

Supporting Information

Identifying Molecular Species on Surfaces by Scanning Tunneling Microscopy: Methyl Pyruvate on Pd(111)

Michael Garvey¹, Yun Bai¹, J. Anibal Boscoboinik^{1,2}, Luke Burkholder¹, Thomas E. Sorensen¹ and Wilfred T. Tysoe¹ *

¹ *Department of Chemistry and Laboratory for Surface Studies, University of Wisconsin-Milwaukee, Milwaukee, WI 53211, USA*

² *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*

E-mail: wtt@uwm.edu

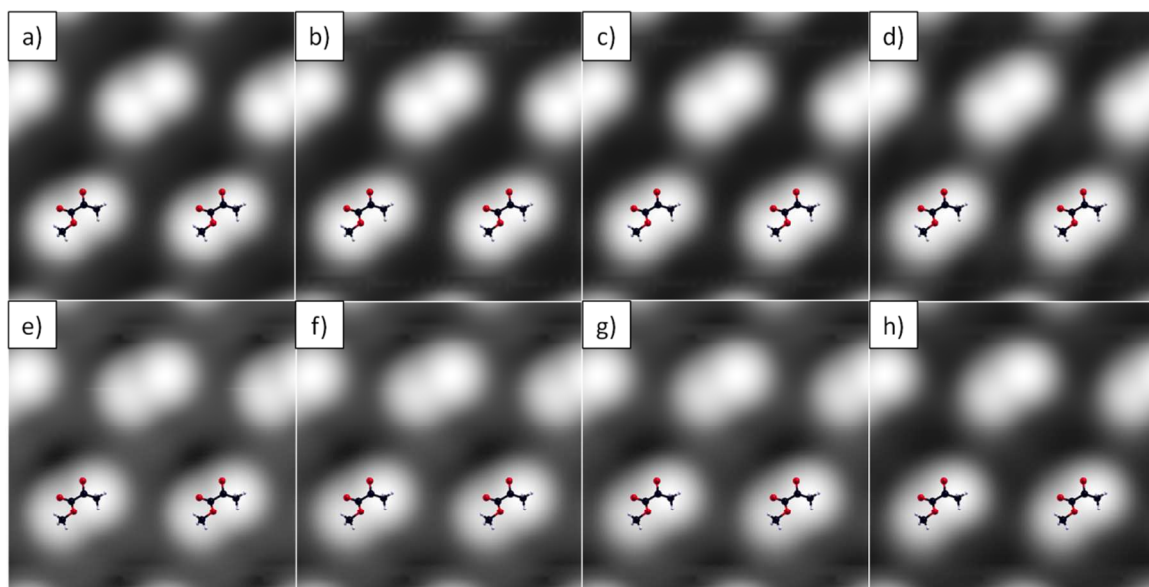


Figure S1: Simulated STM images of the most stable keto form of methyl pyruvate (A30 *cis*) imaged with Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

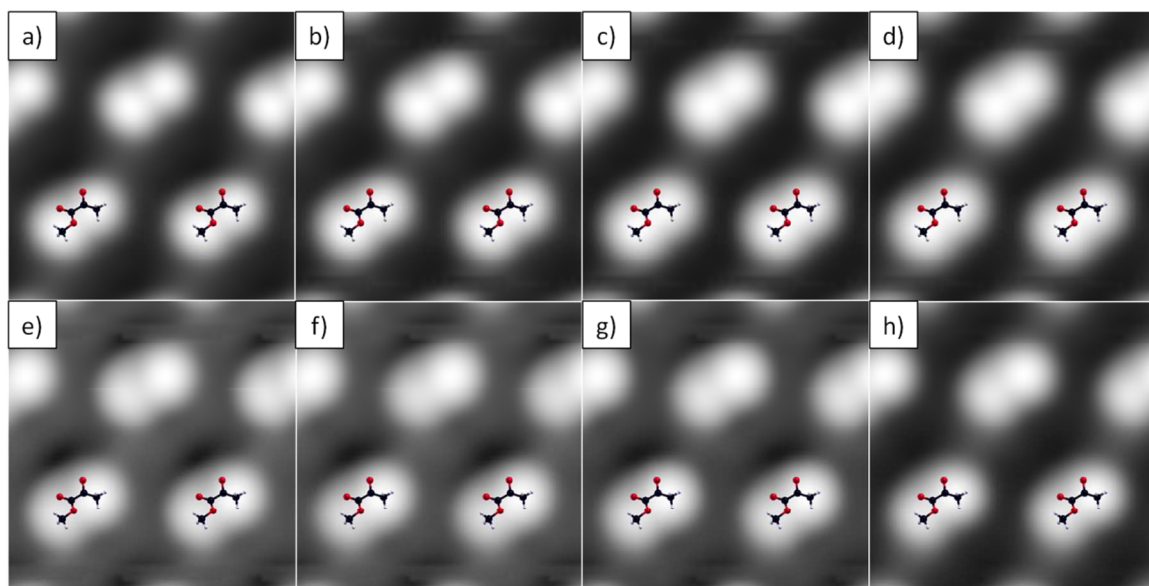


Figure S2: Simulated STM images of the most stable keto form of methyl pyruvate (A30 *cis*) imaged with a CH₃ group on Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

