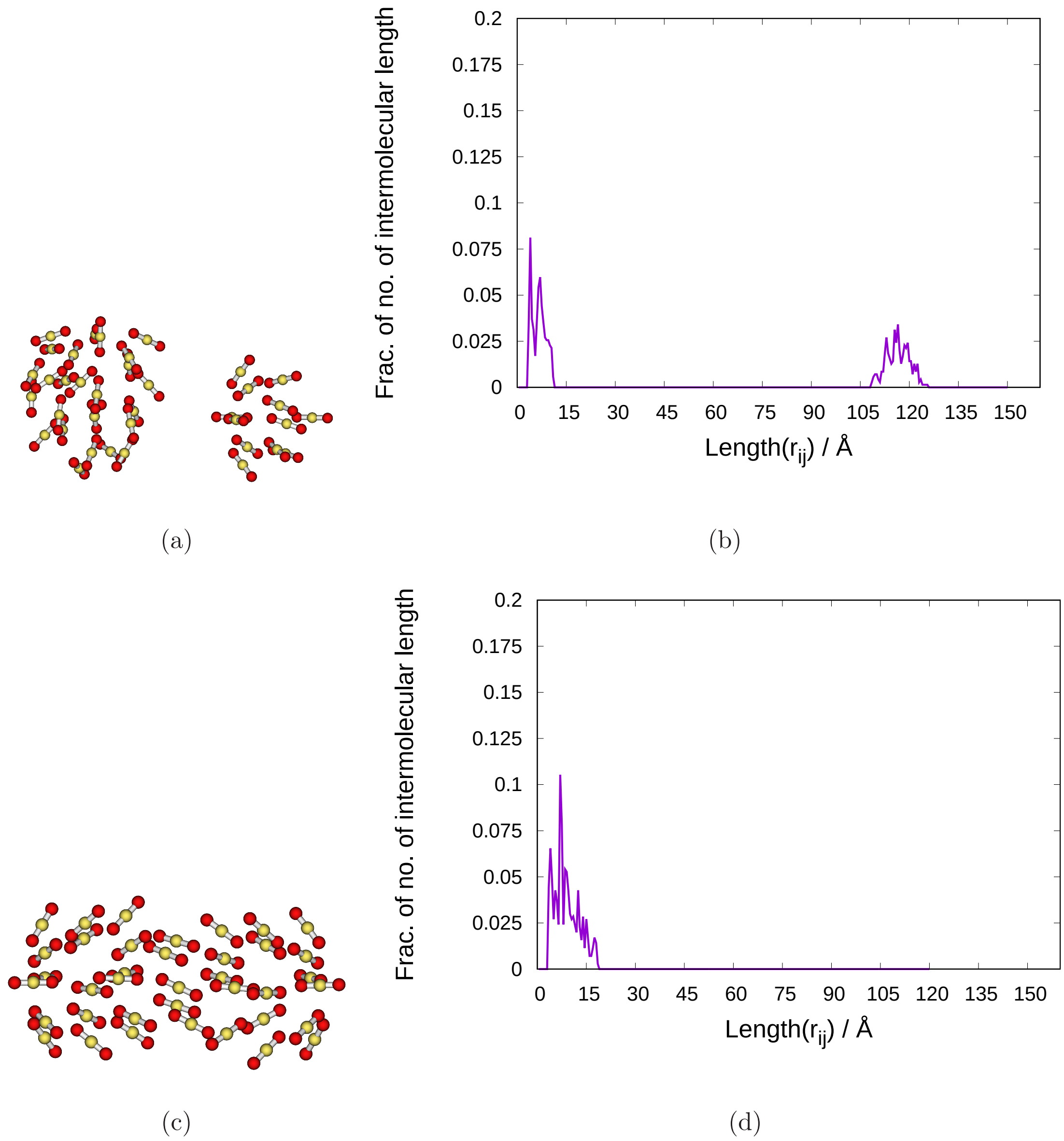


FIG. 32. Structures and fragment patterns for $n = 38$.

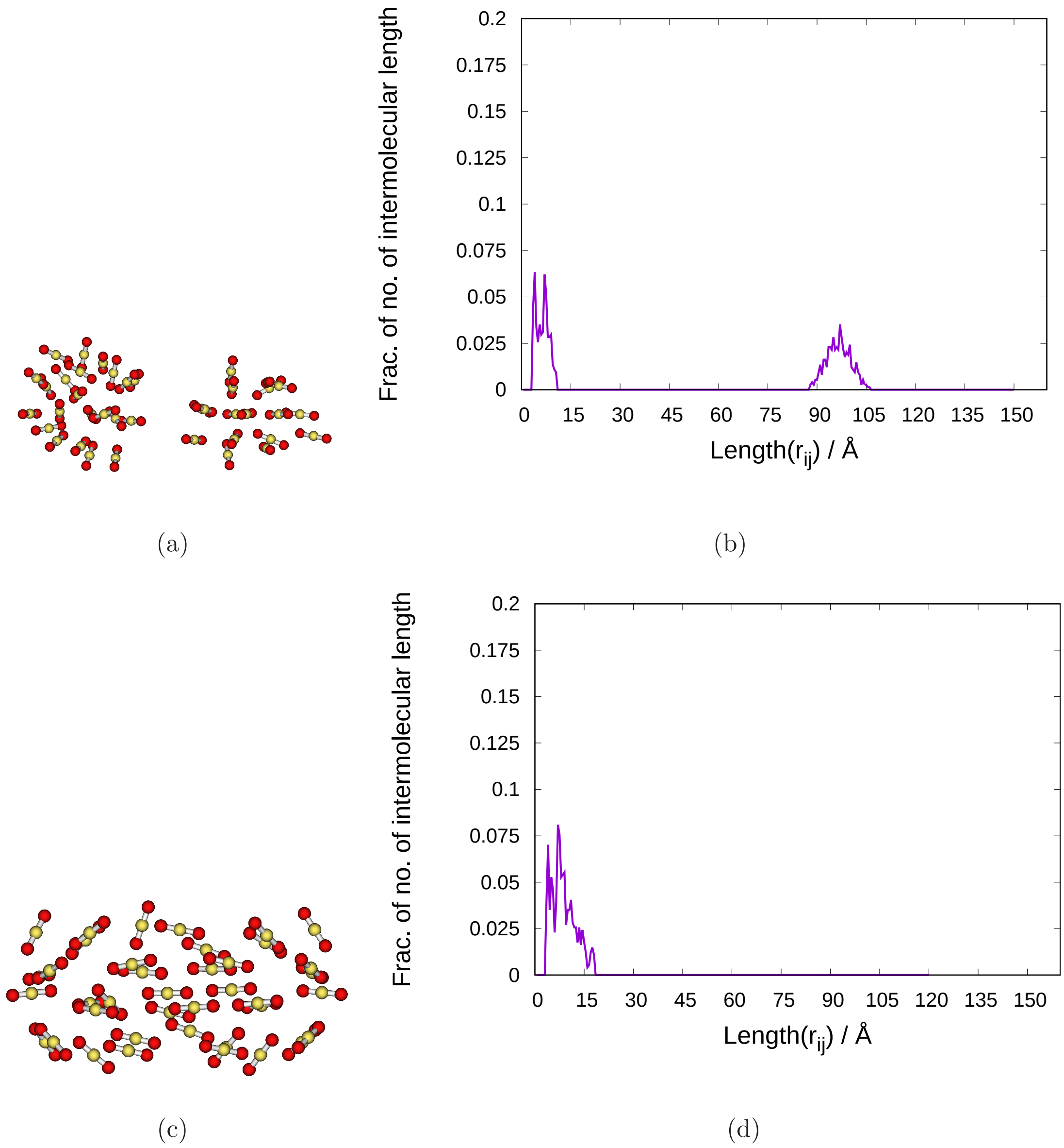


FIG. 33. Structures and fragment patterns for $n = 39$.

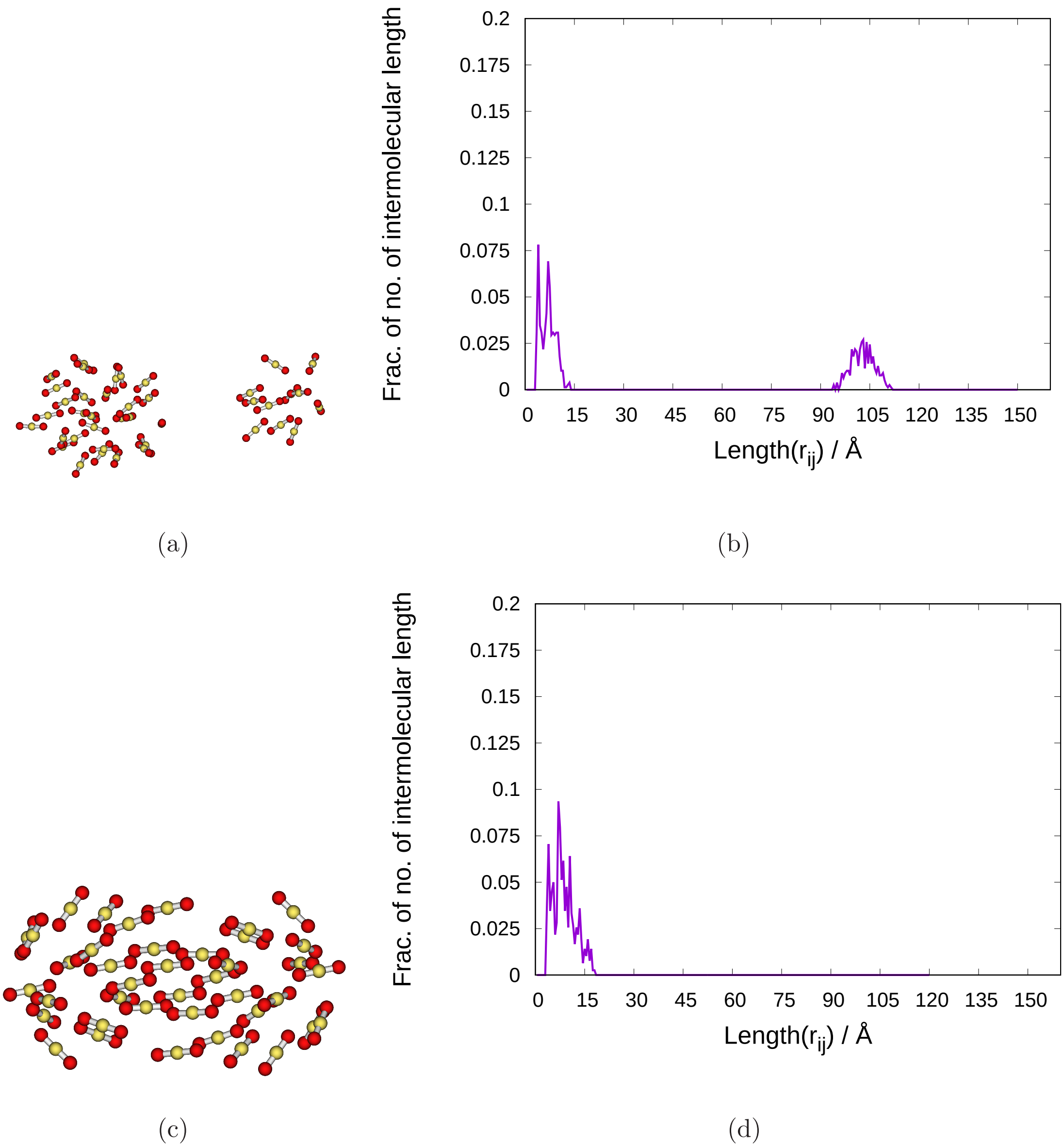
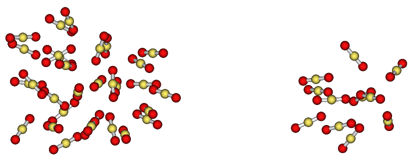
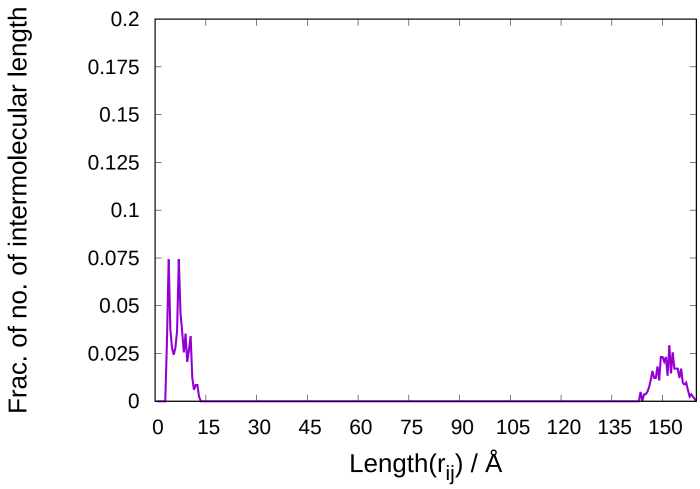


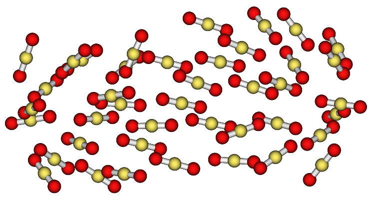
FIG. 34. Structures and fragment patterns for $n = 40$.



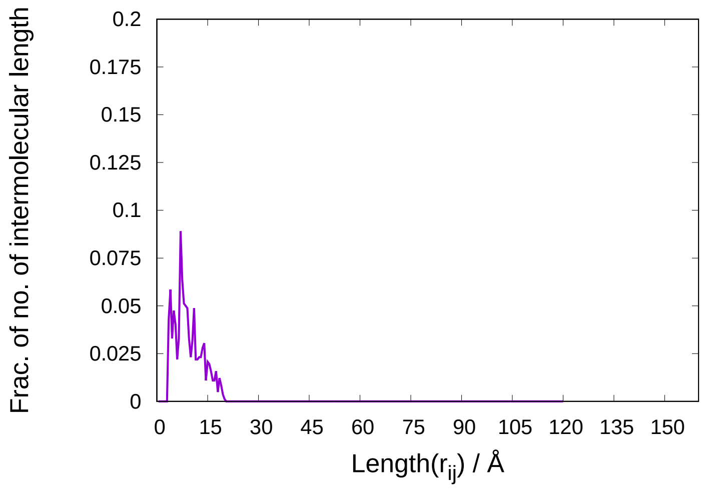
(a)



(b)



(c)



(d)

FIG. 35. Structures and fragment patterns for $n = 41$.

