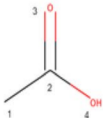


a



acetic acid

b

node index

	1	2	3	4
1	0	1	0	0
2	1	0	1	1
3	0	1	0	0
4	0	1	0	0

node index

adjacency matrix A

c

atom type formal charge implicit Hs

	C	N	O	S	-1	0	+1	0	1	2	3
1	1	0	0	0	0	1	0	0	0	0	1
2	1	0	0	0	0	1	0	1	0	0	0
3	0	0	1	0	0	1	0	1	0	0	0
4	0	0	1	0	0	1	0	0	1	0	0

node index

node features matrix X

d

bond type

	1	2	3
(1,2)	1	0	0
(2,3)	0	1	0
(2,4)	1	0	0

edge indices

edge features matrix E