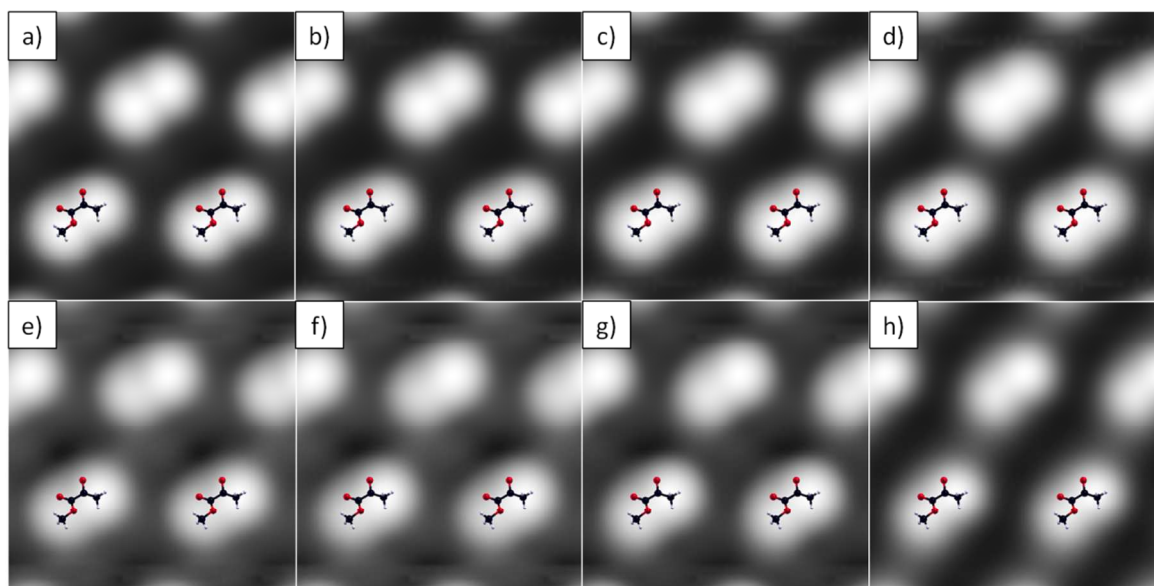


Figure S3: Simulated STM images of the most stable keto form of methyl pyruvate (A30 *cis*) imaged with a CO group Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

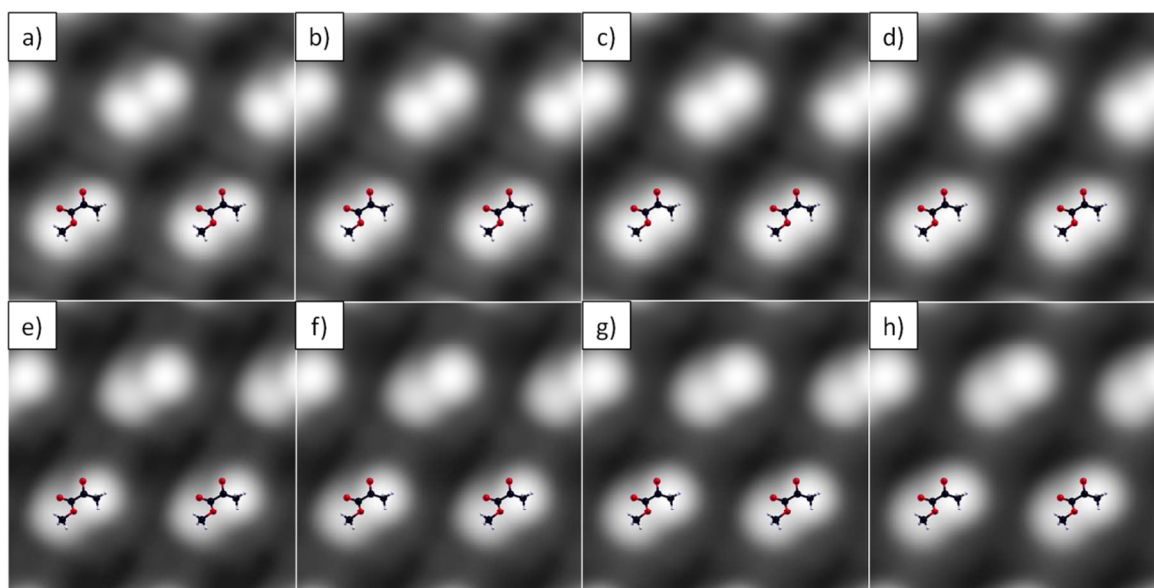


Figure S4: Simulated STM images of the most stable keto form of methyl pyruvate (A30 *cis*) imaged with Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