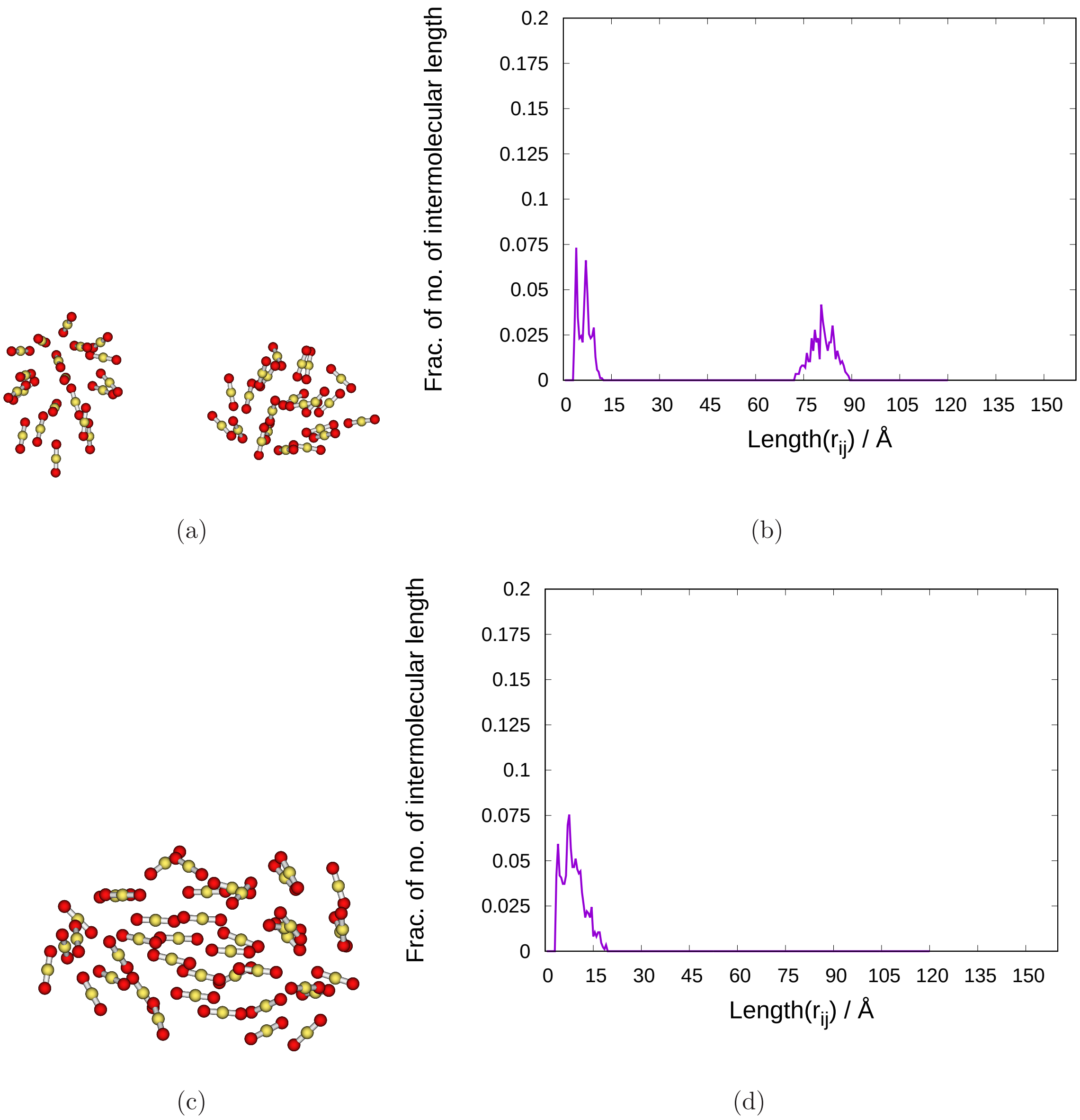


FIG. 36. Structures and fragment patterns for $n = 42$.

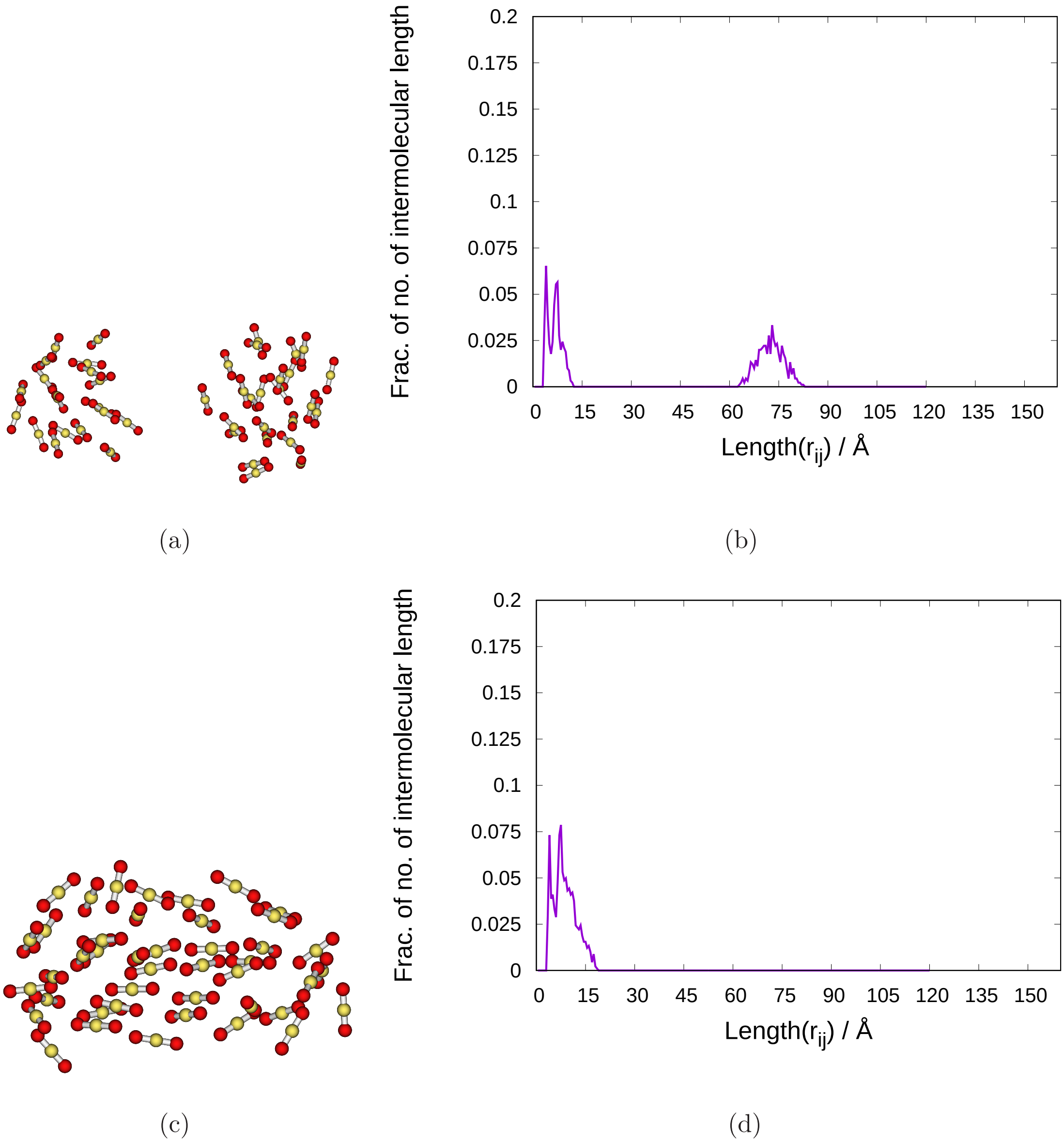


FIG. 37. Structures and fragment patterns for $n = 43$.

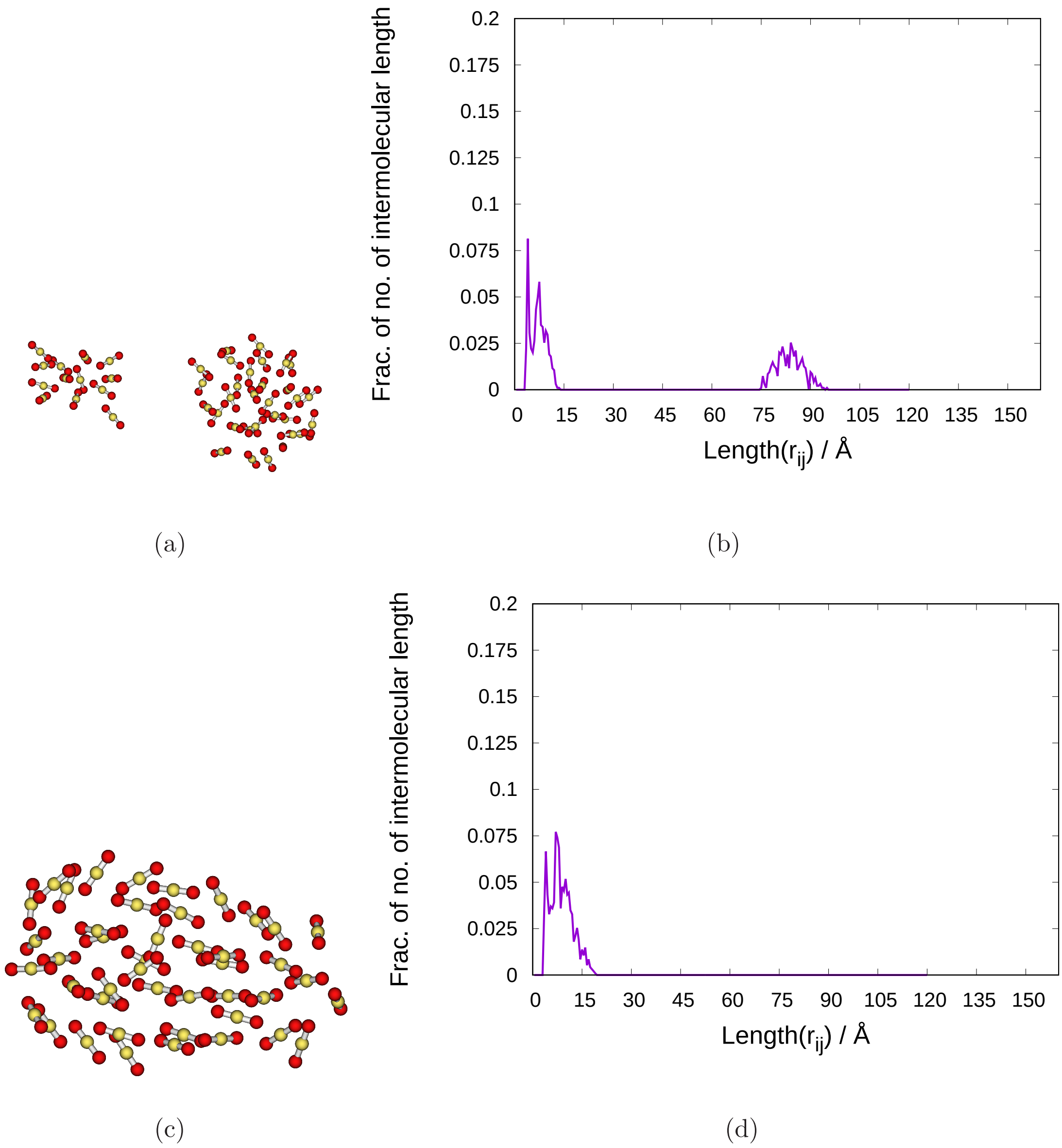


FIG. 38. Structures and fragment patterns for $n = 44$.

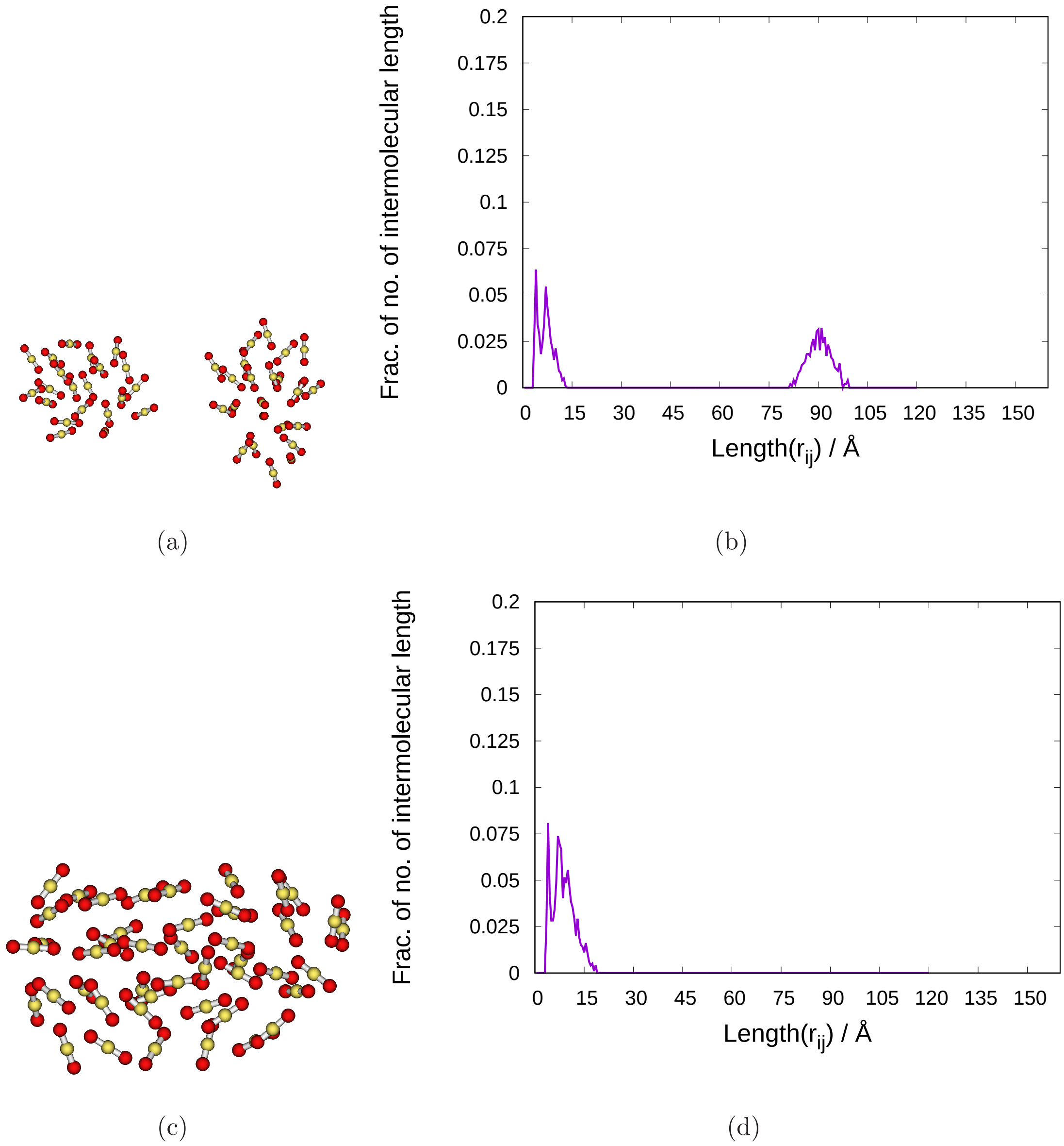
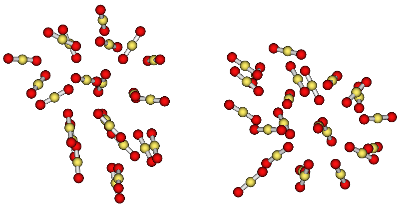
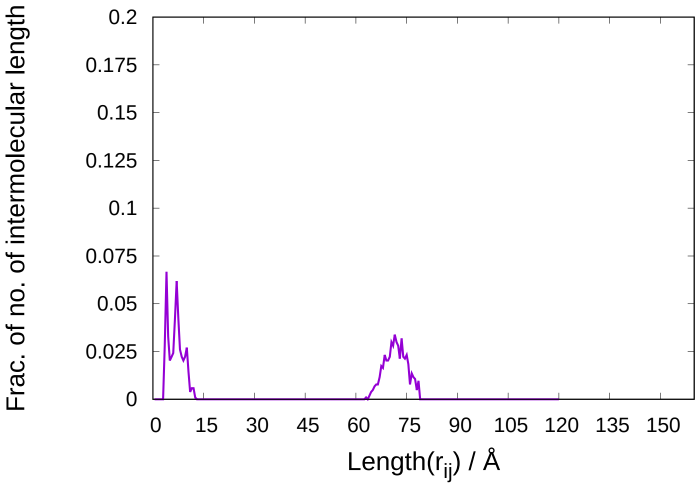


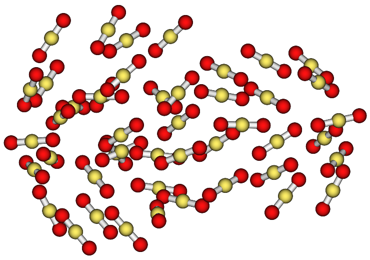
FIG. 39. Structures and fragment patterns for $n = 45$.



