

## 叠氮桥对双核镍配合物磁性影响的密度泛函理论研究

边江鱼<sup>1,\*</sup> 岳淑美<sup>1</sup> 张敏<sup>1</sup> 张景萍<sup>2,\*</sup>

(<sup>1</sup> 长春师范大学化学学院, 长春 130032; <sup>2</sup> 东北师范大学化学学院, 长春 130024)

## Effects of Azido Bridge on Magnetic Properties of Dinuclear Nickel Complexes: Density Functional Theory Studies

BIAN Jiang-Yu<sup>1,\*</sup> YUE Shu-Mei<sup>1</sup> ZHANG Min<sup>1</sup> ZHANG Jing-Ping<sup>2,\*</sup>

(<sup>1</sup>Department of Chemistry, Changchun Normal University, Changchun 130032, P. R. China;

<sup>2</sup>Department of Chemistry, Northeast Normal University, Changchun 130024, P. R. China)

\*Corresponding authors. BIAN Jiang-Yu, Email: bianjy2002@163.com; Tel: +86-43186168210.

ZHANG Jing-Ping, Email: zhangjp162@nenu.edu.cn; Tel: +86-43185099372.

表 S1 UB3PW91/LANL2DZ 水平下不同 Ni-NNN-Ni 二面角( $\tau$ )计算得到的单重态和五重态的总能量( $E$ )、自旋平方算符的平均值/期望值( $S^2$ )和

磁耦合常数( $J_{ab}$ )

**Table S1 Total energies ( $E$ ), spin angular momentum ( $S^2$ ) for singlet (BS) and quintet (QS) states and the magnetic coupling constant ( $J_{ab}$ ) values for title complex obtained by UB3PW91/LANL2DZ with different Ni-N-N-N-Ni dihedral angle ( $\tau$ )**

$\tau/(\circ)$	$E_{BS}/(\text{a.u.})$	$E_{QS}/(\text{a.u.})$	$\langle S^2 \rangle_{BS}$	$\langle S^2 \rangle_{QS}$	$J_{ab}/\text{cm}^{-1}$
-55.38	-2080.522552	-2080.52202	2.00242	6.012322	-29.12
-53.34	-2080.522027	-2080.52146	2.001412	6.012153	-31.02
-50.42	-2080.522214	-2080.521293	2.0009	6.012039	-50.43
-49.72	-2080.522317	-2080.52117	2.000455	6.011995	-62.78
-49.32	-2080.523019	-2080.521771	2.000625	6.011915	-68.25
-47.28	-2080.522486	-2080.521102	1.999635	6.01177	-75.71
-46.25	-2080.522301	-2080.520861	1.999203	6.01171	-78.80
-45.2	-2080.52232	-2080.520849	1.998917	6.011697	-80.49
-42	-2080.52106	-2080.519414	1.99749	6.011544	-89.99
-40.91	-2080.521298	-2080.519589	1.997104	6.01141	-93.44
-39.81	-2080.520994	-2080.519225	1.996642	6.011329	-96.73
-37.58	-2080.52011	-2080.518196	1.995599	6.011094	-104.59
-36.45	-2080.51997	-2080.51802	1.995254	6.011067	-106.61
-32.99	-2080.518567	-2080.516422	1.993819	6.010729	-117.22
-31.82	-2080.518356	-2080.516171	1.993449	6.010694	-119.36
-27.04	-2080.516475	-2080.514078	1.991782	6.010325	-130.95
-22.12	-2080.514349	-2080.511774	1.990348	6.01	-140.57
-17.09	-2080.511994	-2080.509293	1.989235	6.009764	-147.46
-11.95	-2080.509423	-2080.506656	1.988517	6.009655	-151.02

-6.75	-2080.506641	-2080.503876	1.988239	6.009696	-150.89
-1.5	-2080.503652	-2080.500959	1.988423	6.009891	-147.01
1.13	-2080.50208	-2080.499446	1.988685	6.01004	-143.74
3.76	-2080.500454	-2080.497896	1.989054	6.01022	-139.65
6.38	-2080.498774	-2080.496304	1.989526	6.010425	-134.84
9	-2080.497036	-2080.494666	1.990093	6.010651	-129.38

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