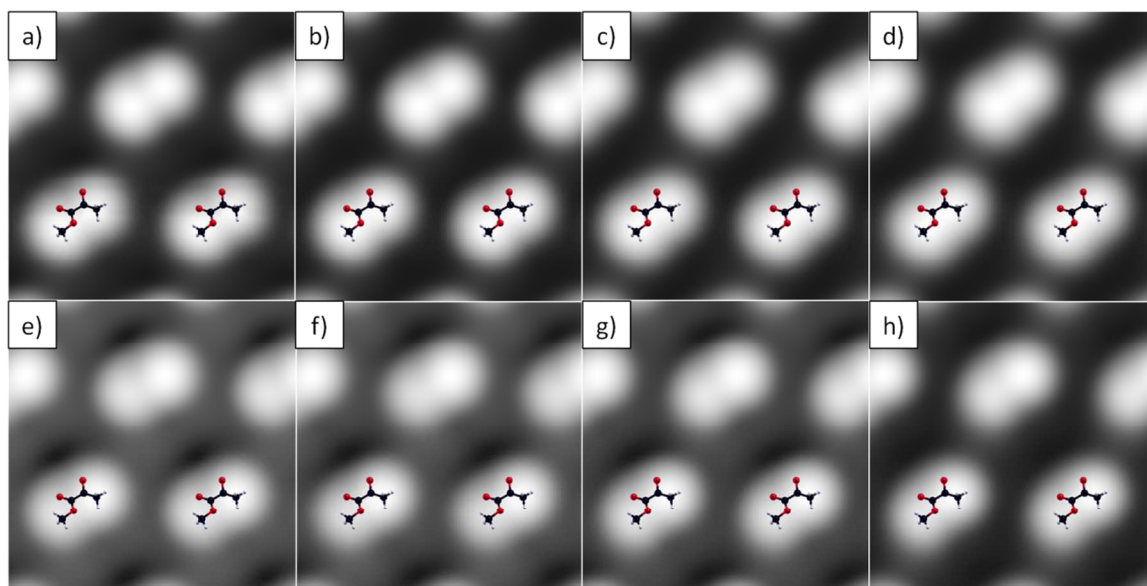


Figure S5: Simulated STM images of the most stable keto form of methyl pyruvate (A30 *cis*) imaged with a CH₃ group on Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

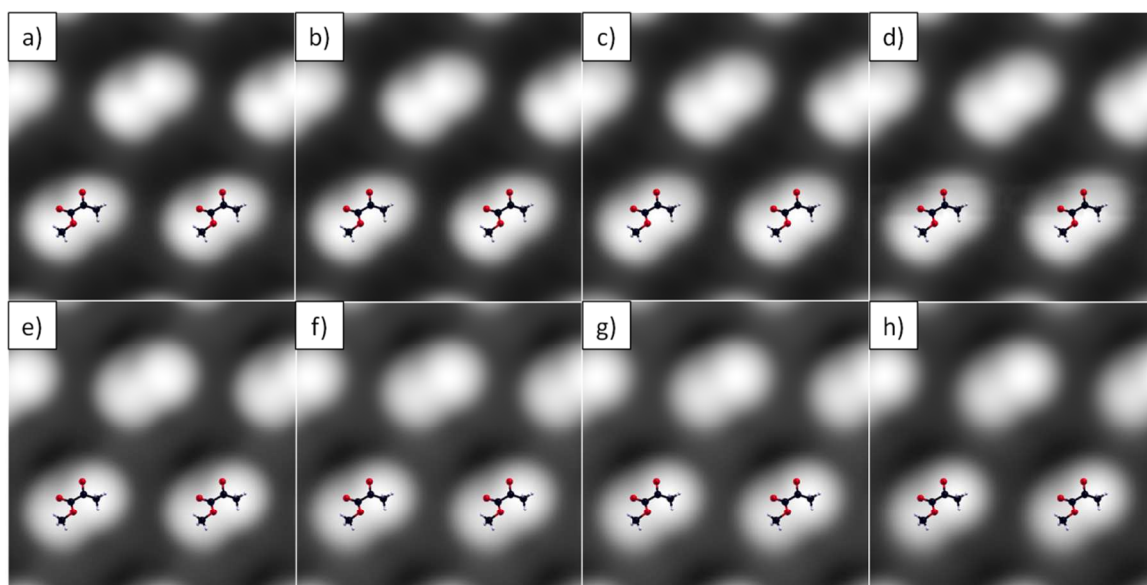


Figure S6: Simulated STM images of the most stable keto form of methyl pyruvate (A30 *cis*) imaged with a CO group on Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

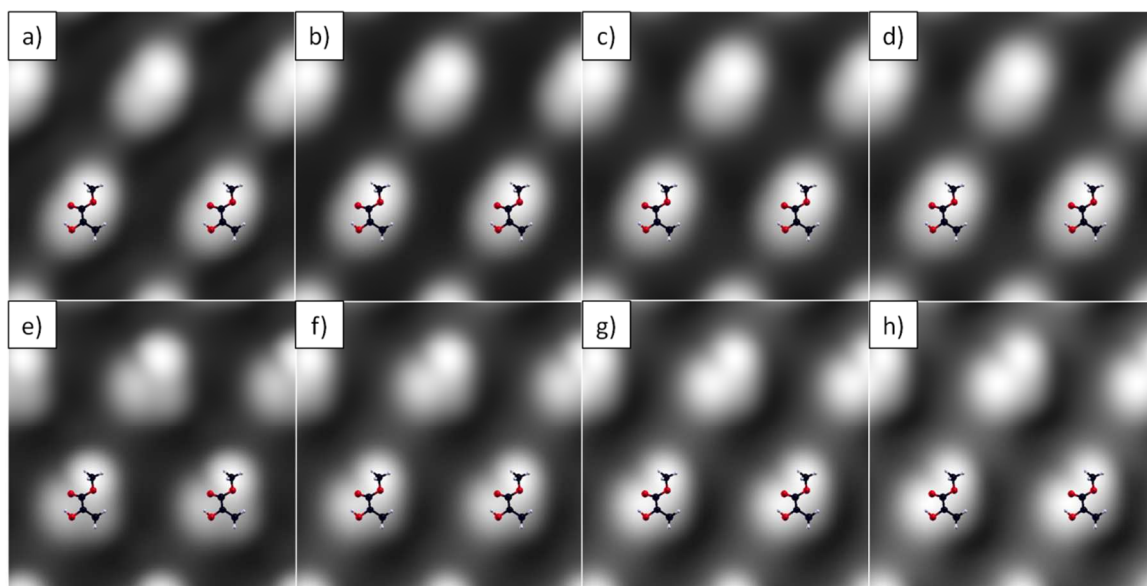


Figure S7: Simulated STM images of the most stable enol form of methyl pyruvate (AB *cis*) imaged with a Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