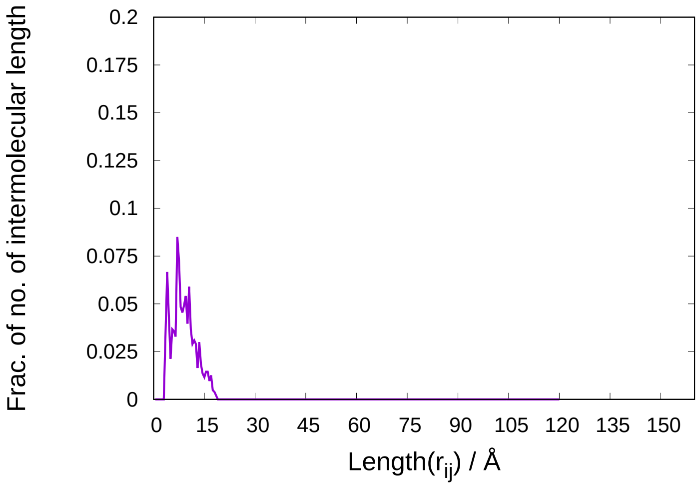
(a)



(b)

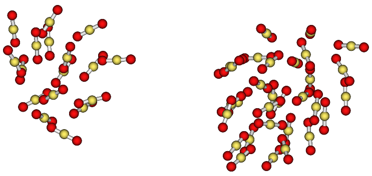


(c)

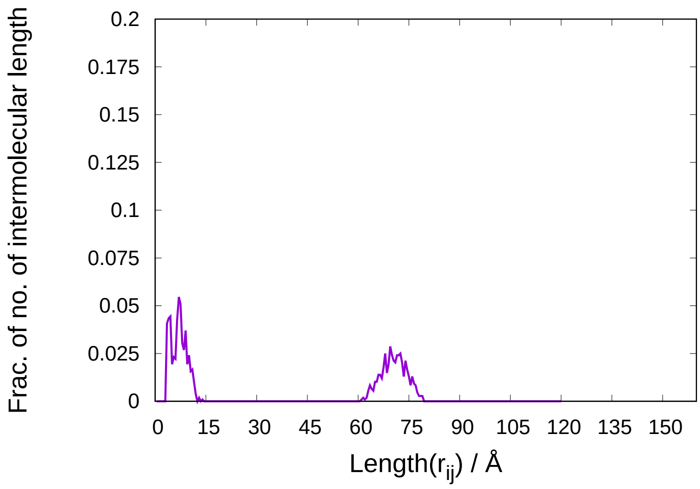


(d)

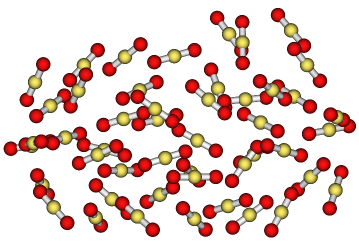
FIG. 40. Structures and fragment patterns for $n = 46$.



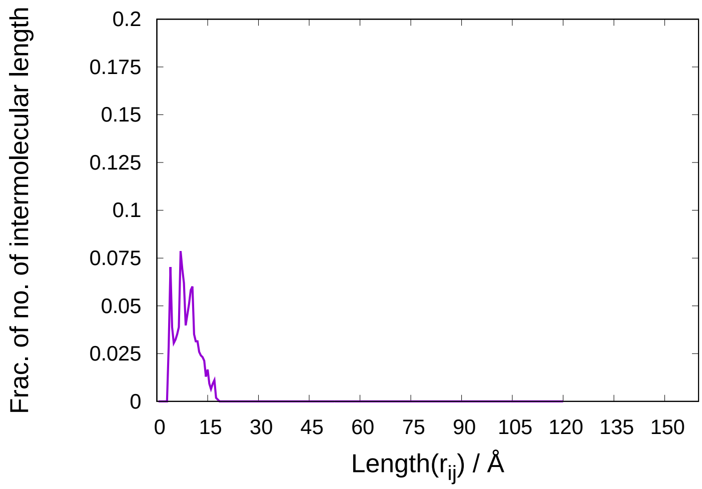
(a)



(b)



(c)



(d)

FIG. 41. Structures and fragment patterns for $n = 47$.

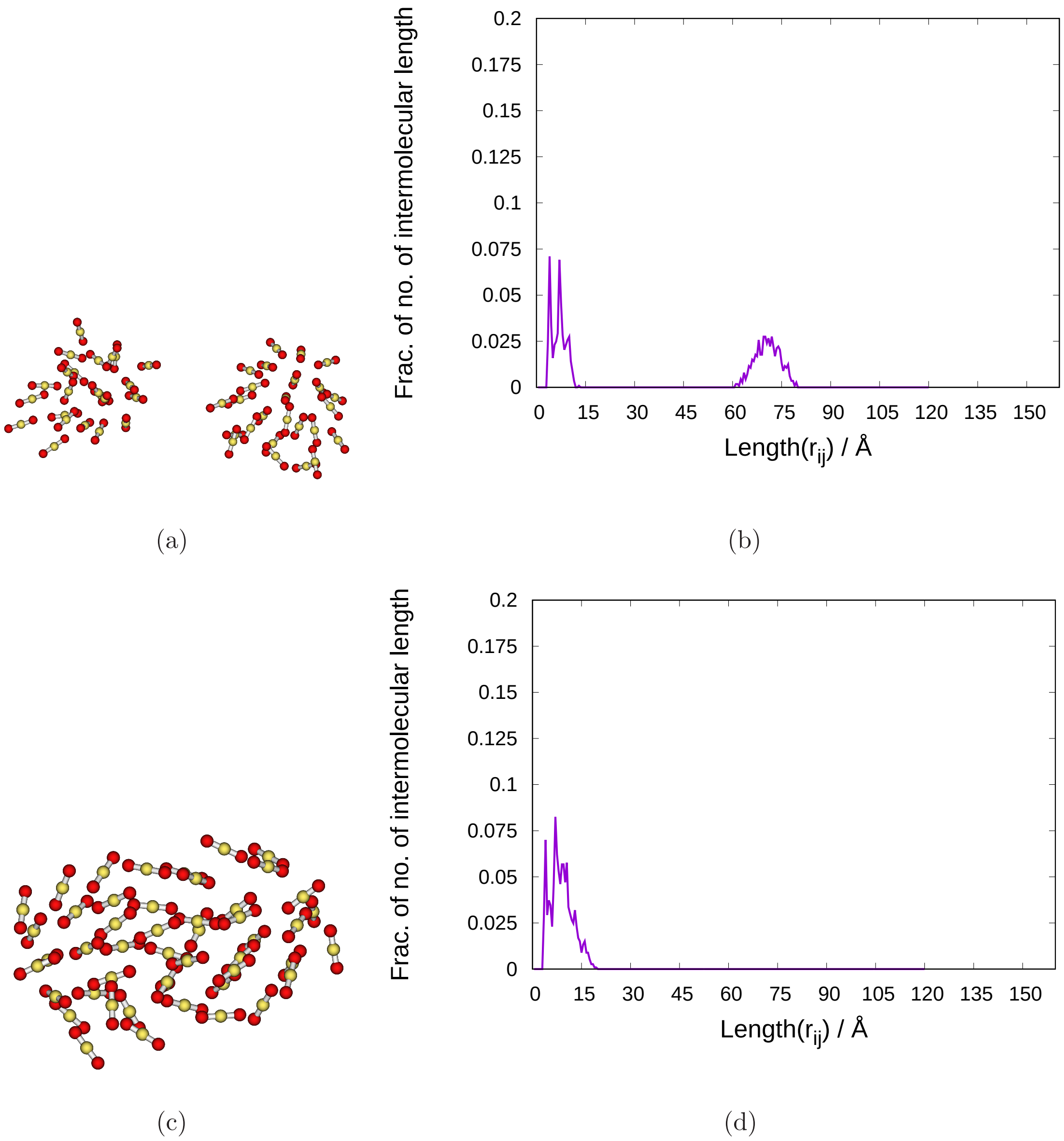
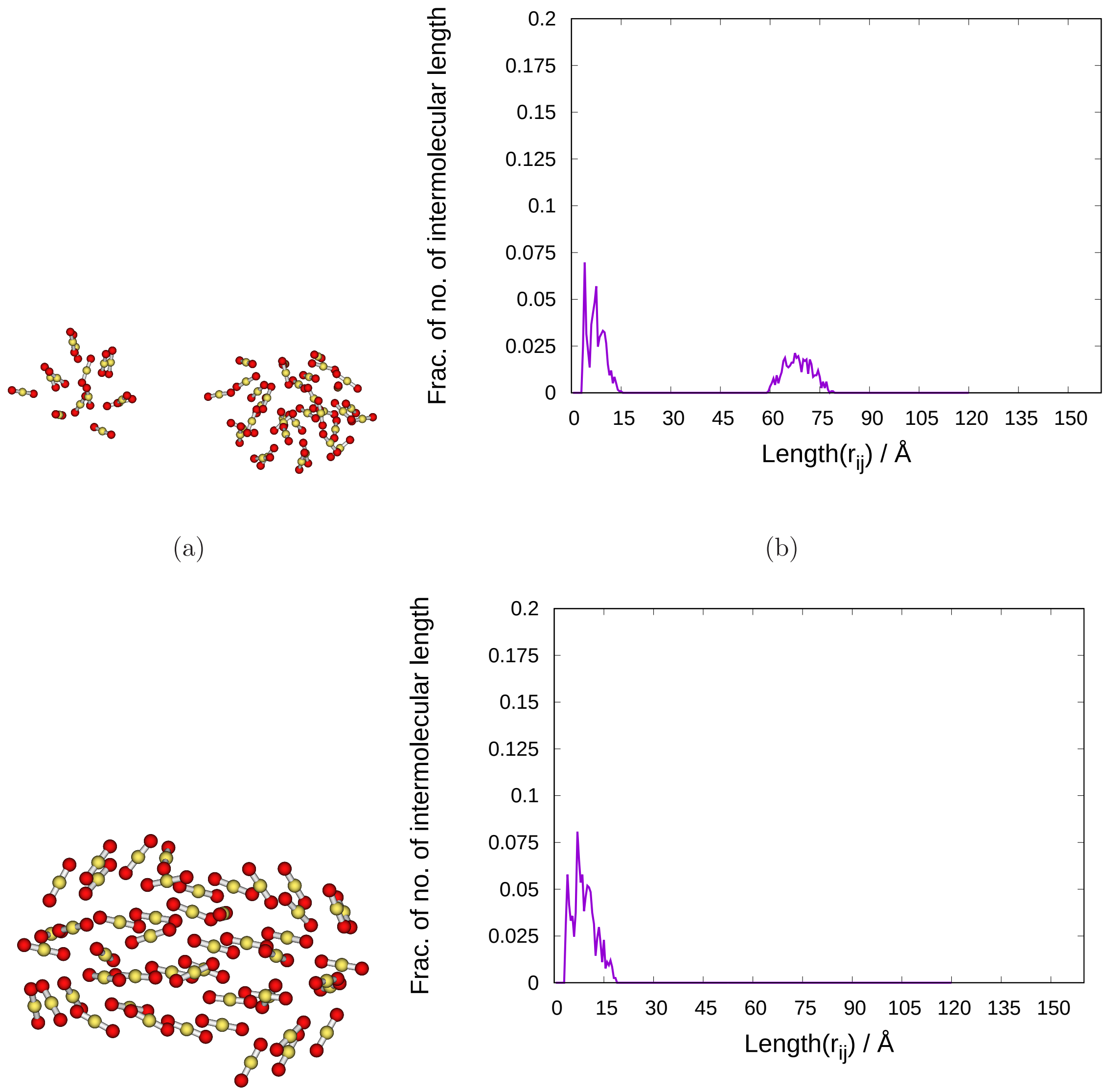


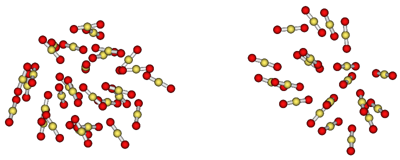
FIG. 42. Structures and fragment patterns for $n = 48$.



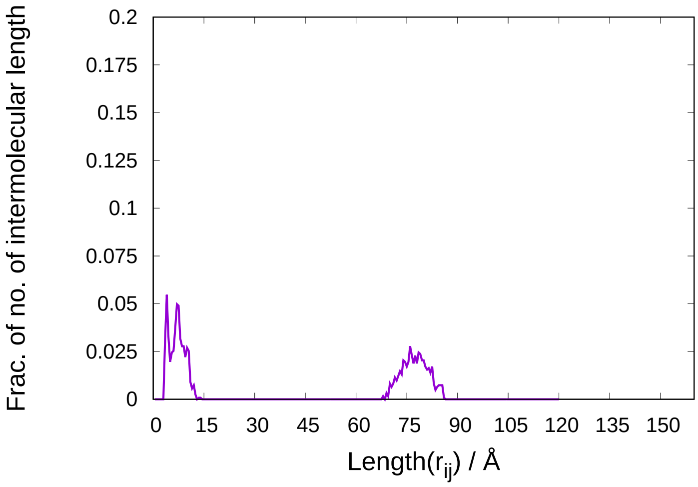
(a) (b)

(c) (d)

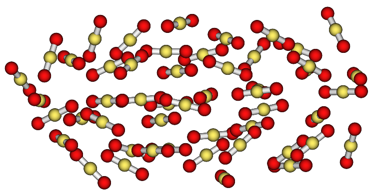
FIG. 43. Structures and fragment patterns for $n = 49$.



