

Discussion

Comment on: An improved microkinetic model  
for the water–gas shift reaction on copper  
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L.T. Fan <sup>a,\*</sup>, Yu-Chuan Lin <sup>a</sup>, Shahram Shafie <sup>a</sup>, Keith L. Hohn <sup>a</sup>,  
Botond Bertók <sup>b</sup>, Ferenc Friedler <sup>b</sup>

<sup>a</sup> Department of Chemical Engineering, Kansas State University, 105 Durland Hall, Manhattan, KS 66506-5102, USA

<sup>b</sup> Department of Computer Science, University of Pannonia, Egyetem u. 10, Veszprem H-8200, Hungary

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A recent paper by Callaghan et al. [1] presents 70 reaction routes ( $RR_i$ s), which correspond to stoichiometrically feasible independent pathways ( $IP_i$ s), for the water–gas shift (WGS) reaction; these 70  $IP_i$ s have been generated from 17 elementary reactions by resorting to a linear algebraic method in conjunction with some heuristics. This is in stark contrast to the 116  $IP_i$ s obtained by us from the same set of 17 elementary reactions. Obviously, the former is substantially fewer than the latter. Our results have been obtained by resorting to the inordinately effective graph–theoretic, algorithmic method based on P-graphs (process graph) [2–6] in less than 2 s on a PC (Intel Pentium 4, CPU 3.06 GHz; and 1G RAM) upon inputting the 17 elementary reactions. The method comprises three algorithms

crafted from two sets of axioms, and thus, it does not require any heuristic to implement; this is totally unlike the method employed by Callaghan et al. [1]; moreover, P-graphs are unique bipartite graphs that are rigorously defined mathematically [7–11]. Both sets of  $IP_i$ s are listed in Table 1 for comparison. Note that the 116  $IP_i$ s identified by us contain all the 70  $IP_i$ s identified by Callaghan et al. [1]. The authors have cited the P-graph based method in their earlier papers [5,6], but surprisingly not in [1].

To determine potentially dominant pathways through further energetic, computational, mechanistic and/or experimental exploration on the basis of an incomplete set of  $IP_i$ s would indeed be precarious. It is mandatory that the  $IP_i$ s be rigorously and exhaustively identified at the outset.

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\* Corresponding author. Tel.: +1 785 532 5584; fax: +1 785 532 7372.

E-mail address: [fan@cheme.ksu.edu](mailto:fan@cheme.ksu.edu) (L.T. Fan).

Table 1  
Comparison of the stoichiometrically feasible independent pathways identified in our work with those identified by Callaghan et al. [1]

