

# Energia relativa complejos Fe-A $\beta$

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## 1 Introduction

Table 1: Energías de los complejos Fe-A $\beta$  de los complejos de reactividad

| Complejo  | Carga | Multiplicidad | Energía Hartrees | $\Delta G$ kcal/mol |
|-----------|-------|---------------|------------------|---------------------|
| <b>20</b> | +1    | Sextete       | -2423.492708     | 0.00                |
| <b>20</b> | +1    | Quartete      | -2423.485153     | 4.71                |
| <b>20</b> | +1    | Doublete      | -2423.458126     | 21.56               |
| <b>21</b> | +1    | Sextete       | -2347.050992     | 0.00                |
| <b>21</b> | +1    | Quartete      | -2347.034643     | 10.19               |
| <b>21</b> | +1    | Doublete      | -2347.017302     | 21.01               |
| <b>22</b> | 0     | Sextete       | -3107.938996     | 0.00                |
| <b>22</b> | 0     | Quartete      | -3107.931175     | 4.88                |
| <b>22</b> | 0     | Doublete      | -3107.899759     | 24.46               |
| <b>23</b> | 0     | Sextete       | -3107.941741     | 0.00                |
| <b>23</b> | 0     | Quartete      | -3107.925669     | 10.02               |
| <b>23</b> | 0     | Doublete      | -3107.917643     | 15.03               |
| <b>24</b> | 0     | Sextete       | -3107.942357     | 0.00                |
| <b>24</b> | 0     | Quartete      | -3107.930664     | 7.29                |
| <b>24</b> | 0     | Doublete      | -3107.895642     | 29.13               |
| <b>25</b> | 0     | Sextete       | -3031.435602     | 0.00                |
| <b>25</b> | 0     | Quartete      | -3031.416789     | 11.73               |
| <b>25</b> | 0     | Doublete      | -3031.297455     | 86.13               |
| <b>26</b> | -1    | Sextete       | -3030.916269     | 0.00                |
| <b>27</b> | -1    | Quartete      | -3030.969515     | 0.00                |
| <b>27</b> | -1    | Sextete       | -3030.969006     | 0.32                |
| <b>27</b> | -1    | Doublete      | -3030.942460     | 16.87               |
| <b>28</b> | 0     | Sextete       | -3181.745505     | 0.00                |
| <b>28</b> | 0     | Quartete      | -3181.744497     | 0.63                |
| <b>28</b> | 0     | Doublete      | -3181.723136     | 13.95               |
| <b>29</b> | 0     | Sextete       | -3258.176616     | 0.00                |
| <b>29</b> | 0     | Quartete      | -3258.175694     | 0.57                |

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| Complejo  | Carga | Multiplicidad | Energía Hartrees | $\Delta G$ kcal/mol |
|-----------|-------|---------------|------------------|---------------------|
| <b>30</b> | -1    | Sextete       | -3107.429976     | 0.00                |
| <b>30</b> | -1    | Quartete      | -3107.412676     | 10.79               |
| <b>30</b> | -1    | Doublete      | -3107.390350     | 24.71               |
| <b>31</b> | 0     | quintete      | -2347.264453     | 0.00                |
| <b>31</b> | 0     | triplete      | -2347.245340     | 11.92               |
| <b>31</b> | 0     | singlete      | -2347.224517     | 24.90               |
| <b>32</b> | 0     | septete       | -2497.591866     | 0.00                |
| <b>32</b> | 0     | quintete      | -2497.586661     | 3.25                |
| <b>32</b> | 0     | triplete      | -2497.568696     | 14.45               |
| <b>32</b> | 0     | singlete      | -2497.550126     | 26.02               |
| <b>33</b> | 1     | quintete      | -2497.981055     | 0.00                |
| <b>33</b> | 1     | triplete      | -2497.970854     | 6.36                |
| <b>33</b> | 1     | singlete      | -2497.968055     | 8.11                |
| <b>34</b> | 0     | Sextete       | -3181.806239     | 0.00                |
| <b>36</b> | 0     | septete       | -2574.047554     | 0.00                |
| <b>36</b> | 0     | quintete      | -2574.035098     | 7.77                |
| <b>37</b> | 0     | Sextete       | -2498.226149     | 0.00                |
| <b>38</b> | +1    | Sextete       | -2498.627704     | 0.00                |
| <b>39</b> | +1    | Sextete       | -2498.627019     | 0.00                |