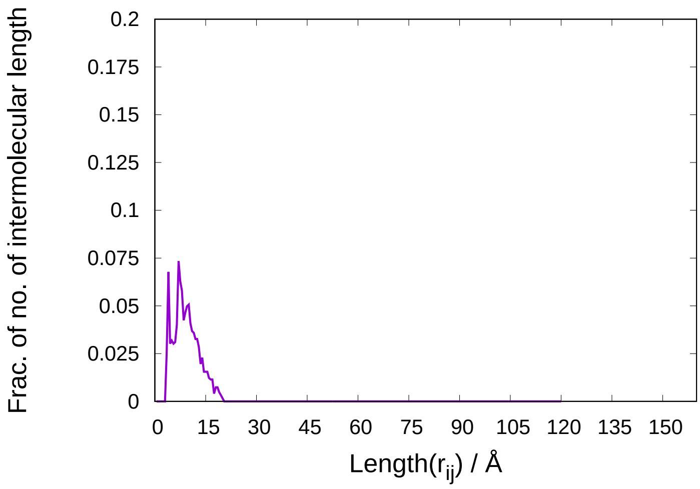
(a)



(b)

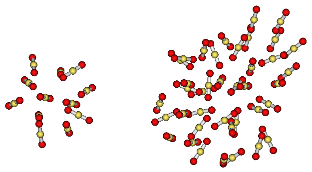


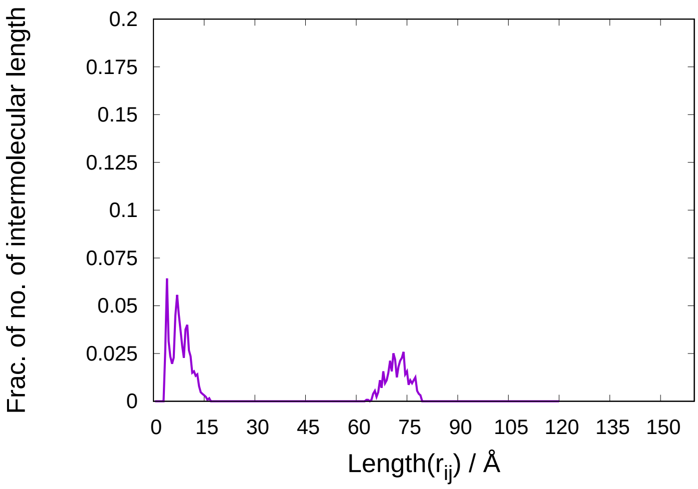
(c)



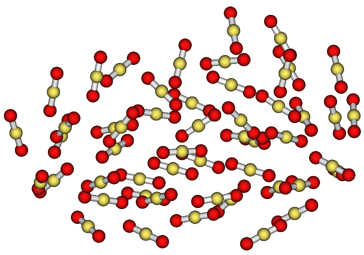
(d)

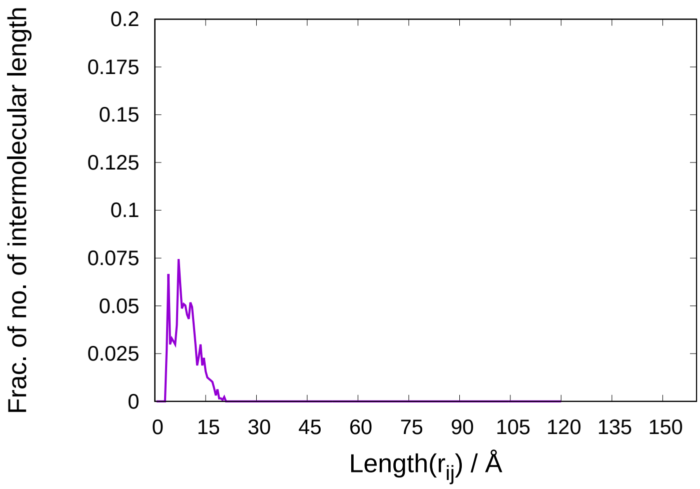
FIG. 44. Structures and fragment patterns for $n = 50$.





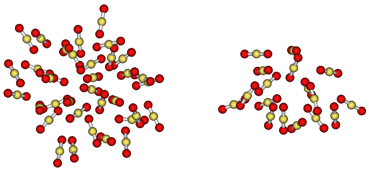
(a) (b)



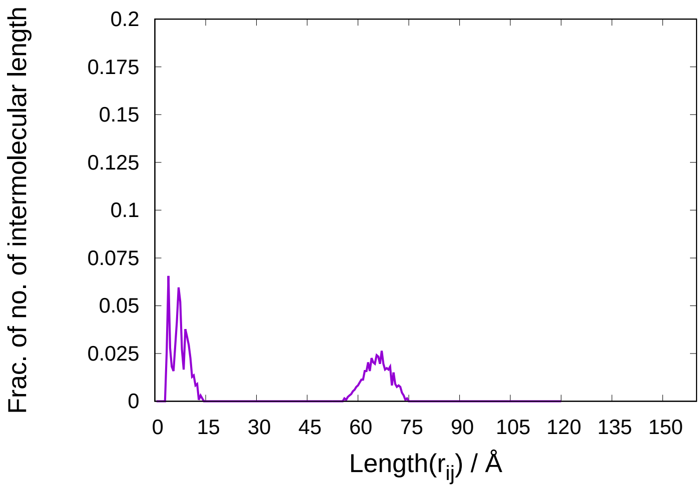


(c) (d)

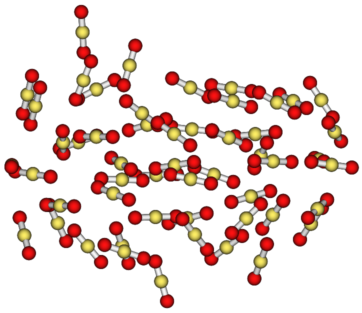
FIG. 45. Structures and fragment patterns for $n = 51$.



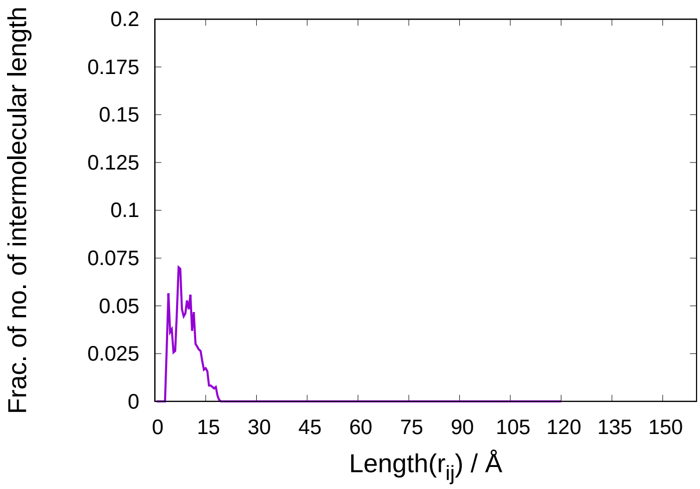
(a)



(b)



(c)



(d)

FIG. 46. Structures and fragment patterns for $n = 52$.

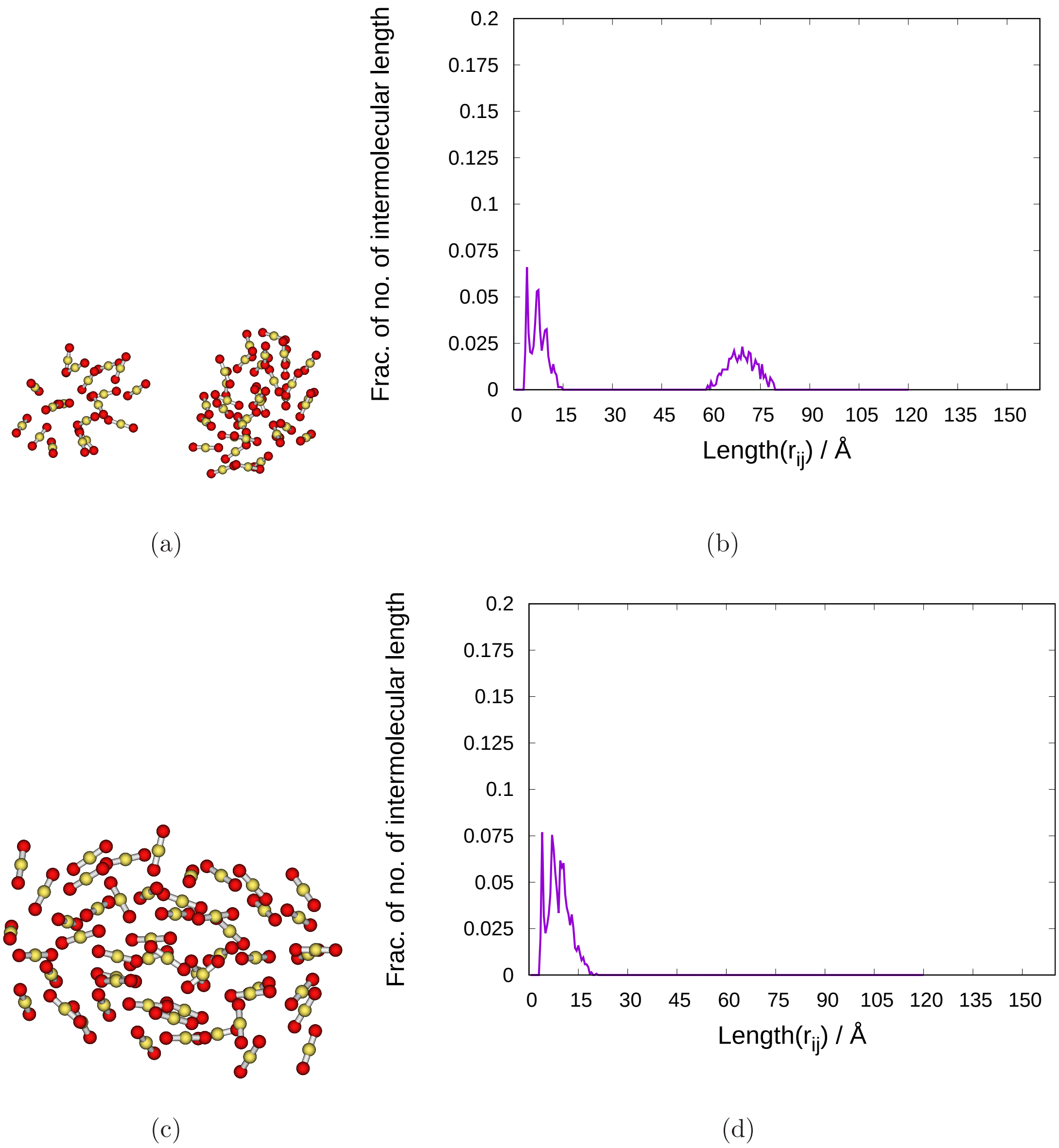
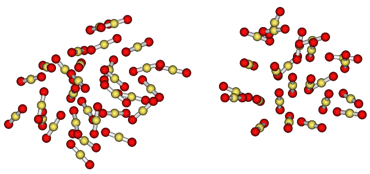
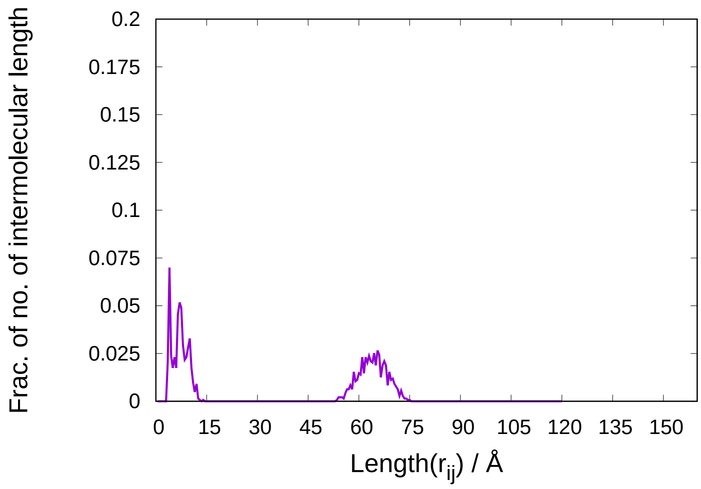
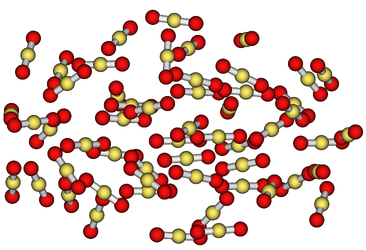


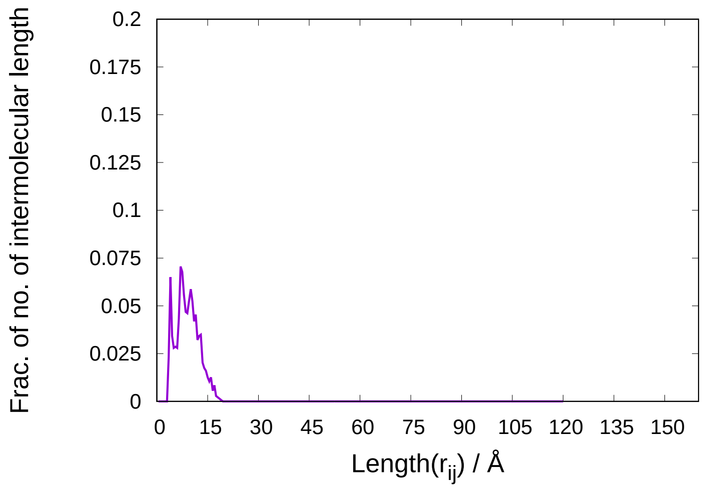
FIG. 47. Structures and fragment patterns for $n = 53$.





(a) (b)





(c) (d)

FIG. 48. Structures and fragment patterns for $n = 54$.