Our work			Callaghan et al. (2003)		
Designation (IP <sub><i>i</i></sub> )	Mechanism	$\Delta H_{\text{fi}}^{\circ}$ (kcal/mol)	Designation (RR <sub><i>i</i></sub> )	Mechanism	$\Delta H_{\text{fi}}^{\circ}$ (kcal/mol)
IP <sub>1</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_8 + s_{11}$	-11	RR <sub>1</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_8 + s_{11}$	-11
IP <sub>2</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_7 + s_9$	-11	RR <sub>2</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_7 + s_9$	-11
IP <sub>3</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_{10}$	-11	RR <sub>3</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_{10}$	-11
IP <sub>4</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_7 - s_{13}$	-11	RR <sub>4</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_7 - s_{13}$	-11
IP <sub>5</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_{10} + s_{11} - s_{12} + s_{13}$	-11	RR <sub>5</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_{10} + s_{11} - s_{12} + s_{13}$	-11
IP <sub>6</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_9 + s_{10} + s_{13}$	-11	RR <sub>6</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_9 + s_{10} + s_{13}$	-11
IP <sub>7</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_{11} - s_{12} + s_{13}$	-11	RR <sub>7</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_{11} - s_{12} + s_{13}$	-11
IP <sub>8</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_8 + 2s_{10} - s_{12} + s_{13}$	-11	RR <sub>8</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_8 + 2s_{10} - s_{12} + s_{13}$	-11
IP <sub>9</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_9 + s_{12} + s_{13}$	-11	RR <sub>9</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_9 + s_{12} + s_{13}$	-11
IP <sub>10</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + s_9 + s_{11} + s_{13}$	-11	RR <sub>10</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + s_9 + s_{11} + s_{13}$	-11
IP <sub>11</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_{11} - 2s_{12} + s_{13}$	-11	RR <sub>11</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_{11} - 2s_{12} + s_{13}$	-11
IP <sub>12</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_9 + s_{13}$	-11	RR <sub>12</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_9 + s_{13}$	-11
IP <sub>13</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_7 + 2s_{10} + s_{13}$	-11	RR <sub>13</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_7 + 2s_{10} + s_{13}$	-11
IP <sub>14</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_7 + 2s_8 + 2s_{11} + s_{13}$	-11	RR <sub>14</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_7 + 2s_8 + 2s_{11} + s_{13}$	-11
IP <sub>15</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_8 + s_{12} - s_{13}$	-11	RR <sub>15</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_8 + s_{12} - s_{13}$	-11
IP <sub>16</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_8 + s_9 + s_{12}$	-11	RR <sub>16</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_8 + s_9 + s_{12}$	-11
IP <sub>17</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_7 + s_{11} - s_{12}$	-11	RR <sub>17</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 + s_7 + s_{11} - s_{12}$	-11
IP <sub>18</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 + s_{15}$	-11	RR <sub>18</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 + s_{15}$	-11
IP <sub>19</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{12} + s_{15}$	-11	RR <sub>19</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{12} + s_{15}$	-11
IP <sub>20</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 + s_{14}$	-11	RR <sub>20</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 + s_{14}$	-11
IP <sub>21</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} + s_{14}$	-11	RR <sub>21</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} + s_{14}$	-11
IP <sub>22</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} + s_{14}$	-11	RR <sub>22</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} + s_{14}$	-11
IP <sub>23</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{13} + 2s_{14}$	-11	RR <sub>23</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{13} + 2s_{14}$	-11
IP <sub>24</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{13} + 2s_{15}$	-11	RR <sub>24</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{13} + 2s_{15}$	-11
IP <sub>25</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{14} + s_{15}$	-11	RR <sub>25</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{14} + s_{15}$	-11
IP <sub>26</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{12} + s_{14}$	-11	RR <sub>26</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{12} + s_{14}$	-11
IP <sub>27</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{12} + s_{14}$	-11	RR <sub>27</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{12} + s_{14}$	-11
IP <sub>28</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} + s_{13} + s_{15}$	-11	RR <sub>28</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} + s_{13} + s_{15}$	-11
IP <sub>29</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} + s_{13} + s_{15}$	-11	RR <sub>29</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} + s_{13} + s_{15}$	-11
IP <sub>30</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{12} - s_{13} + 2s_{14}$	-11	RR <sub>30</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{12} - s_{13} + 2s_{14}$	-11
IP <sub>31</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{12} + s_{14} + s_{15}$	-11	RR <sub>31</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{12} + s_{14} + s_{15}$	-11
IP <sub>32</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{12} + s_{13} + 2s_{15}$	-11	RR <sub>32</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{12} + s_{13} + 2s_{15}$	-11
IP <sub>33</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_7 - s_{12} + s_{16}$	-11	RR <sub>33</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_7 - s_{12} + s_{16}$	-11
IP <sub>34</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_8 + s_{16}$	-11	RR <sub>34</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_6 + s_8 + s_{16}$	-11
IP <sub>35</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + 2s_7 - s_8 + 2s_{15} - s_{16}$	-11	RR <sub>35</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + 2s_7 - s_8 + 2s_{15} - s_{16}$	-11
IP <sub>36</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_7 - s_8 + 2s_9 - s_{16}$	-11	RR <sub>36</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + 2s_7 - s_8 + 2s_9 - s_{16}$	-11
IP <sub>37</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_{10} + s_{11} - s_{16}$	-11	RR <sub>37</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_{10} + s_{11} - s_{16}$	-11
IP <sub>38</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_7 + 2s_{10} + s_{12} - s_{16}$	-11	RR <sub>38</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_7 + 2s_{10} + s_{12} - s_{16}$	-11
IP <sub>39</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_{11} - s_{12} - s_{16}$	-11	RR <sub>39</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_{11} - s_{12} - s_{16}$	-11
IP <sub>40</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_{11} - s_{13} - 2s_{16}$	-11	RR <sub>40</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_{11} - s_{13} - 2s_{16}$	-11
IP <sub>41</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - 2s_{12} + s_{13} + 2s_{17}$	-11	RR <sub>41</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - 2s_{12} + s_{13} + 2s_{17}$	-11
IP <sub>42</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 - s_7 + 2s_8 + s_{13} + 2s_{17}$	-11	RR <sub>42</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 - s_7 + 2s_8 + s_{13} + 2s_{17}$	-11
IP <sub>43</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_9 + s_{12} - s_{16}$	-11	RR <sub>43</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + 2s_9 + s_{12} - s_{16}$	-11
IP <sub>44</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{12} + 2s_{14} + s_{16}$	-11	RR <sub>44</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{12} + 2s_{14} + s_{16}$	-11
IP <sub>45</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{12} + 2s_{15} - s_{16}$	-11	RR <sub>45</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{12} + 2s_{15} - s_{16}$	-11
IP <sub>46</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{12} + s_{14} + s_{17}$	-11	RR <sub>46</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{12} + s_{14} + s_{17}$	-11

