

496  
MW $\text{C}_4\text{H}_2\text{N}_2$ **(2Z)-2-Butenedinitrile**  
Maleonitrile $\text{C}_{2v}$ 

$r_0$	$\text{\AA}^{\text{a}}$
H–C	1.099(5)
C=C	1.340(3)
C–C	1.428(3)
C≡N	1.160(3)

$\theta_0$	$\text{deg}^{\text{a}}$
H–C=C	122.2(5)
C–C=C	123.1(3)
N≡C–C	178.4(3) <sup>b)</sup>

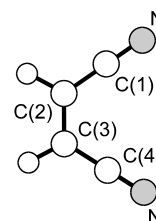
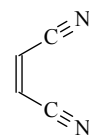
$r_s$	$\text{\AA}^{\text{a}}$
H–C	1.099(3)
C=C	1.338(2)
C–C	1.446(2)
C≡N	1.143(2)

$\theta_s$	$\text{deg}^{\text{a}}$
H–C=C	122.2(3)
C–C=C	122.6(2)
N≡C–C	177.2(2) <sup>b)</sup>

$r_e$	$\text{\AA}^{\text{a}}$
H–C	1.075(5)
C=C	1.341(5)
C–C	1.429(5)
C≡N	1.157(5)

$\theta_e$	$\text{deg}^{\text{a}}$
H–C=C	119.4(5)
C–C=C	123.2(5)
N≡C–C	178.4(5) <sup>b)</sup>

Atom	$ a_s  [\text{\AA}]$	$ b_s  [\text{\AA}]$
C(2)	0.66921	1.14084
C(1)	1.44868	0.07722
N	2.11075	1.00891
H	1.25523	2.07052

<sup>a)</sup> Uncertainties were not estimated in the original paper, except for  $r_e$ .<sup>b)</sup> Bent out.

Halter, R.J., Fimmen, R.L., McMahon, R.J., Peebles, S.A., Kuczkowski, R.L., Stanton, J.F.:  
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