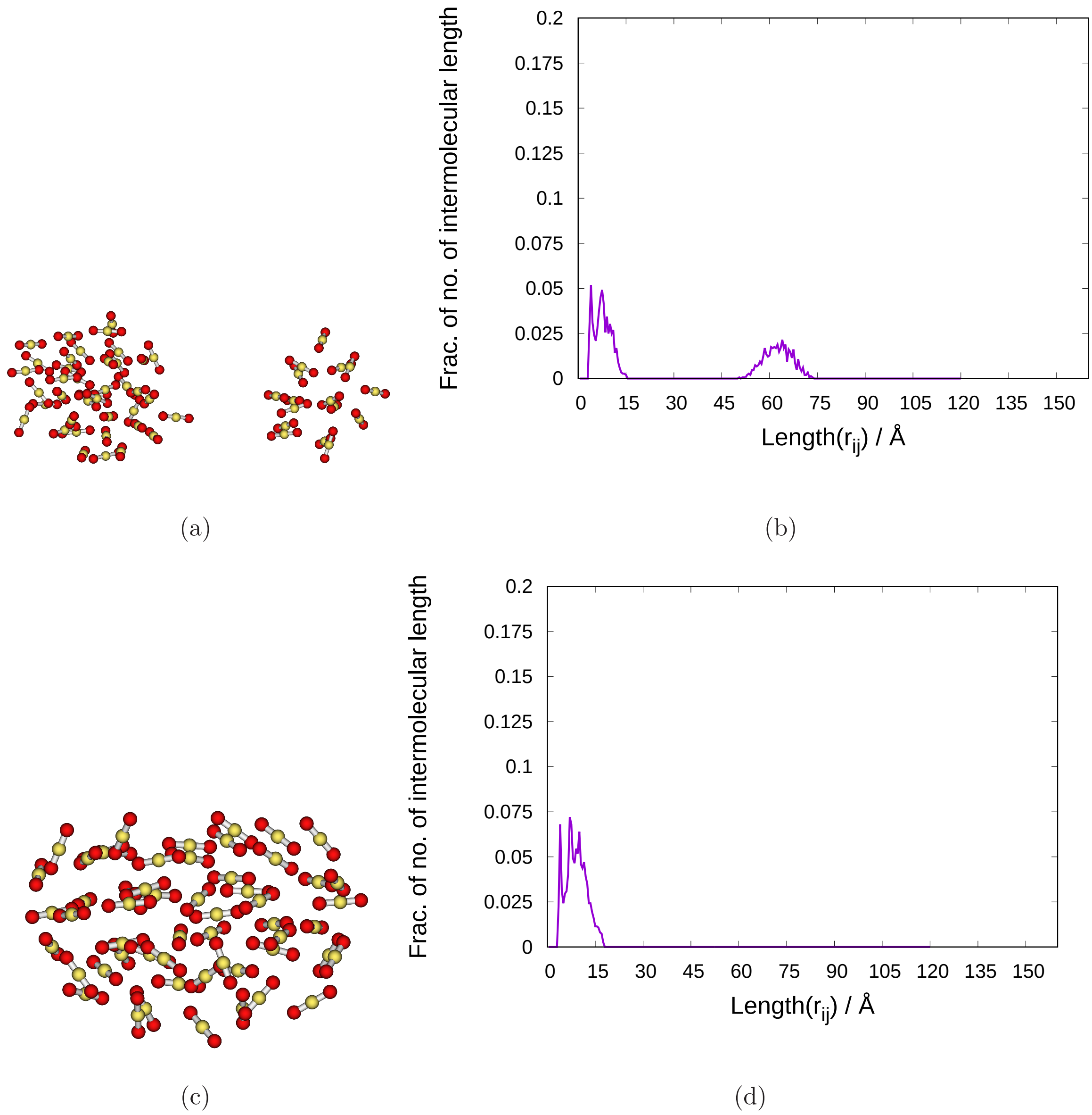
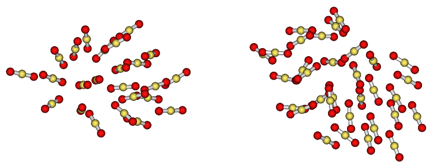
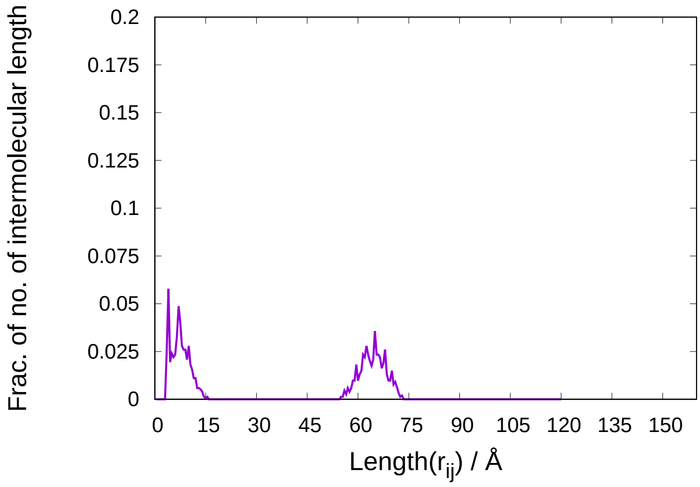


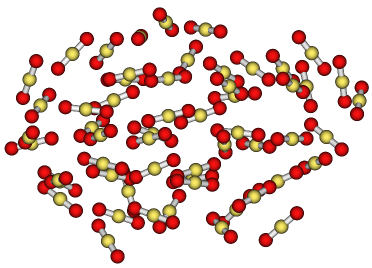
FIG. 49. Structures and fragment patterns for $n = 55$.



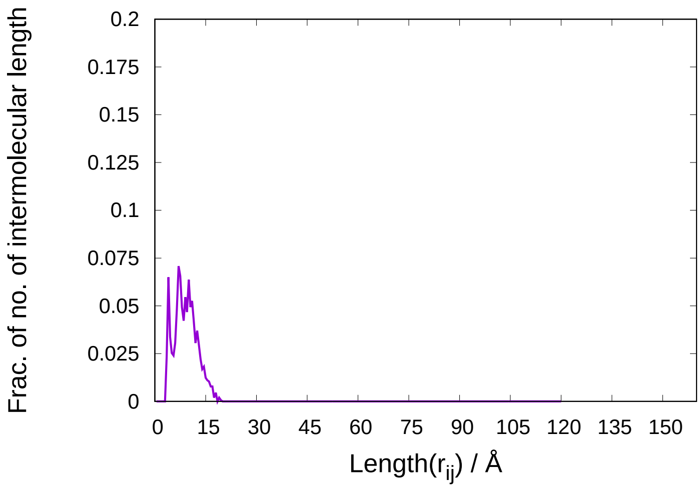
(a)



(b)



(c)



(d)

FIG. 50. Structures and fragment patterns for $n = 56$.

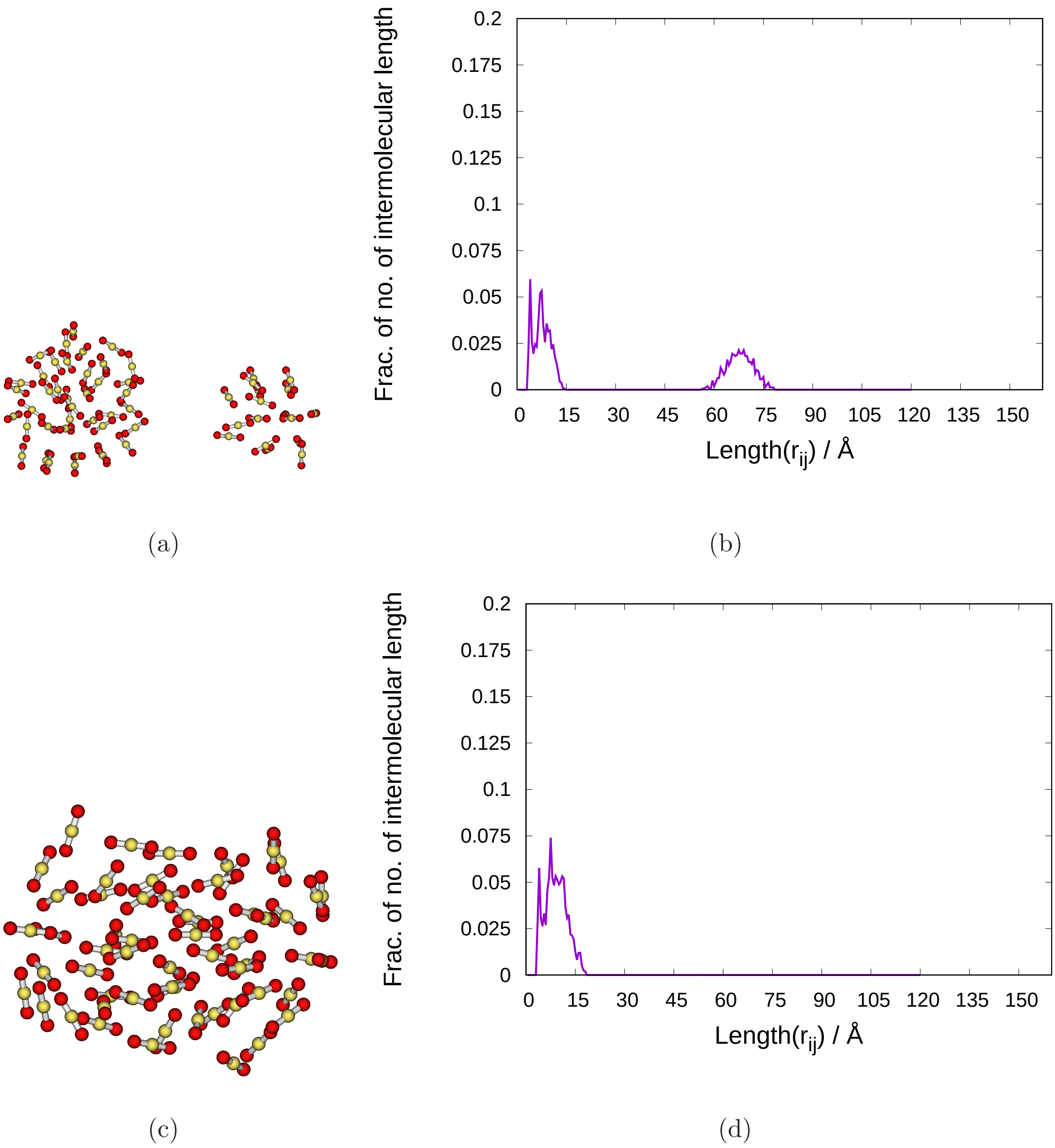
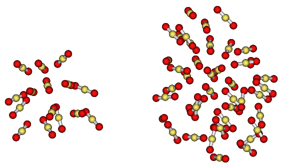
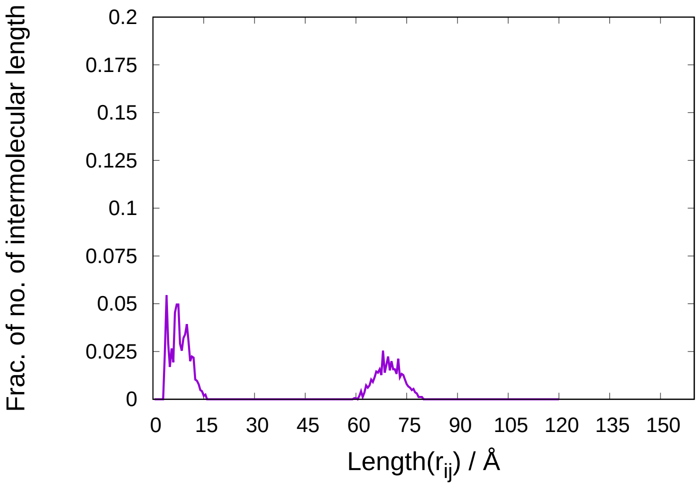


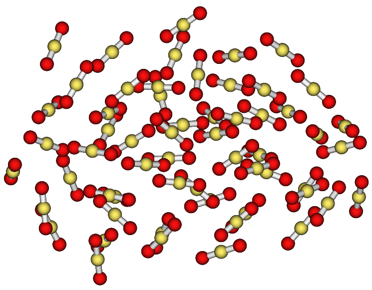
FIG. 51. Structures and fragment patterns for $n = 57$.



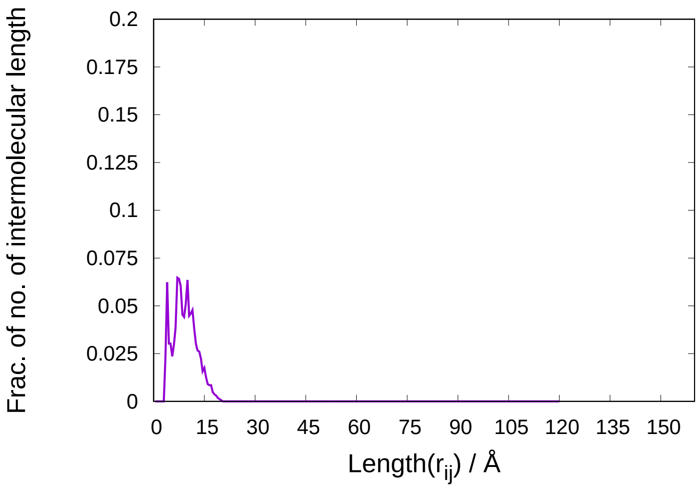
(a)



(b)

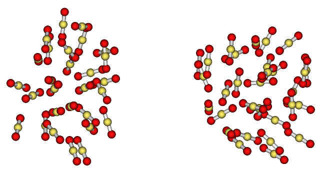


(c)

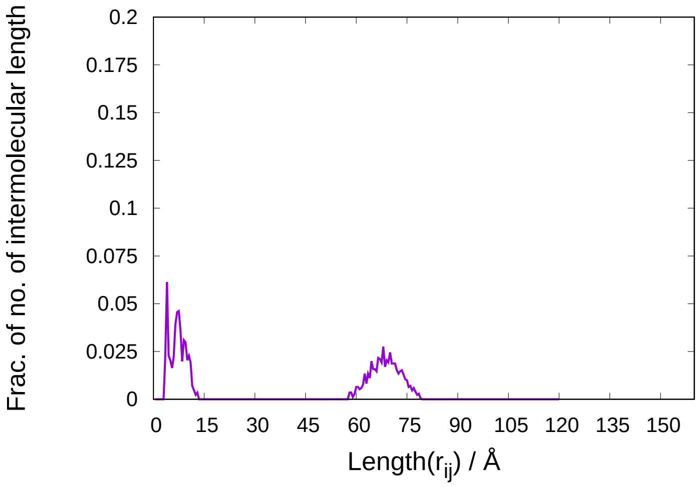


(d)

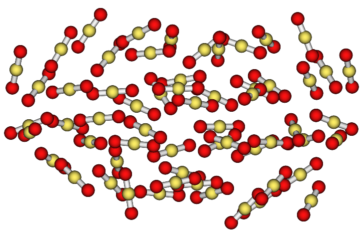
FIG. 52. Structures and fragment patterns for $n = 58$.