IP <sub>47</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{12} - s_{16} + 2s_{17}$	-11
IP <sub>48</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{13} - 2s_{16} + 2s_{17}$	-11
IP <sub>49</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{15} - s_{16} + s_{17}$	-11
IP <sub>50</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + s_9 + s_{11} - s_{16}$	-11
IP <sub>51</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_8 + 2s_{10} - s_{16}$	-11
IP <sub>52</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_{11} - s_{16}$	-11
IP <sub>53</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + 2s_{12} + 2s_{15} - s_{16}$	-11
IP <sub>54</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + 2s_{13} + 2s_{15} + s_{16}$	-11
IP <sub>55</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + 2s_{14} + s_{16}$	-11
IP <sub>56</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_9 + 2s_{12} - s_{16}$	-11
IP <sub>57</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_9 + 2s_{13} + s_{16}$	-11
IP <sub>58</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 - s_{12} + s_{13} + 2s_{17}$	-11
IP <sub>59</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{13} + s_{15} + s_{17}$	-11
IP <sub>60</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{14} + s_{17}$	-11
IP <sub>61</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 - s_{16} + 2s_{17}$	-11
IP <sub>62</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_9 + s_{10} + s_{12} - s_{16}$	-11
IP <sub>63</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} - s_{12} + s_{13} + s_{17}$	-11
IP <sub>64</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} + s_{12} + s_{15} - s_{16}$	-11
IP <sub>65</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} - s_{16} + s_{17}$	-11
IP <sub>66</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 - s_{12} + s_{17}$	-11
IP <sub>67</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{17}$	-11
IP <sub>68</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} + s_{15} - s_{16}$	-11
IP <sub>69</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 - s_{16} + s_{17}$	-11
IP <sub>70</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{13} + s_{17}$	-11
IP <sub>71</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 + s_9 - s_{11} + s_{17}$	-11
IP <sub>72</sub>	$s_1 + s_2 + s_3 + s_5 + 2s_6 + s_7 - s_{11} - s_{13} + s_{17}$	-11
IP <sub>73</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 + s_{13} + s_{15}$	-11
IP <sub>74</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{12} + s_{13} + s_{15}$	-11
IP <sub>75</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} + s_{13} + 2s_{15} - s_{17}$	-11
IP <sub>76</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + 2s_9 - s_{11} + s_{13} + s_{17}$	-11
IP <sub>77</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - 2s_{12} + s_{13} + s_{17}$	-11
IP <sub>78</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 - s_{12} + s_{13} + s_{17}$	-11
IP <sub>79</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{13} + 2s_{14} - s_{17}$	-11
IP <sub>80</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} + s_{14} + s_{15} - s_{17}$	-11
IP <sub>81</sub>	$s_1 + s_2 + s_3 + s_5 + 2s_7 - s_8 + s_9 + s_{15} - s_{16}$	-11
IP <sub>82</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 + s_{12} + s_{15} - s_{16}$	-11
IP <sub>83</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{13} - 2s_{16} + s_{17}$	-11
IP <sub>84</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{12} - s_{16} + s_{17}$	-11
IP <sub>85</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 - s_{13} + s_{14}$	-11
IP <sub>86</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 - s_{12} + s_{14} + s_{16}$	-11
IP <sub>87</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 - s_{13} - s_{16} + s_{17}$	-11
IP <sub>88</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} - s_{13} + s_{14} - s_{16}$	-11
IP <sub>89</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 - s_9 + s_{11} + s_{15}$	-11
IP <sub>90</sub>	$s_1 + s_2 + s_3 + s_5 + 2s_6 + s_8 - s_9 + s_{15} + s_{16}$	-11
IP <sub>91</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{12} + s_{13} + s_{15}$	-11
IP <sub>92</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + 2s_{13} + s_{15} + s_{16}$	-11
IP <sub>93</sub>	$s_1 + s_2 + s_3 + s_5 - s_7 + 2s_8 + s_{11} + s_{13} + s_{17}$	-11
IP <sub>94</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} - s_{12} + s_{13} + s_{17}$	-11
IP <sub>95</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + 2s_{14} - s_{15} + s_{16}$	-11
IP <sub>96</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{14} - s_{15} + s_{17}$	-11
IP <sub>97</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 - s_9 + 2s_{11} + s_{15} - s_{16}$	-11

