

**SUPPLEMENTARY MATERIAL**

**Table 1S.** Energies (a.u.), relative energies (kJ/mol) and frequencies ( $\text{cm}^{-1}$ ) of the reaction

Species	B3LYP/6-311++G**		G3	
	$E_T$	$E_T$	$E_{\text{rel}}$	Frequency
R(S) (OH+HCNS)	-567.45521422	-566.5769609	0	-
IM1	-567.16678154	-566.8538058	-726.9	-
IM2	-567.18728663	-566.8890179	-819.3	-
IM3	-567.12823228	-566.8416173	-694.9	-
IM4	-567.13674575	-566.8226088	-644.9	-
IM5	-567.76642807	-566.8657495	-758.2	-
IM6	-567.17470302	-566.8657494	-758.2	-
IM7	-567.15578905	-566.8434857	-699.8	-
TS1	-567.06713058	-566.7241868	-386.5	521.904i
TS2	-567.06047590	-566.7681519	-502.0	1690.29i
TS3	-567.87015980	-566.7451612	-441.6	1793.12i
TS4	-567.08652907	-566.7504714	-455.6	634.744i
TS5	-567.08006244	-566.7687970	-503.7	638.159i
TS6	-567.00940849	-566.6865265	-287.7	152.696i
P1	-567.29509973	-567.0138667	-518.31	-
P2	-567.06126011	-566.7139276	-615.98	-
P3	-567.50030180	-566.7795535	-531.9	-
R(T)(OH+HCNS)	-566.86141573	-566.6667315	0	-
<sup>3</sup> IM1	-567.11792597	-566.7959261	-339.2	-
<sup>3</sup> IM2	-567.11657878	-566.8037169	-359.7	-
<sup>3</sup> IM3	-567.13735683	-566.806905	-359.6	-
<sup>3</sup> TS1	-567.15712191	-566.740789983	-194.4	547.881i
<sup>3</sup> TS2	-566.87238300	-566.685837306	-50.16	1583.27i
<sup>3</sup> P1	-567.09344566	-566.8367137	-446.3	-
<sup>3</sup> P2	-567.11320645	-566.7948381	-336.3	-