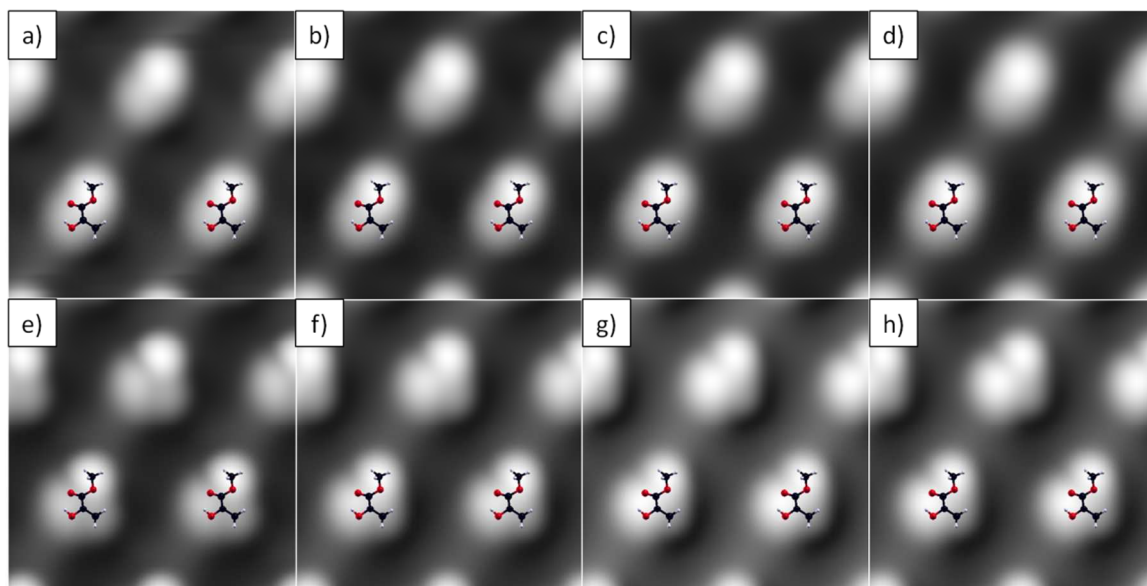


Figure S8: Simulated STM images of the most stable enol form of methyl pyruvate (AB *cis*) imaged with a CH₃ group on Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

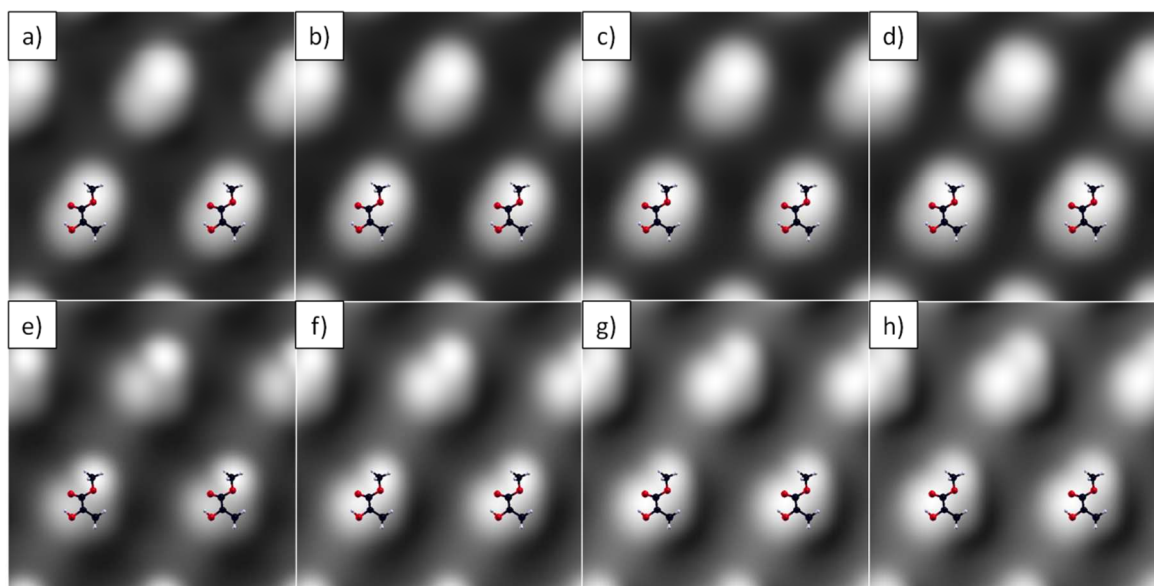


Figure S9: Simulated STM images of the most stable enol form of methyl pyruvate (AB *cis*) imaged with a CO group on Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