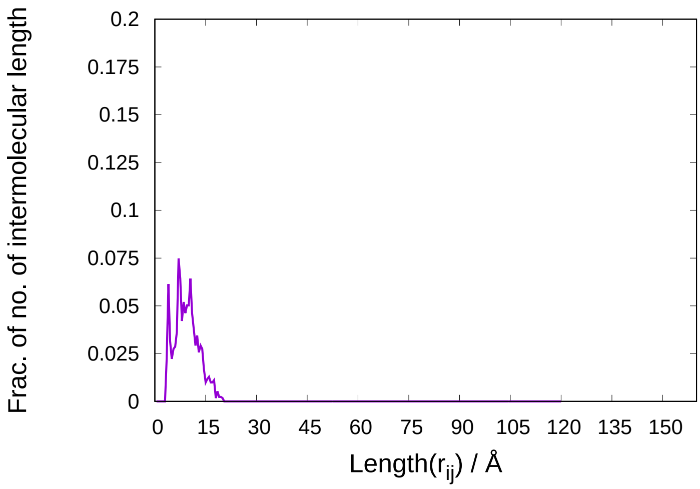
(a)



(b)

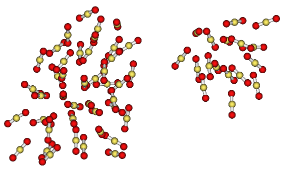


(c)

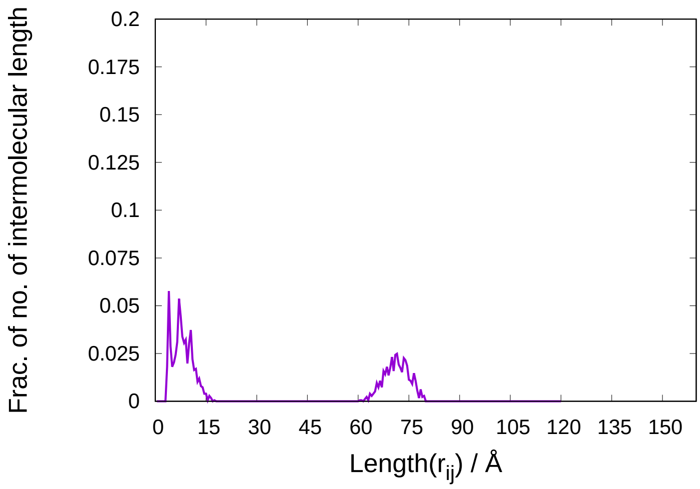


(d)

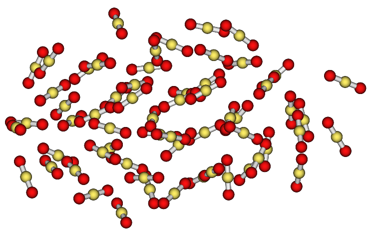
FIG. 53. Structures and fragment patterns for $n = 59$.



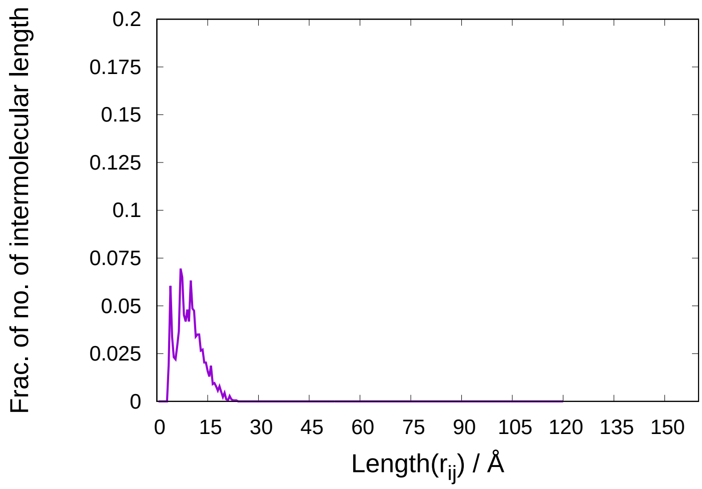
(a)



(b)



(c)



(d)

FIG. 54. Structures and fragment patterns for $n = 60$.

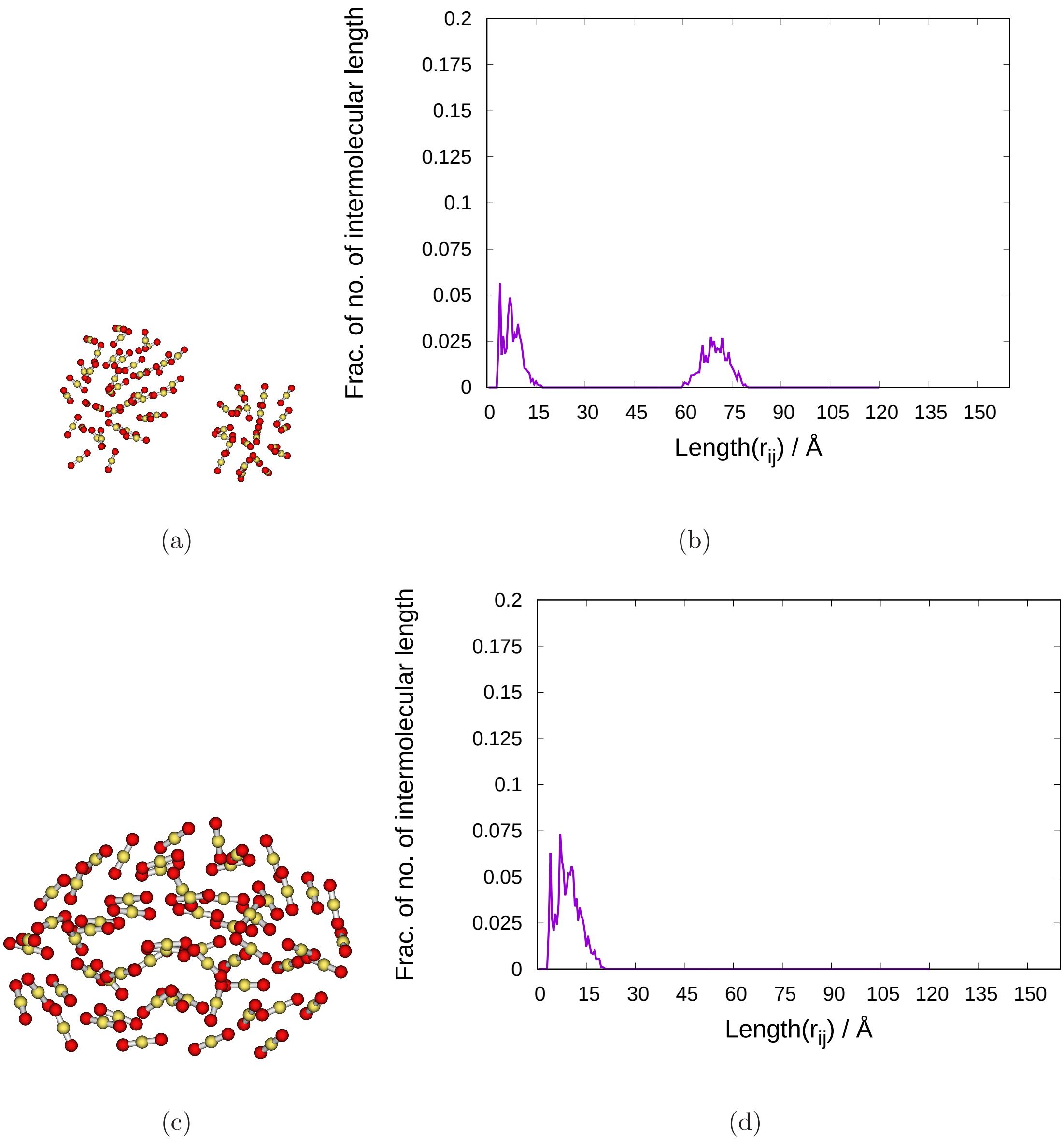


FIG. 55. Structures and fragment patterns for $n = 61$.

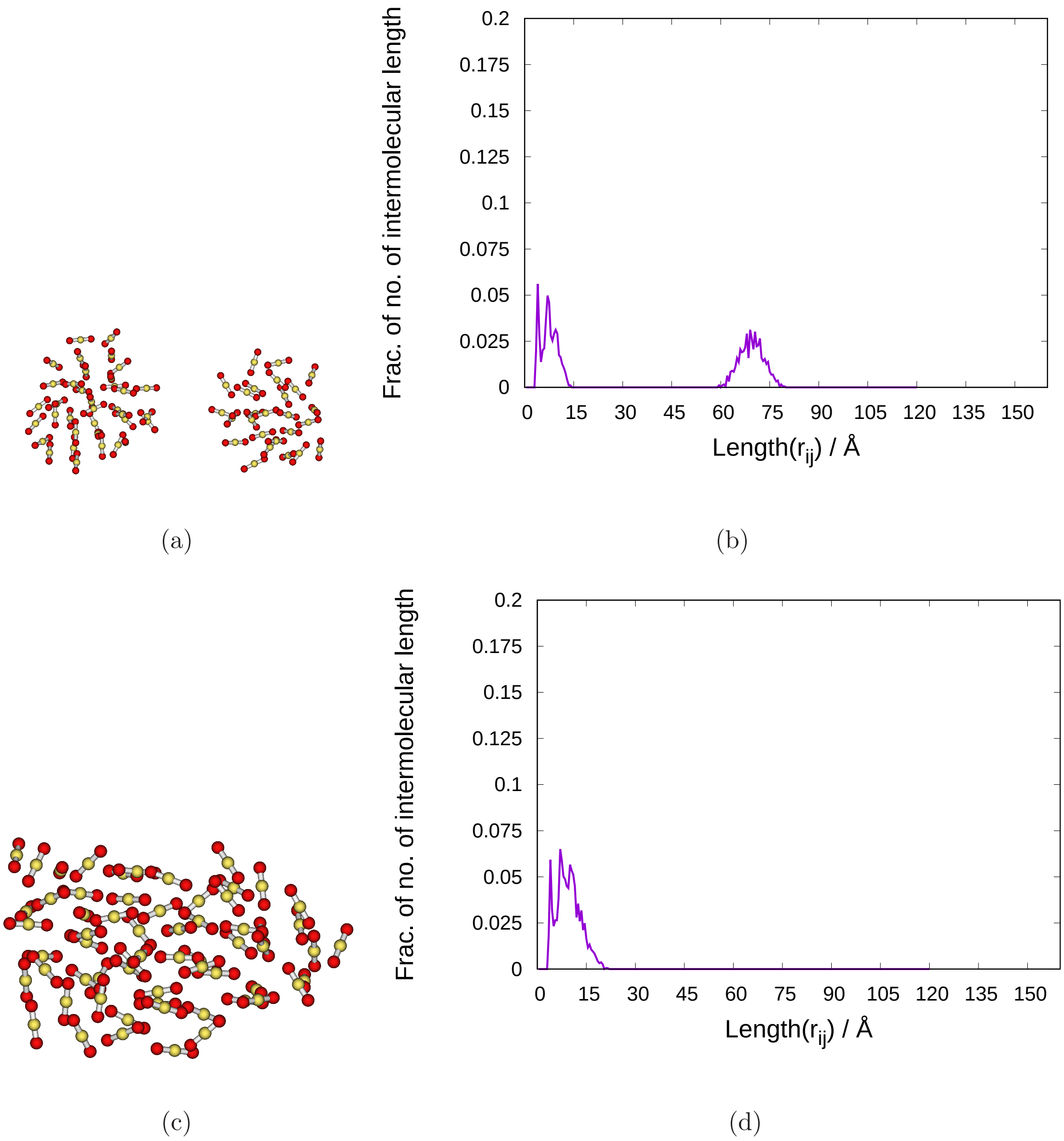
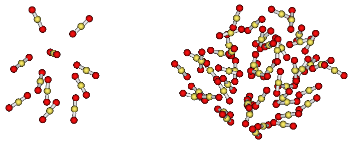
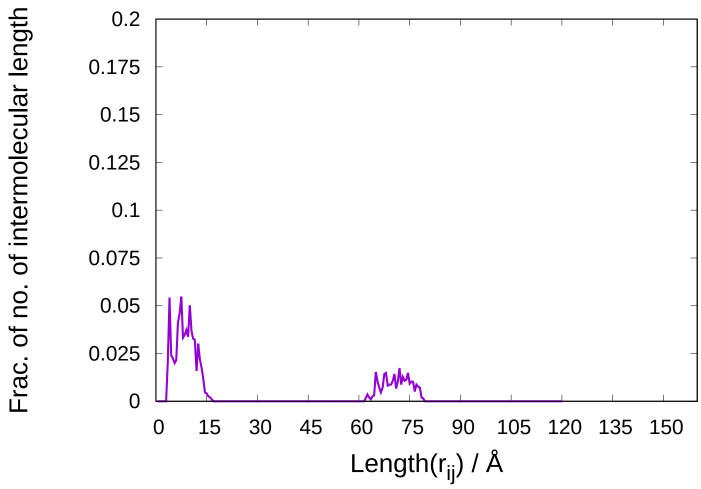


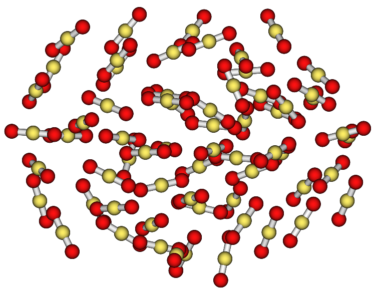
FIG. 56. Structures and fragment patterns for $n = 62$.



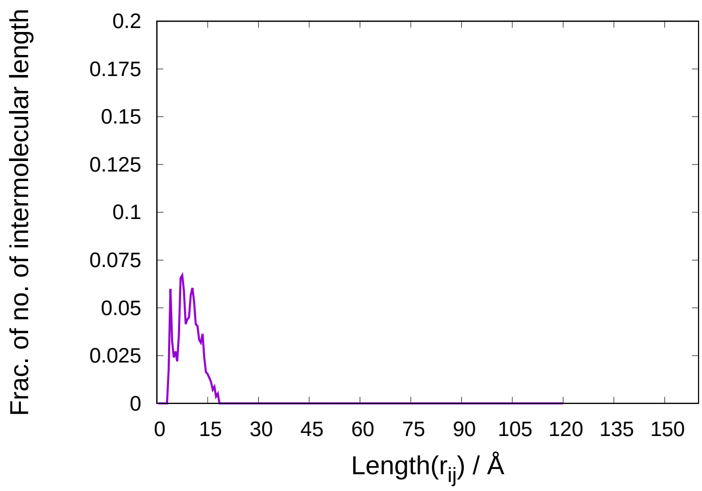
(a)



(b)



(c)



(d)

FIG. 57. Structures and fragment patterns for $n = 63$.