RR <sub>47</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{12} - s_{16} + 2s_{17}$	-11
RR <sub>48</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 - s_{13} - 2s_{16} + 2s_{17}$	-11
RR <sub>49</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_7 + s_{15} - s_{16} + s_{17}$	-11
RR <sub>50</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_7 + s_9 + s_{11} - s_{16}$	-11
RR <sub>51</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 - s_8 + 2s_{10} - s_{16}$	-11
RR <sub>52</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_{11} - s_{16}$	-11
RR <sub>53</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + 2s_{12} + 2s_{15} - s_{16}$	-11
RR <sub>54</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + 2s_{13} + 2s_{15} + s_{16}$	-11
RR <sub>55</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + 2s_{14} + s_{16}$	-11
RR <sub>56</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_9 + 2s_{12} - s_{16}$	-11
RR <sub>57</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_8 + 2s_9 + 2s_{13} + s_{16}$	-11
RR <sub>58</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 - s_{12} + s_{13} + 2s_{17}$	-11
RR <sub>59</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{13} + s_{15} + s_{17}$	-11
RR <sub>60</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 + s_{14} + s_{17}$	-11
RR <sub>61</sub>	$s_1 + s_2 + s_3 - s_4 + s_5 + s_8 - s_{16} + 2s_{17}$	-11
RR <sub>62</sub>	$s_1 + s_2 + s_3 + s_4 + s_5 + s_9 + s_{10} + s_{12} - s_{16}$	-11
RR <sub>63</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} - s_{12} + s_{13} + s_{17}$	-11
RR <sub>64</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} + s_{12} + s_{15} - s_{16}$	-11
RR <sub>65</sub>	$s_1 + s_2 + s_3 + s_5 + s_{10} - s_{16} + s_{17}$	-11
RR <sub>66</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_7 - s_{12} + s_{17}$	-11
RR <sub>67</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{17}$	-11
RR <sub>68</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_{11} + s_{15} - s_{16}$	-11
RR <sub>69</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 + s_9 - s_{16} + s_{17}$	-11
RR <sub>70</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{13} + s_{17}$	-11

(continued on next page)

Table 1 (continued)

Our work			Callaghan et al. (2003)		
Designation (IP <sub><i>i</i></sub> )	Mechanism	$\Delta H_{ri}^{\circ}$ (kcal/mol)	Designation (RR <sub><i>i</i></sub> )	Mechanism	$\Delta H_{ri}^{\circ}$ (kcal/mol)
IP <sub>98</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + 2s_{12} + s_{15} - s_{16}$	-11			
IP <sub>99</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 - s_{15} - s_{16} + 2s_{17}$	-11			
IP <sub>100</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} + s_{12} + s_{15} - s_{16}$	-11			
IP <sub>101</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_{11} - s_{16} + s_{17}$	-11			
IP <sub>102</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{12} - s_{16} + s_{17}$	-11			
IP <sub>103</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{13} + s_{15} + s_{16}$	-11			
IP <sub>104</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{12} - s_{13} + s_{14}$	-11			
IP <sub>105</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_8 + s_{14} + s_{16}$	-11			
IP <sub>106</sub>	$s_1 + s_2 + s_3 + s_5 + s_8 + s_9 + s_{13} + s_{14} + s_{16}$	-11			
IP <sub>107</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 - s_9 + s_{10} + s_{15}$	-11			
IP <sub>108</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_{10} - s_{11} + s_{12} + s_{15}$	-11			
IP <sub>109</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 + s_{10} - s_{11} + s_{17}$	-11			
IP <sub>110</sub>	$s_1 + s_2 + s_3 + s_5 + s_6 - s_9 + s_{10} - s_{12} + s_{17}$	-11			
IP <sub>111</sub>	$s_1 + s_2 + s_3 + s_5 + s_9 + s_{10} - s_{11} + s_{13} + s_{17}$	-11			
IP <sub>112</sub>	$s_1 + s_2 + s_3 + s_5 - s_7 + 2s_{10} - s_{11} + s_{13} + s_{17}$	-11			
IP <sub>113</sub>	$s_1 + s_2 + s_3 + s_5 - s_8 - s_9 + 2s_{10} + s_{15} - s_{16}$	-11			
IP <sub>114</sub>	$s_1 + s_2 + s_3 + s_5 - s_9 + s_{10} + s_{11} + s_{15} - s_{16}$	-11			
IP <sub>115</sub>	$s_1 + s_2 + s_3 + s_5 + s_7 - s_8 + s_{10} + s_{15} - s_{16}$	-11			
IP <sub>116</sub>	$s_1 + s_2 + s_3 + s_5 - s_7 + s_8 + s_{10} + s_{13} + s_{17}$	-11			

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