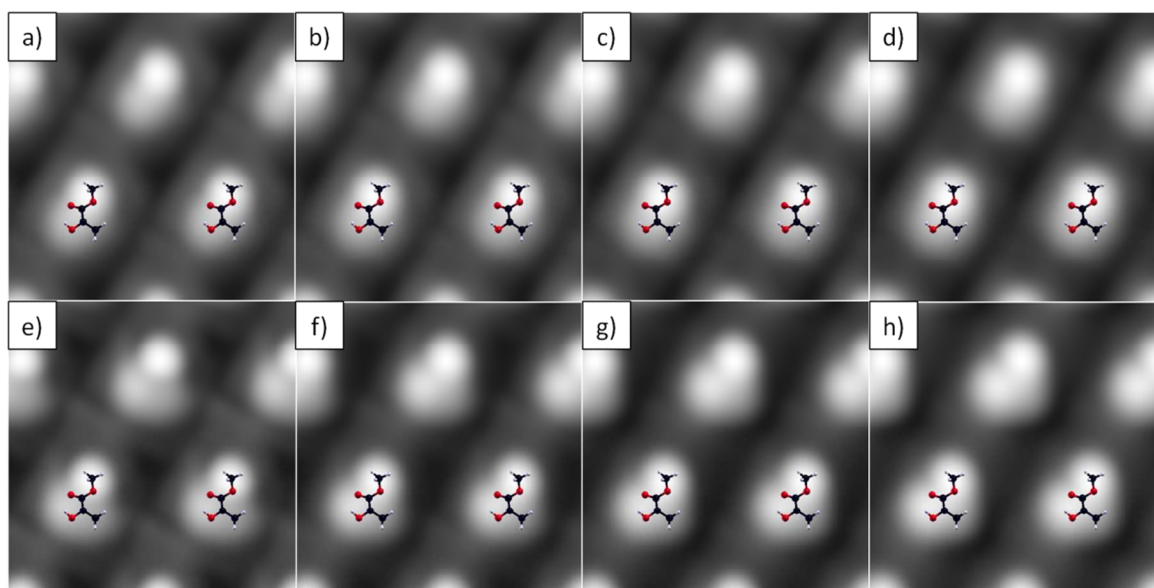


Figure S10: Simulated STM images of the most stable enol form of methyl pyruvate (AB *cis*) imaged with a Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

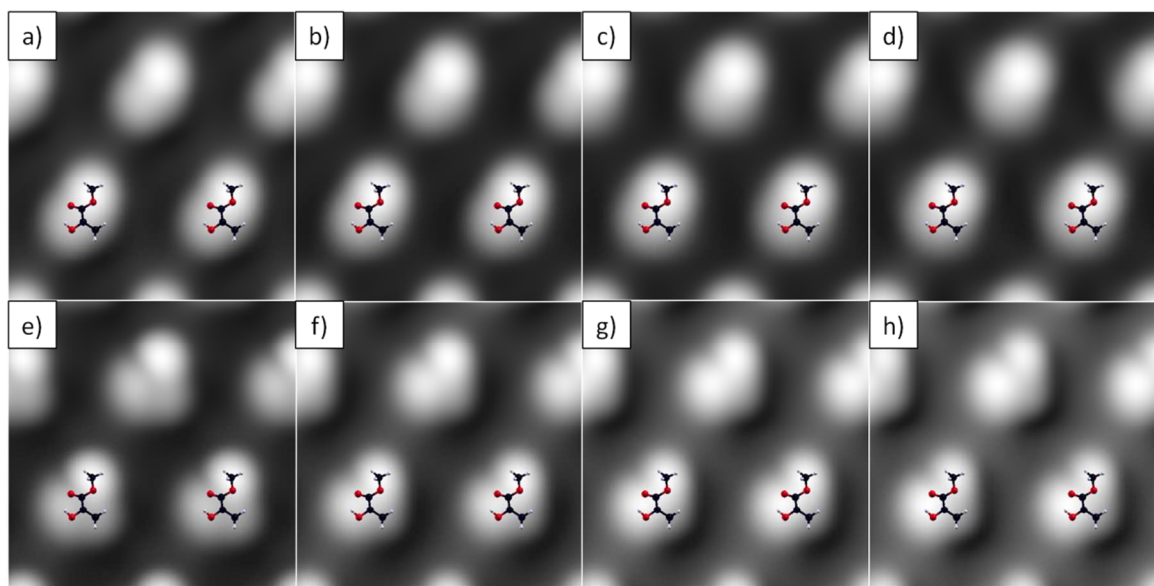


Figure S11: Simulated STM images of the most stable enol form of methyl pyruvate (AB *cis*) imaged with a CH₃ group on Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

