

NBO/NLMO STERIC ANALYSIS

Occupied NLMO contributions dE(i) (kcal/mol) to total steric exchange energy

NLMOs (i) in unit	1	dE(i)
1. BD (1) H 1-	O 2	-46.39
2. BD (1) O 2-	H 3	-42.86
5. CR (1) O 2		140.95
7. LP (1) O 2		-65.91
8. LP (2) O 2		-5.04

Steric exchange energy, unit 1: -19.25 kcal/mol

NLMOs (i) in unit	2	dE(i)
3. BD (1) O 4-	H 5	-47.18
4. BD (1) O 4-	H 6	-47.18
6. CR (1) O 4		139.09
9. LP (1) O 4		-35.01
10. LP (2) O 4		-34.69

Steric exchange energy, unit 2: -24.97 kcal/mol

 Total steric exchange energy: -44.22 kcal/mol

Pairwise steric exchange energies dE(i,j) (kcal/mol) and associated pre-NLMO overlaps S(i,j) for disjoint (no common atoms) interactions between NLMOs i,j:

Threshold for printing: 0.50 kcal/mol
 (Intermolecular threshold: 0.05 kcal/mol)

NLMO (i)	NLMO (j)	PNLMO S(i,j)	dE(i,j) kcal/mol
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within unit 1
 None above threshold

sum within unit 1: 0.00

between units 1 and 2

1. BD (1) H 1-	O 2	10. LP (2) O 4	-0.1473	7.58
2. BD (1) O 2-	H 3	10. LP (2) O 4	0.0067	-0.06
5. CR (1) O 2		10. LP (2) O 4	0.0043	-0.08
7. LP (1) O 2		9. LP (1) O 4	-0.0175	0.12

sum between units 1 and 2: 7.60

within unit 2

sum within unit 2: 0.00

 Total disjoint NLMO steric exchange energy from pairwise sum: 7.60