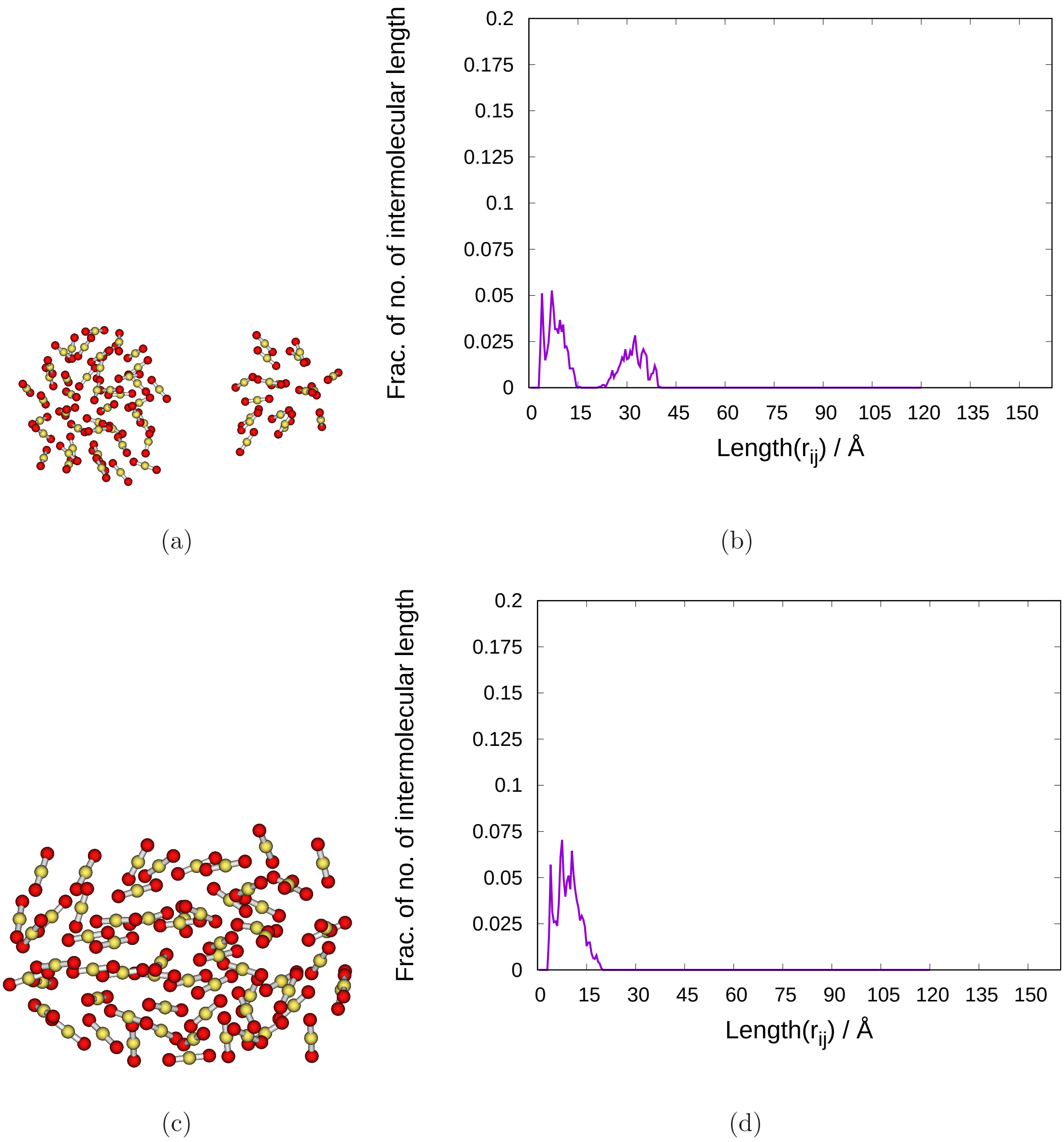


FIG. 58. Structures and fragment patterns for $n = 64$.

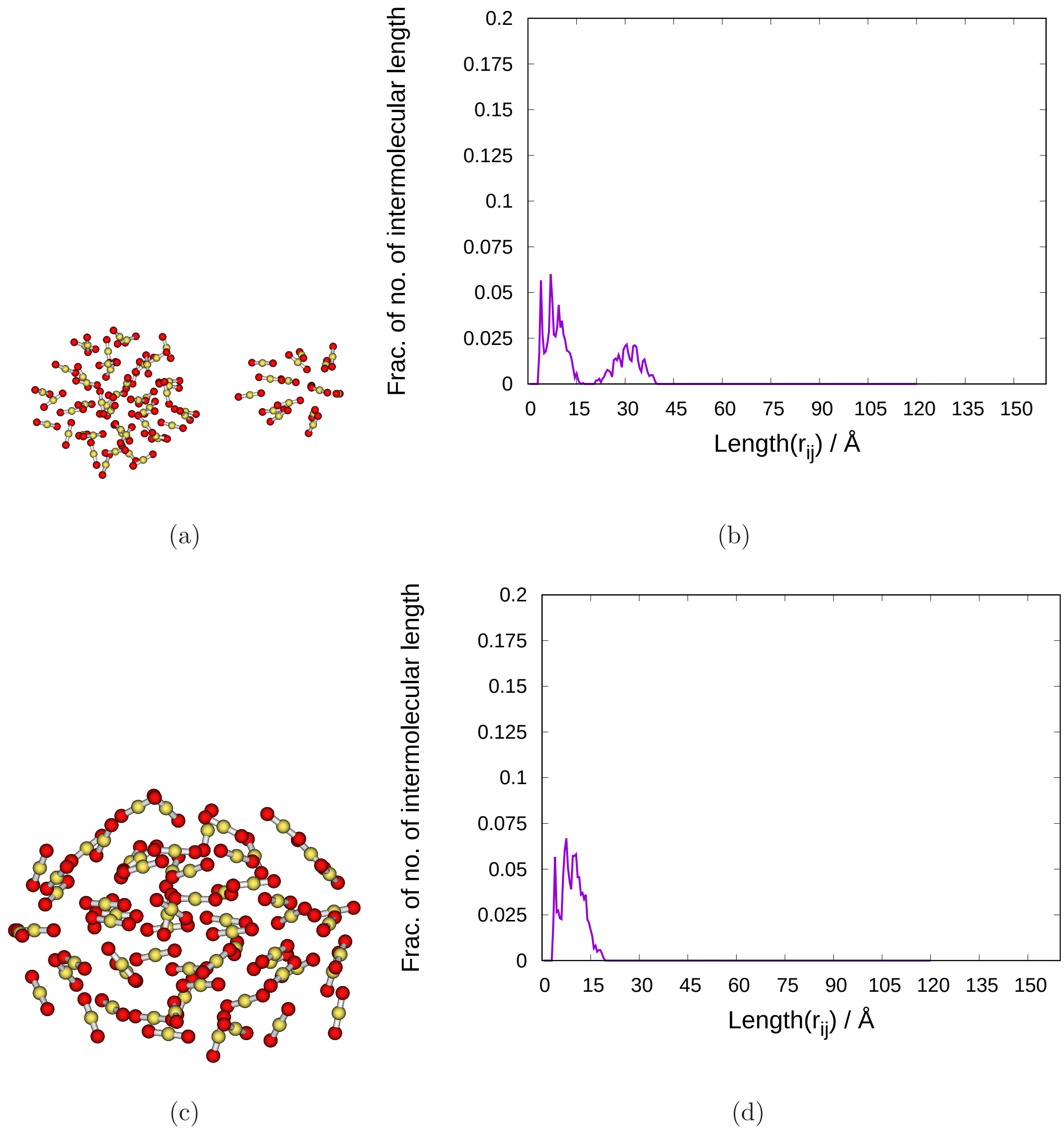
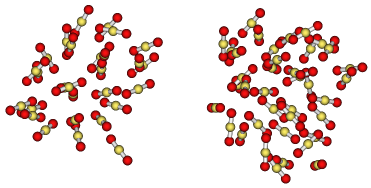
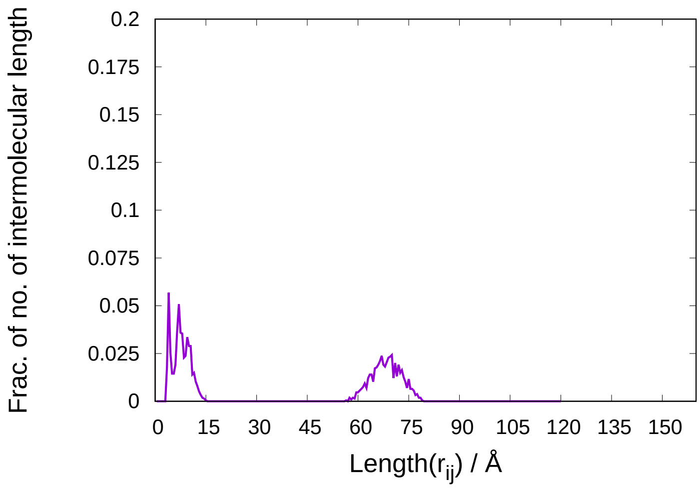


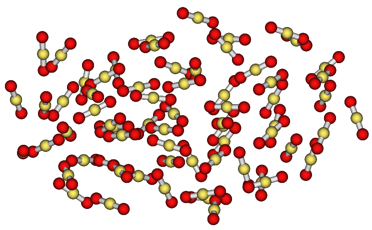
FIG. 59. Structures and fragment patterns for $n = 65$.



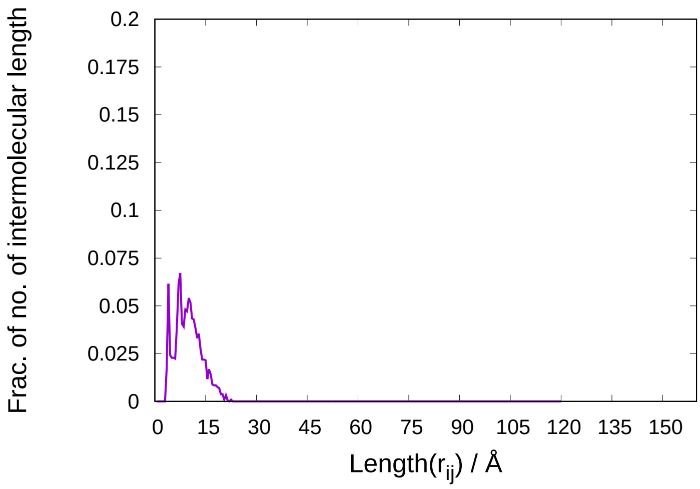
(a)



(b)



(c)



(d)

FIG. 60. Structures and fragment patterns for $n = 66$.

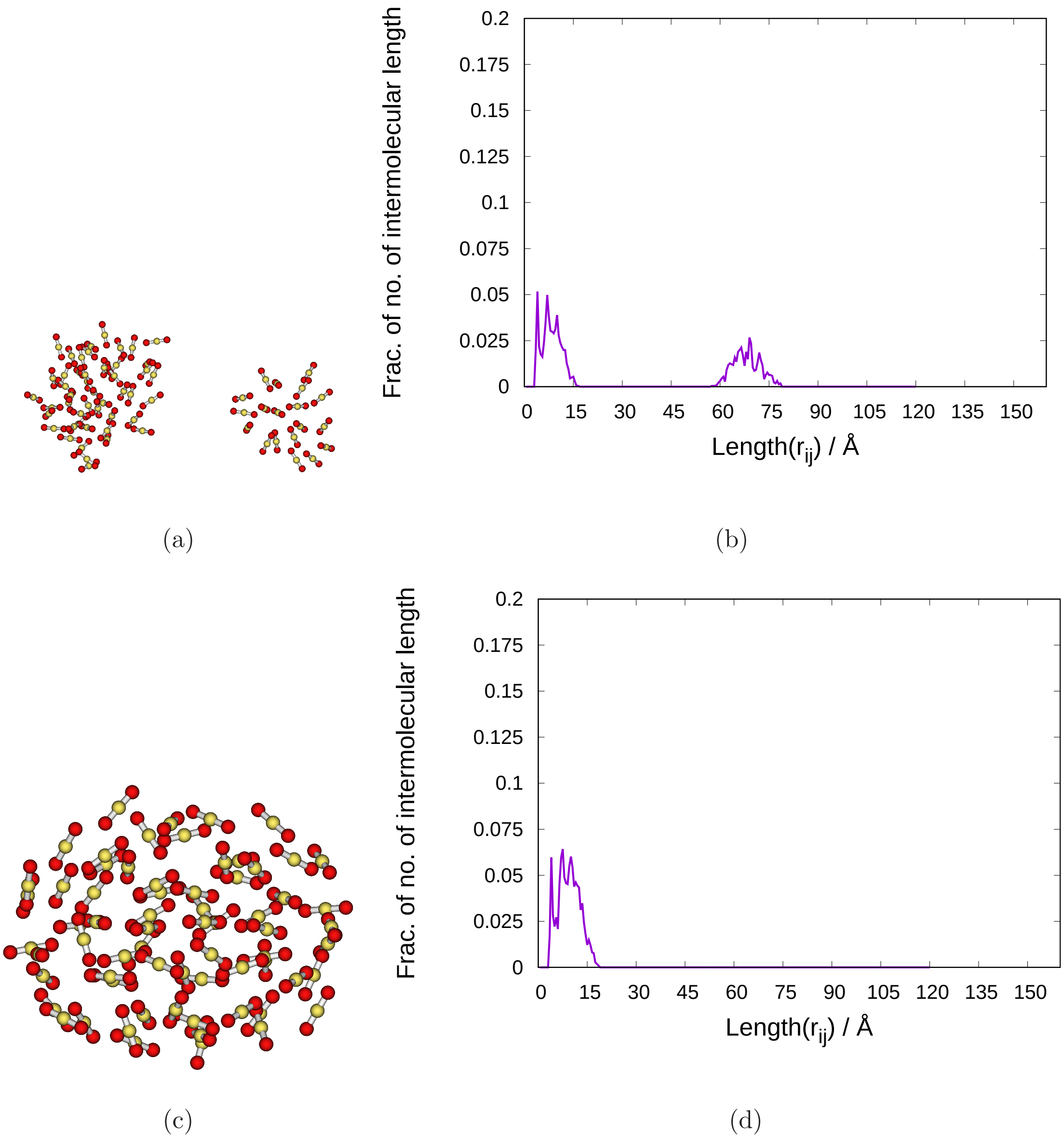
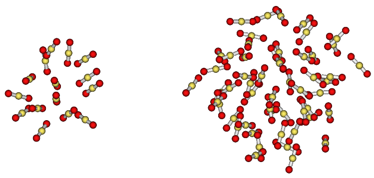
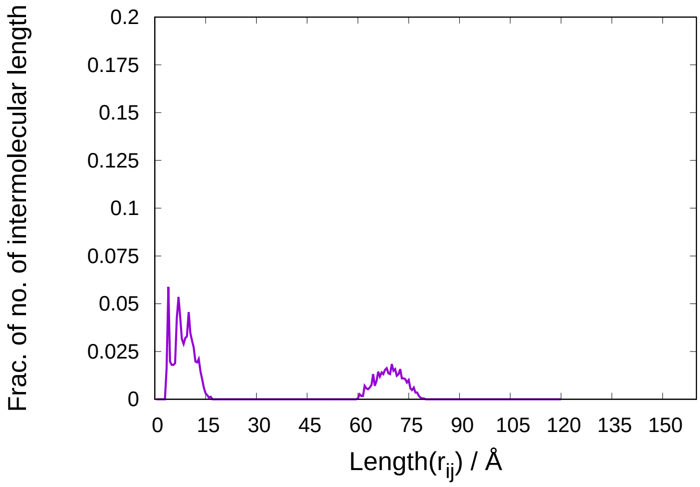


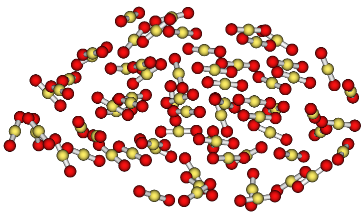
FIG. 61. Structures and fragment patterns for $n = 67$.