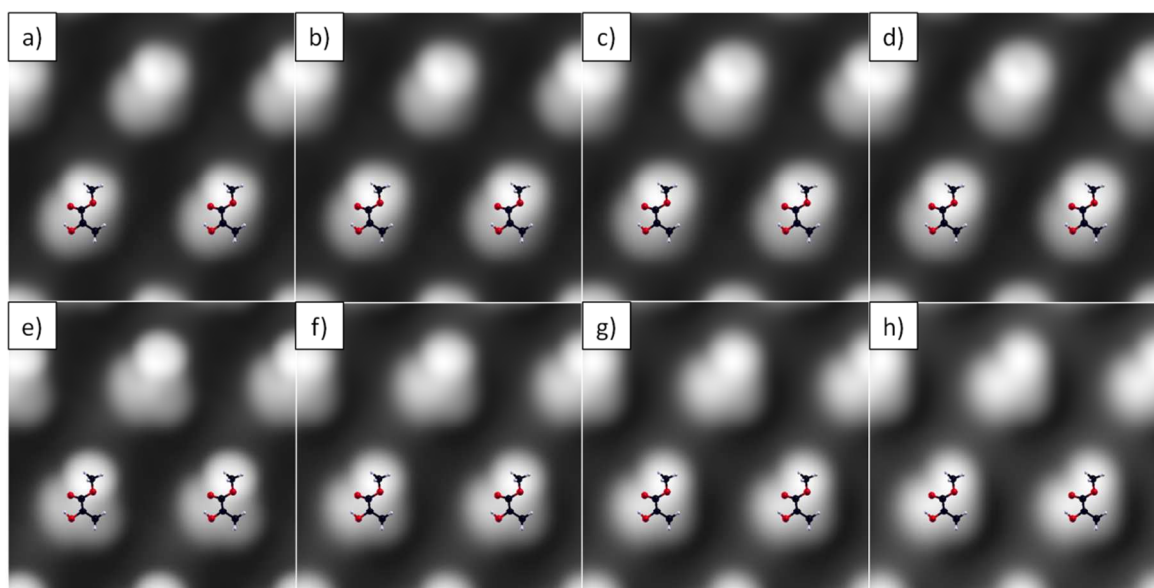


Figure S12: Simulated STM images of the most stable enol form of methyl pyruvate (AB *cis*) imaged with a CO group on Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

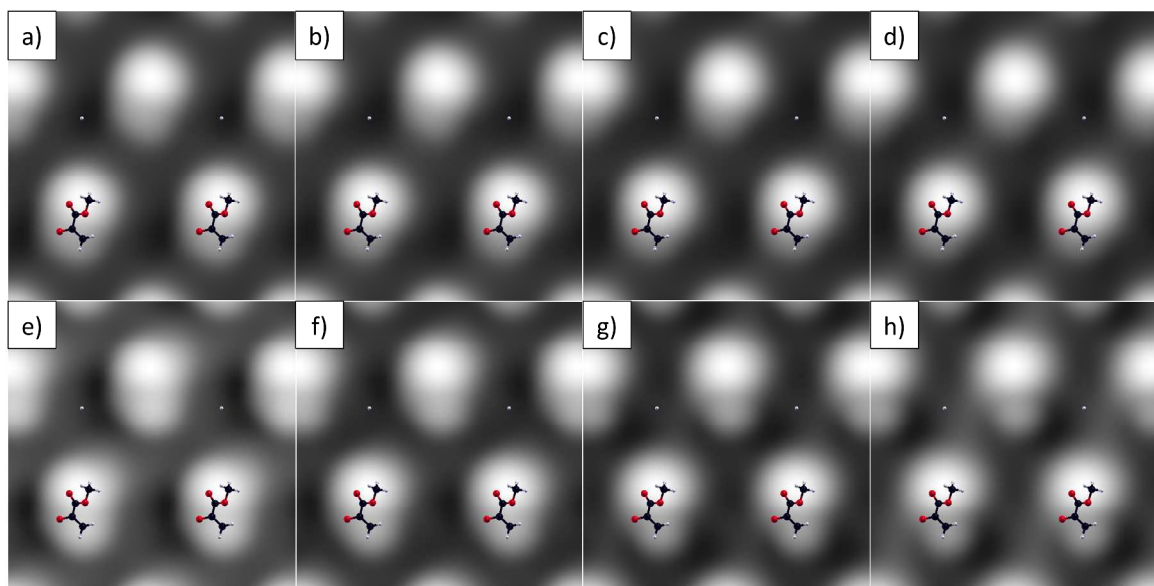


Figure S13: Simulated STM images of the most stable enolate form of methyl pyruvate (BA *cis*) imaged with a Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

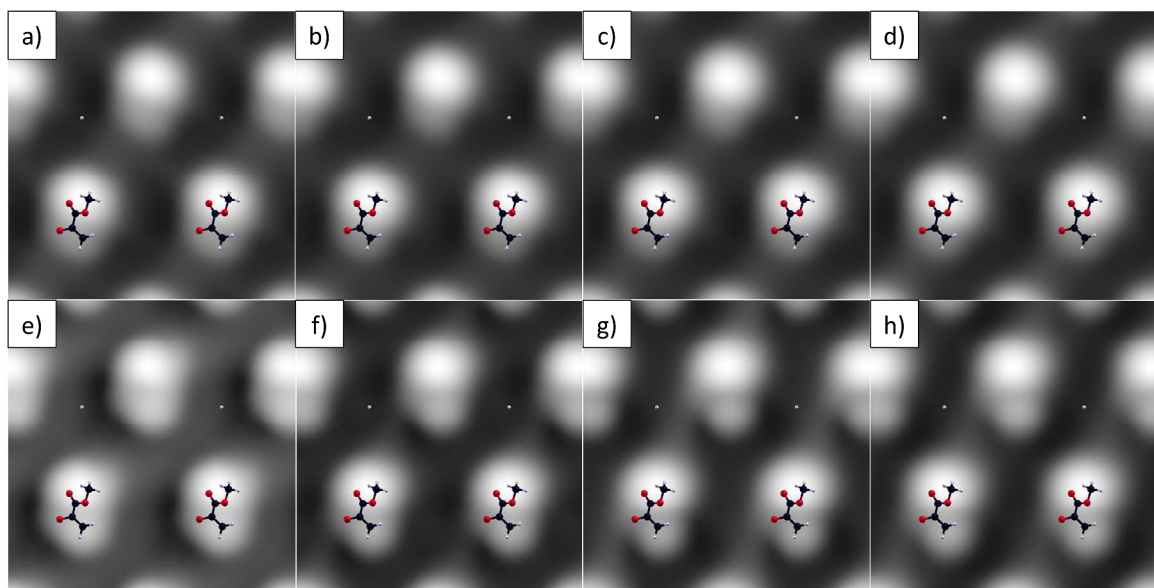


Figure S14: Simulated STM images of the most stable enolate form of methyl pyruvate (BA *cis*) imaged with a CH₃ group on Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

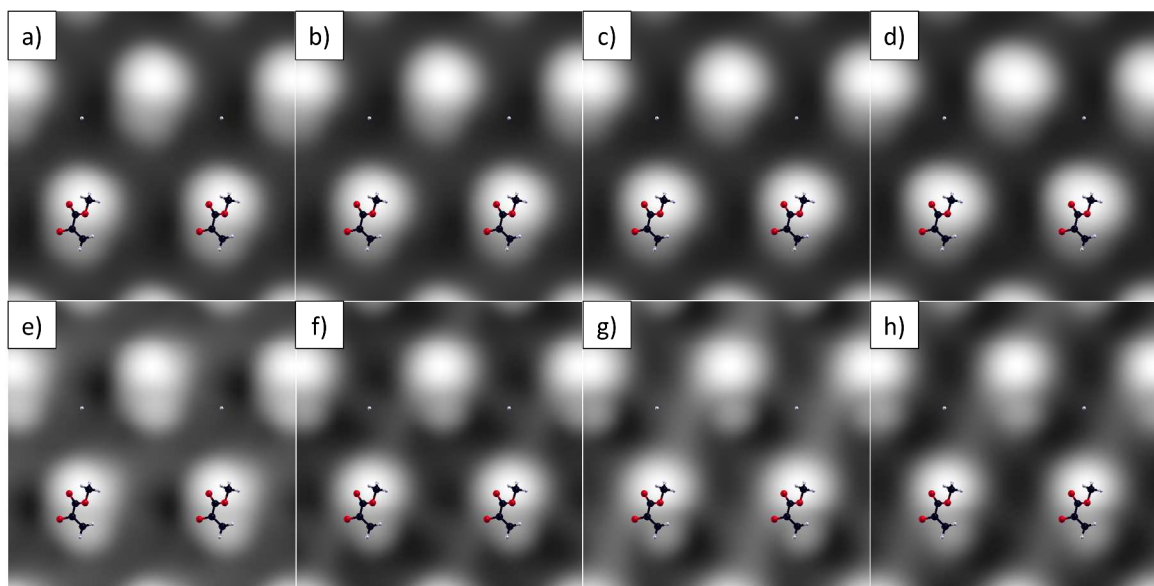


Figure S15: Simulated STM images of the most stable enolate form of methyl pyruvate (BA *cis*) imaged with a CO group on Au on W(110) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

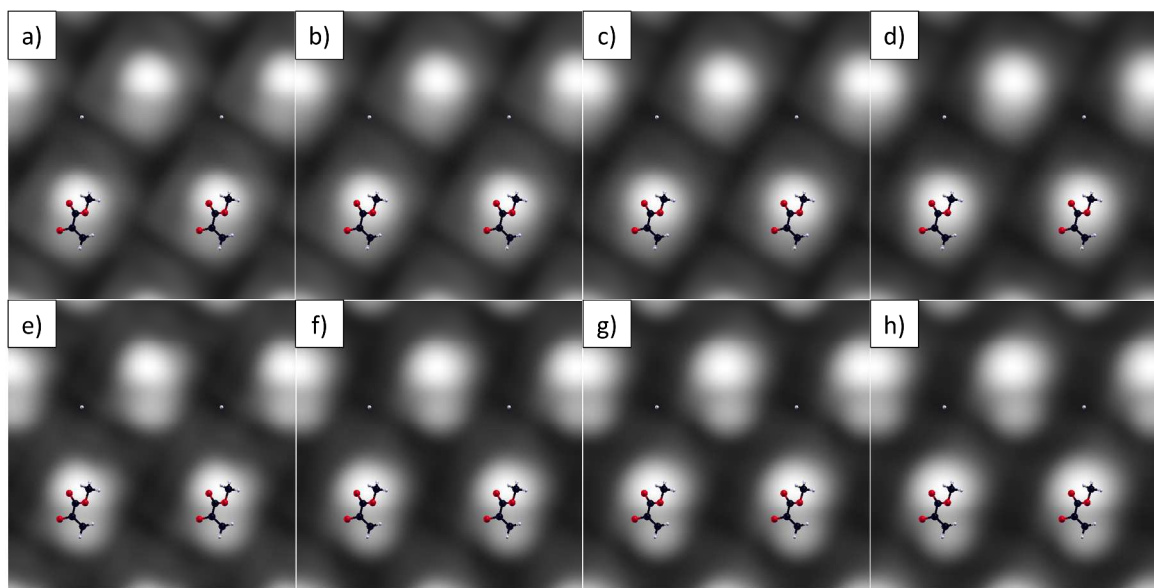


Figure S16: Simulated STM images of the most stable enolate form of methyl pyruvate (BA *cis*) imaged with a Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