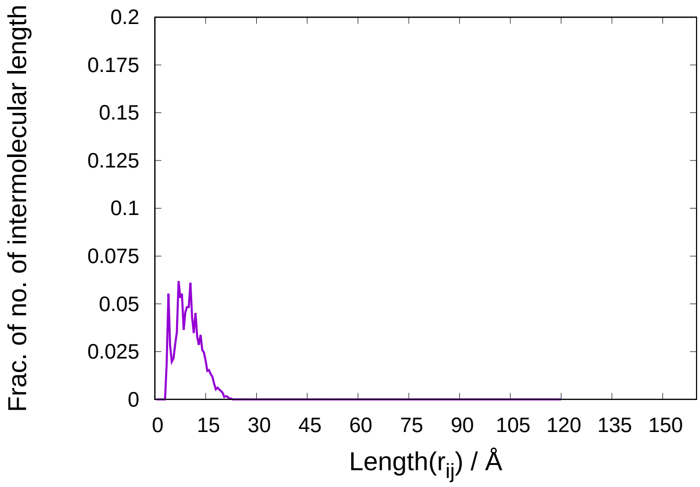
(a)



(b)



(c)



(d)

FIG. 62. Structures and fragment patterns for $n = 68$.

TABLES

TABLE I. Parameters used in empirical potential energy function for E_{LJ} part.

Interaction type	σ [Å]	ϵ [$kJ.mol^{-1}$]
$C-C$	2.82400	0.21867
$C-O$	2.92500	0.36999
$O-O$	3.02600	0.62524

TABLE II. Parameters used for neutral CO_2 molecule in empirical potential energy function for E_{Coul} part.

Site	Z[Å]	Q(e)
1	-1.5232	0.1216
2	-1.0663	-0.6418
3(C)	0.0	1.0404
4	1.0663	-0.6418
5	1.5232	0.1216

TABLE III. Charges found from Quantum Chemical Calculations at different levels.

	For CO_2 molecule	For CO_2^+ molecule
Atom	Charge (Mulliken)	Charge (Mulliken)
at	DFT(B3LYP)/6-311++G(3df,3pd)	level
O	-0.515	-0.100
C	+1.030	+1.200
O	-0.515	-0.100
at	DFT(ωB97xD)/6-311++G(3df,3pd)	level
O	-0.524	-0.153
C	+1.048	+1.306
O	-0.524	-0.153
at	DFT(MPW1PW91)/6-311++G(3df,3pd)	level
O	-0.573	-0.144
C	+1.146	+1.288
O	-0.573	-0.144
at	MP2/6-311++G(3df,3pd)	level
O	-0.640	-0.193
C	+1.280	+1.386
O	-0.640	-0.193

TABLE IV. Parameters used for two $(CO_2)^+$ molecules in empirical potential energy function for E_{Coul} part.

Site	Z[Å]	Q(e)
1	-1.5232	0.1216 + 0.25
2	-1.0663	-0.6418
3(C)	0.0	1.0404 + 0.50
4	1.0663	-0.6418
5	1.5232	0.1216 + 0.25

TABLE V. Parameters used in AMSA/SA.

Number of coordinates to be optimized	:	3 $\times$ Total no. of molecule
Number of Euler angles to be optimized	:	3 $\times$ Total no. of molecule
Initial AMSA/SA temperature	:	0.150
Cooling schedule after i^{th} step	:	$T_{i+1} = T_i \times 0.90$
Reheating schedule	:	70 steps
Reheating rate	:	$T_{new}^{initial} = T_{current}^{initial} \times 0.9990$
Number of Metropolis sampling at a particular T	:	$NOVER \times$ (3 $\times$ Total no. of molecule)
r_{mut}^{min},r_{mut}^{max} in AMSA	:	0.10,0.25
Initial mutation step for changing coordinates in AMSA	:	0.5
Initial mutation step for changing Euler angles in AMSA	:	40.0

TABLE VI. Cost values at different points of simulation for $NOVER = 100$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.48343	0.48587
140	1.04325	0.47093	0.47525
210	1.04221	0.47093	1.20017
280	1.04117	0.47093	1.36721
350	1.04103	0.38036	0.39006
420	1.03909	0.38036	0.48551
490	1.03805	0.38036	1.01619
560	1.03701	0.38036	0.91902
630	1.03597	0.38036	0.59553
700	1.03494	0.38036	1.33089
770	1.03390	0.38036	0.64341
840	1.03287	0.38036	1.46443
910	1.03184	0.38036	0.78841
980	1.03080	0.38036	0.72207
1050	1.02977	0.38036	0.60360
1120	1.02874	0.38036	1.11512
1190	1.02771	0.38036	0.69058

TABLE VII. Cost values at different points of simulation for $NOVER = 500$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.38521	0.44768
140	1.04325	0.38457	0.79743
210	1.04221	0.38457	0.49375
280	1.04117	0.38457	0.42578
350	1.04103	0.20514	0.21315
420	1.03909	0.20514	0.60731
490	1.03805	0.20514	0.38778
560	1.03701	0.20514	0.53704
630	1.03597	0.20514	0.40173
700	1.03494	0.20514	0.32664
770	1.03390	0.20514	0.41538
840	1.03287	0.20514	0.41020
910	1.03184	0.20514	0.42931
980	1.03080	0.20514	0.45582
1050	1.02977	0.20514	0.49306
1120	1.02874	0.20514	0.52262
1190	1.02771	0.20514	0.32870

TABLE VIII. Cost values at different points of simulation for $NOVER = 1000$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.30858	0.31167
140	1.04325	0.30858	0.53878
210	1.04221	0.30858	0.36518
280	1.04117	0.30858	0.32088
350	1.04013	0.30858	0.33312
420	1.03909	0.30858	0.37217
490	1.03805	0.30858	0.36169
560	1.03701	0.15792	0.16224
630	1.03597	0.15792	0.53366
700	1.03494	0.15792	0.55790
770	1.03390	0.15792	0.41420
840	1.03287	0.15792	0.80074
910	1.03184	0.15792	0.23296
980	1.03080	0.15792	0.49966
1050	1.02977	0.15792	0.18210
1120	1.02874	0.15792	0.46452
1190	1.02771	0.15792	0.79198

TABLE IX. Cost values at different points of simulation for $NOVER = 1500$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.35094	0.35510
140	1.04325	0.35094	0.38086
210	1.04221	0.22788	0.23500
280	1.04117	0.16496	0.16954
350	1.04103	0.10367	0.10904
420	1.03909	0.10367	0.46486
490	1.03805	0.08623	0.09167
560	1.03701	0.08623	0.10531
630	1.03597	0.08623	0.46806
700	1.03494	0.08623	0.22454
770	1.03390	0.08623	0.37146
840	1.03287	0.08623	0.16550
910	1.03184	0.08623	0.26846
980	1.03080	0.08623	0.20649
1050	1.02977	0.08623	0.33046
1120	1.02874	0.08623	0.24377
1190	1.02771	0.08623	0.36384

TABLE X. Cost values at different points of simulation for $NOVER = 2000$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.22908	0.23306
140	1.04325	0.22908	0.48207
210	1.04221	0.22908	0.49227
280	1.04117	0.22908	0.26172
350	1.04013	0.16942	0.17316
420	1.03909	0.16942	0.22353
490	1.03805	0.13765	0.14278
560	1.03701	0.13765	0.34043
630	1.03597	0.13765	0.34300
700	1.03494	0.13765	0.24835
770	1.03390	0.13765	0.47998
840	1.03287	0.10403	0.10841
910	1.03184	0.10403	0.26535
980	1.03080	0.10403	0.41504
1050	1.02977	0.10403	0.38843
1120	1.02874	0.10403	0.19457
1190	1.02771	0.10403	0.13594

TABLE XI. Cost values at different points of simulation for $NOVER = 5000$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.18793	0.19154
140	1.04325	0.08839	0.09199
210	1.04221	0.07763	0.08087
280	1.04117	0.07763	0.37537
350	1.04013	0.07763	0.15777
420	1.03909	0.07763	0.20982
490	1.03805	0.07385	0.07845
560	1.03701	0.07385	0.22313
630	1.03597	0.07385	0.15449
700	1.03494	0.07163	0.07742
770	1.03390	0.03877	0.04789
840	1.03287	0.00512	0.00849
910	1.03184	0.00512	0.35362
980	1.03080	0.00512	0.09466
1050	1.02977	0.00512	0.08018
1120	1.02874	0.00512	0.14387
1190	1.02771	0.00512	0.09009

TABLE XII. Cost values at different points of simulation for $NOVER = 7000$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.08737	0.09117
140	1.04325	0.08737	0.17828
210	1.04221	0.08737	0.12161
280	1.04117	0.08737	0.18650
350	1.04013	0.00685	0.01057
420	1.03909	0.00685	0.14763
490	1.03805	0.00685	0.39916
560	1.03701	0.00685	0.32401
630	1.03597	0.00685	0.14981
700	1.03494	0.00685	0.15880
770	1.03390	0.00685	0.19332
840	1.03287	0.00685	0.34095
910	1.03184	0.00685	0.04590
980	1.03080	0.00685	0.08342
1050	1.02977	0.00685	0.18409
1120	1.02874	0.00685	0.08923
1190	1.02771	0.00685	0.09656

TABLE XIII. Cost values at different points of simulation for $NOVER = 10000$ in AMSA ($< Cost >$s are given in $(kJ/mol)^2$).

Step	$Temp. \times 10^4$	$< Cost >_{global\ best}$	$< Cost >_{local\ best}$
70	1.04430	0.00324	0.00710
140	1.04325	0.00324	0.27407
210	1.04221	0.00324	0.09972
280	1.04117	0.00324	0.21870
350	1.04013	0.00324	0.39814
420	1.03909	0.00324	0.34161
490	1.03805	0.00324	0.20581
560	1.03701	0.00324	0.07954
630	1.03597	0.00324	0.03212
700	1.03494	0.00324	0.14591
770	1.03390	0.00324	0.08494
840	1.03287	0.00324	0.02016
910	1.03184	0.00324	0.11874
980	1.03080	0.00324	0.39141
1050	1.02977	0.00324	0.15989
1120	1.02874	0.00324	0.10287
1190	1.02771	0.00324	0.40275

TABLE XIV. Critical analysis of results obtained by AMSA/SA for $n = 43$ [energies are given in kJ/mol and $< Cost >$s are given in $(kJ/mol)^2$].

Fig. No.	Total no. AMSA/SA steps	$NOVER$	Metropolis Test at a particular T [$= NOVER \times (3 \times n)$]	$< Cost >_{best}$ in AMSA	$-E_{best}$ in AMSA	AMSA steps required to reach best solution	$< Cost >_{best}$ in SA	$-E_{best}$ in SA	SA steps required to reach best solution
2(a) & 2(g)	1200	100	12900	0.38036	-714.23296	350	0.75639	-665.72532	1190
3(a) & 3(g)	1200	500	64500	0.20514	-736.83633	350	0.43929	-706.63083	1188
4(a) & 4(g)	1200	1000	129000	0.15792	-742.92883	560	0.31487	-722.68150	1190
5(a) & 5(g)	1200	1500	193500	0.08623	-752.17536	490	0.30244	-724.28416	1190
6(a) & 6(g)	1200	2000	258000	0.10403	-749.87992	840	0.16873	-741.53293	1186
7(a) & 7(g)	1200	5000	645000	0.00512	-767.45524	840	0.30992	-723.31925	1178
8(a) & 8(g)	1200	7000	903000	0.00685	-768.11578	350	0.00617	-755.33615	1191
9(a) & 9(g)	1200	10000	1290000	0.00324	- 768.58213	70	0.26766	-728.77170	1186
10(a) & 10(g)	5000	2000	258000	0.00765	-758.23877	3710	0.24731	-731.39627	4898
11(a) & 11(g)	3300	5000	645000	0.00346	-764.52849	140	0.00617	-747.89913	3281
12(a) & 12(g)	5000	5000	645000	0.00555	-768.28380	4970	0.11870	-747.98752	4967

TABLE XV. Energies for all sizes in (KJ/mol)[$d = E_{One\ Unit} - E_{Splitted}$]

Size (n)	Splitted	One Unit	d	Size (n)	Splitted	One Unit	d
20	-324.72022	-291.15004	33.57018	45	-789.34037	-801.67536	-12.33499
21	-344.45872	-311.69767	32.76105	46	-811.10347	-825.11902	-14.01555
22	-364.35030	-331.86870	32.48160	47	-822.70783	-846.94397	-24.23614
23	-381.15093	-353.86007	27.29086	48	-848.45750	-867.90360	-19.44610
24	-398.04086	-374.87096	23.16990	49	-869.87163	-893.32635	-23.45472
25	-416.83526	-393.72001	23.11526	50	-875.85333	-892.37570	-16.52237
26	-436.43333	-412.37624	24.05709	51	-902.95821	-931.42583	-28.46763
27	-458.18277	-435.86701	22.31576	52	-922.14885	-934.12258	-11.97373
28	-478.59370	-458.04241	20.55129	53	-938.67257	-965.59451	-26.92194
29	-493.65937	-475.18916	18.47021	54	-959.22965	-986.26647	-27.03682
30	-513.86536	-495.86286	18.00250	55	-969.52434	-1006.64882	-37.12447
31	-543.98609	-525.54570	18.44039	56	-990.24262	-1023.10364	-32.86102
32	-561.72678	-544.46912	17.25766	57	-1022.26563	-1037.21522	-14.94960
33	-577.54272	-567.88860	9.65412	58	-1032.29014	-1067.54698	-35.25684
34	-595.58925	-590.68753	4.90173	59	-1059.03064	-1088.45552	-29.42488
35	-638.57571	-612.14943	26.42628	60	-1062.31488	-1085.14397	-22.82908
36	-657.57400	-627.76141	29.81259	61	-1082.53898	-1131.84671	-49.30773
37	-664.06611	-651.10942	12.95669	62	-1103.97396	-1137.92098	-33.94701
38	-685.28561	-669.58689	15.69872	63	-1118.67696	-1175.65553	-56.97857
39	-710.89499	-685.03391	25.86108	64	-1139.88057	-1182.01649	-42.13592
40	-721.93235	-710.82903	11.10331	65	-1149.01797	-1210.93152	-61.91354
41	-742.64792	-729.77556	12.87236	66	-1183.97190	-1209.16986	-25.19796
42	-744.16362	-734.90150	9.26212	67	-1193.97032	-1250.96555	-56.99523
43	-753.85723	-768.58213	-14.72490	68	-1222.53142	-1251.87295	-29.34153
44	-772.08320	-782.3079	-10.22476				