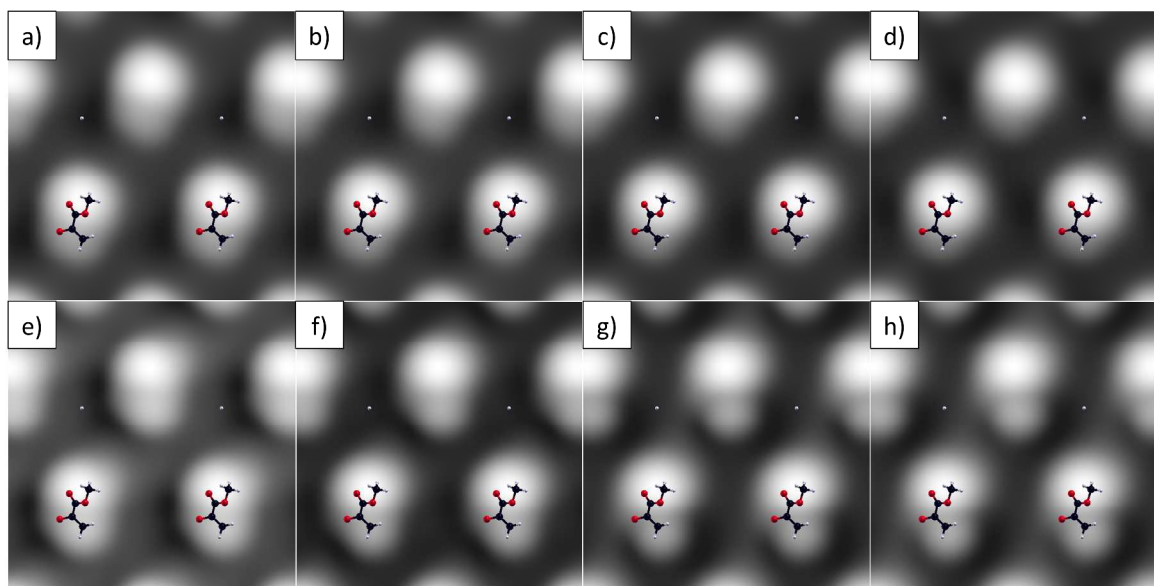


Figure S17: Simulated STM images of the most stable enolate form of methyl pyruvate (BA *cis*) imaged with a CH₃ group on Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

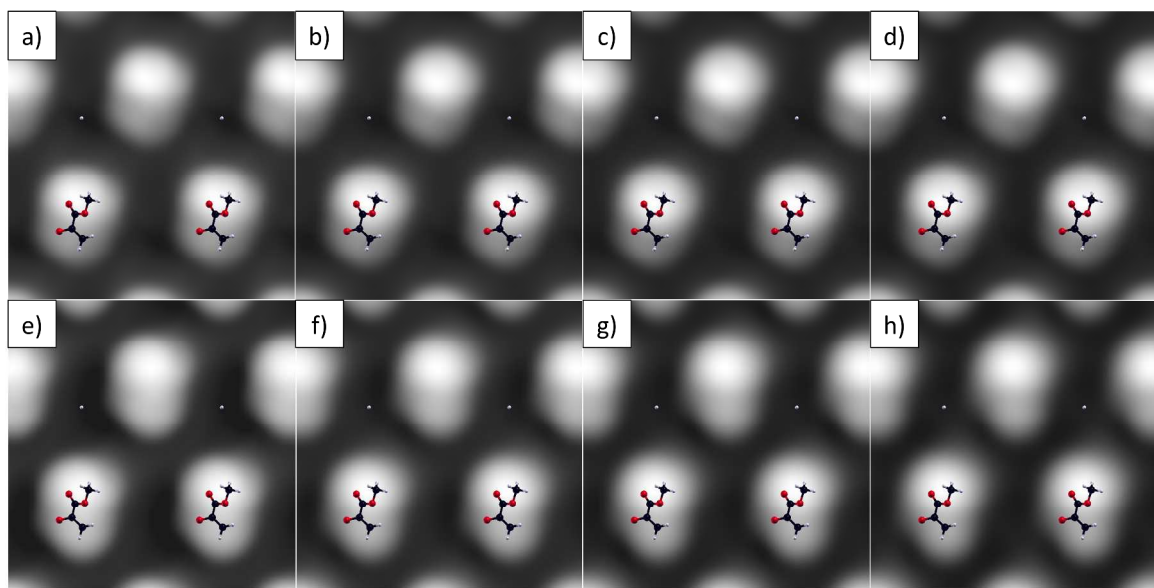


Figure S18: Simulated STM images of the most stable enolate form of methyl pyruvate (BA *cis*) imaged with a CO group on Au on W(111) tip at varied bias: a) -0.1 V, b) -0.2 V, c) -0.3 V, d) -0.4 V e) +0.1 V, f) +0.2 V, g) +0.3 V, h) +0.4 V

File: Atom coordinates for the most stable enol form of methyl pyruvate depicted in Fig. 7 of the manuscript (MP_enol_cis_AB.xyz)